



## Full wwPDB EM Validation Report ⓘ

Apr 6, 2026 – 12:03 AM UTC

PDB ID : 9B0Q / pdb\_00009b0q  
EMDB ID : EMD-44050  
Title : In situ human top-back di-ribosome structure (Composite map)  
Authors : Wei, Z.; Yong, Z.  
Deposited on : 2024-03-12  
Resolution : 3.20 Å (reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

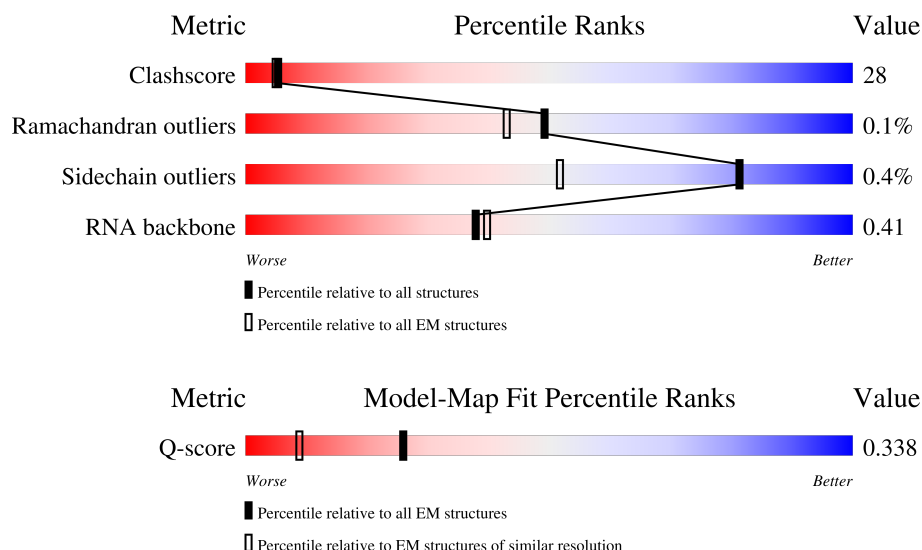
EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



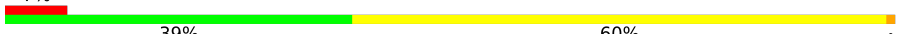
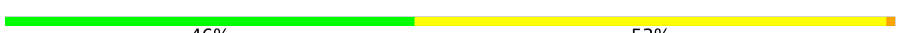
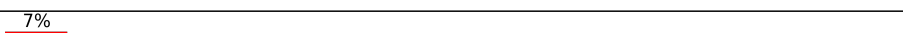
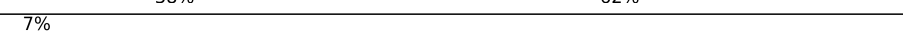
| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| RNA backbone          | 8273                        | 3508                        | -                                                        |
| Q-score               | -                           | 25397                       | 15020 ( 2.70 - 3.70 )                                    |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain                                          |
|-----|-------|--------|-----------------------------------------------------------|
| 1   | CH    | 125    | <div> <div>7%</div> <div>42%</div> <div>56%</div> </div>  |
| 1   | cH    | 125    | <div> <div>16%</div> <div>38%</div> <div>61%</div> </div> |
| 2   | SE    | 262    | <div> <div>42%</div> <div>57%</div> </div>                |

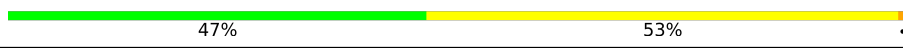
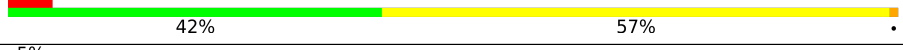
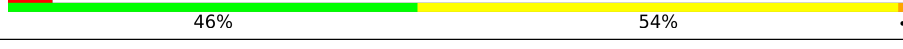
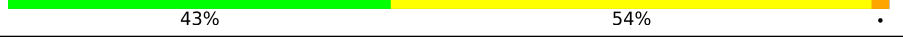
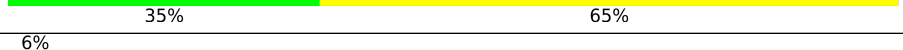
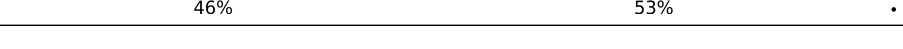
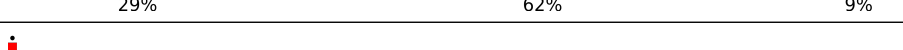
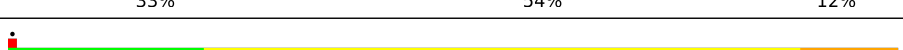
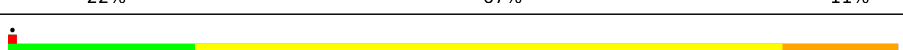
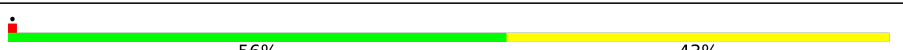
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| Mol | Chain | Length | Quality of chain                                                                                 |
|-----|-------|--------|--------------------------------------------------------------------------------------------------|
| 2   | sE    | 262    |  49% 50%       |
| 3   | SI    | 206    |  50% 50%       |
| 3   | sI    | 206    |  48% 52%       |
| 4   | SL    | 153    |  5% 47% 52%    |
| 4   | sL    | 153    |  7% 39% 60%    |
| 5   | SX    | 141    |  46% 53%       |
| 5   | sX    | 141    |  52% 48%       |
| 6   | SG    | 237    |  5% 43% 56%    |
| 6   | sG    | 237    |  5% 38% 61%    |
| 7   | SJ    | 185    |  42% 58%       |
| 7   | sJ    | 185    |  42% 58%       |
| 8   | SY    | 131    |  40% 60%       |
| 8   | sY    | 131    |  45% 54%     |
| 9   | se    | 58     |  16% 43% 57% |
| 10  | SA    | 221    |  7% 38% 62%  |
| 10  | sA    | 221    |  7% 33% 66%  |
| 11  | SB    | 214    |  35% 64%     |
| 11  | sB    | 214    |  38% 61%     |
| 12  | SH    | 189    |  8% 36% 62%  |
| 12  | sH    | 189    |  9% 42% 56%  |
| 13  | SV    | 83     |  47% 53%     |
| 13  | sV    | 83     |  23% 76%     |
| 14  | Sa    | 102    |  45% 53%     |
| 14  | sa    | 102    |  43% 54%     |
| 15  | SC    | 222    |  43% 57%     |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 15  | sC    | 222    |    |
| 16  | SN    | 150    |    |
| 16  | sN    | 150    |    |
| 17  | SO    | 140    |    |
| 17  | sO    | 140    |    |
| 18  | SW    | 129    |    |
| 18  | sW    | 129    |    |
| 19  | Sb    | 83     |    |
| 19  | sb    | 83     |    |
| 20  | L7    | 120    |    |
| 20  | l7    | 120    |    |
| 21  | L8    | 156    |  |
| 21  | l8    | 156    |  |
| 22  | LA    | 248    |  |
| 22  | lA    | 248    |  |
| 23  | LB    | 402    |  |
| 23  | lB    | 402    |  |
| 24  | LC    | 368    |  |
| 24  | lC    | 368    |  |
| 25  | LD    | 293    |  |
| 25  | lD    | 293    |  |
| 26  | LE    | 247    |  |
| 26  | lE    | 247    |  |
| 27  | LF    | 225    |  |
| 27  | lF    | 225    |  |

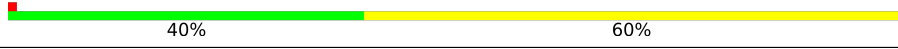
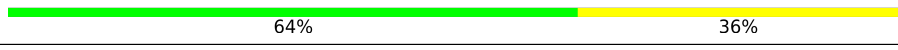
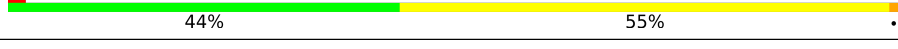
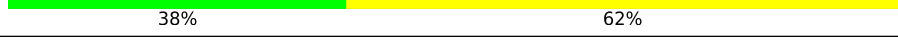
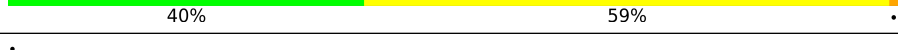
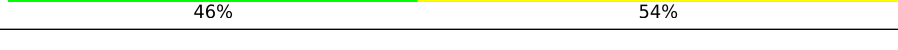
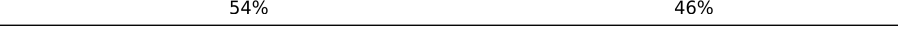
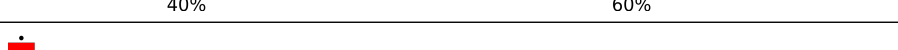
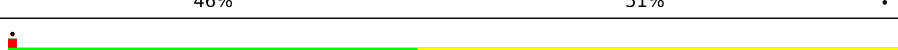
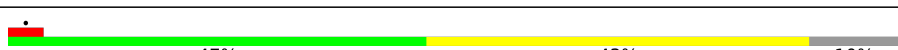
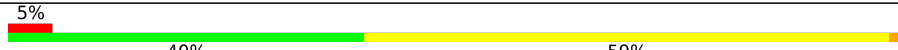
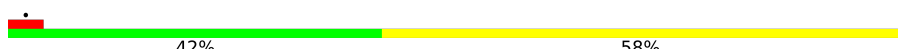
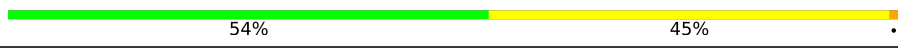
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| Mol | Chain | Length | Quality of chain                                                      |
|-----|-------|--------|-----------------------------------------------------------------------|
| 28  | LG    | 241    | <div> <div>5%</div> <div>53%</div> <div>47%</div> </div>              |
| 28  | IG    | 241    | <div> <div>5%</div> <div>59%</div> <div>41%</div> </div>              |
| 29  | LH    | 190    | <div> <div>48%</div> <div>52%</div> </div>                            |
| 29  | IH    | 190    | <div> <div>46%</div> <div>53%</div> <div>.</div> </div>               |
| 30  | LI    | 213    | <div> <div>51%</div> <div>44%</div> <div>5%</div> </div>              |
| 30  | II    | 213    | <div> <div>53%</div> <div>41%</div> <div>5%</div> </div>              |
| 31  | LJ    | 176    | <div> <div>5%</div> <div>46%</div> <div>53%</div> <div>.</div> </div> |
| 31  | IJ    | 176    | <div> <div>7%</div> <div>49%</div> <div>51%</div> </div>              |
| 32  | LL    | 210    | <div> <div>5%</div> <div>55%</div> <div>45%</div> </div>              |
| 32  | IL    | 210    | <div> <div>.</div> <div>50%</div> <div>49%</div> </div>               |
| 33  | LM    | 139    | <div> <div>39%</div> <div>60%</div> <div>.</div> </div>               |
| 33  | IM    | 139    | <div> <div>.</div> <div>39%</div> <div>58%</div> <div>.</div> </div>  |
| 34  | LN    | 203    | <div> <div>49%</div> <div>50%</div> <div>.</div> </div>               |
| 34  | IN    | 203    | <div> <div>49%</div> <div>50%</div> </div>                            |
| 35  | LO    | 201    | <div> <div>52%</div> <div>47%</div> <div>.</div> </div>               |
| 35  | IO    | 201    | <div> <div>48%</div> <div>52%</div> </div>                            |
| 36  | LP    | 153    | <div> <div>50%</div> <div>50%</div> </div>                            |
| 36  | IP    | 153    | <div> <div>54%</div> <div>45%</div> <div>.</div> </div>               |
| 37  | LQ    | 187    | <div> <div>49%</div> <div>51%</div> </div>                            |
| 37  | IQ    | 187    | <div> <div>51%</div> <div>49%</div> </div>                            |
| 38  | LR    | 187    | <div> <div>5%</div> <div>48%</div> <div>52%</div> </div>              |
| 38  | IR    | 187    | <div> <div>6%</div> <div>52%</div> <div>48%</div> </div>              |
| 39  | LS    | 175    | <div> <div>54%</div> <div>46%</div> </div>                            |
| 39  | IS    | 175    | <div> <div>56%</div> <div>43%</div> <div>.</div> </div>               |
| 40  | LT    | 159    | <div> <div>.</div> <div>47%</div> <div>53%</div> <div>.</div> </div>  |

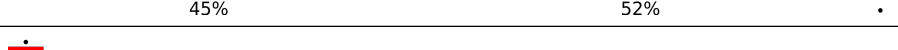
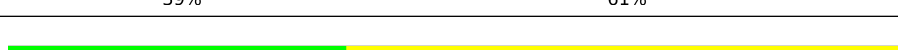
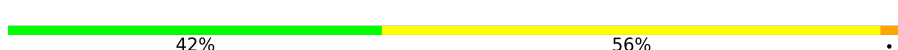
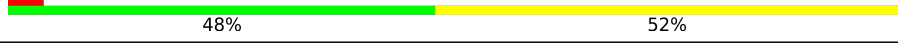
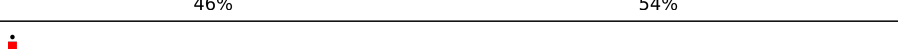
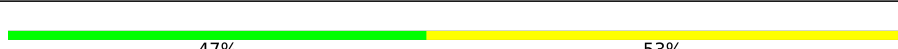
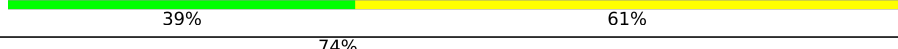
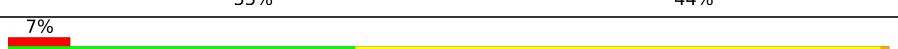
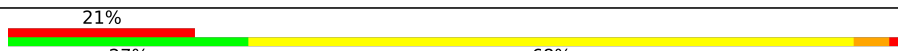
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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 40  | IT    | 159    |    |
| 41  | LU    | 101    |    |
| 41  | IU    | 101    |    |
| 42  | LV    | 131    |    |
| 42  | IV    | 131    |    |
| 43  | LX    | 120    |    |
| 43  | IX    | 120    |    |
| 44  | LY    | 134    |    |
| 44  | IY    | 134    |    |
| 45  | LZ    | 135    |    |
| 45  | IZ    | 135    |    |
| 46  | La    | 147    |  |
| 46  | la    | 147    |  |
| 47  | Lb    | 121    |  |
| 47  | lb    | 121    |  |
| 48  | Lc    | 98     |  |
| 48  | lc    | 98     |  |
| 49  | Ld    | 107    |  |
| 49  | ld    | 107    |  |
| 50  | Le    | 128    |  |
| 50  | le    | 128    |  |
| 51  | Lf    | 109    |  |
| 51  | lf    | 109    |  |
| 52  | Lg    | 114    |  |
| 52  | lg    | 114    |  |

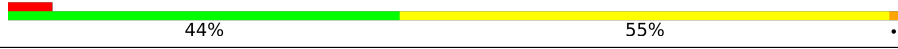
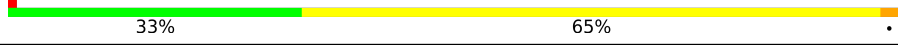
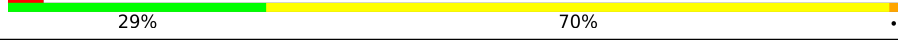
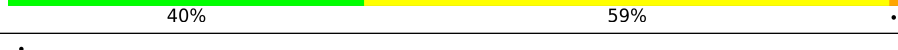
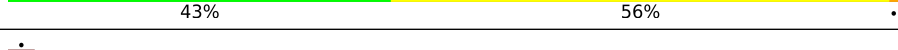
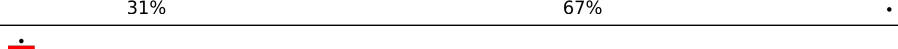
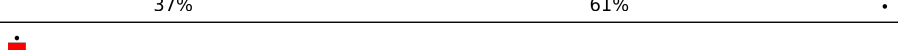
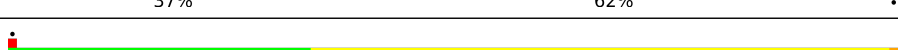
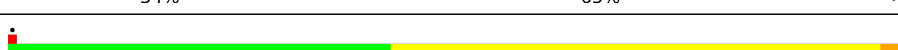
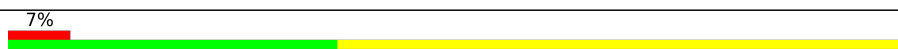
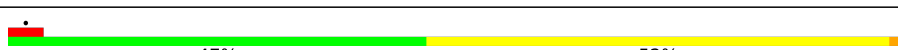
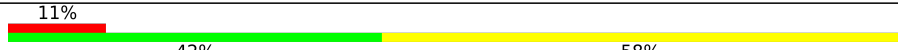
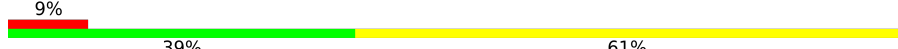
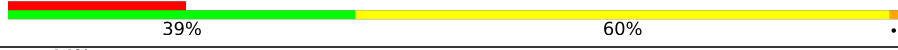
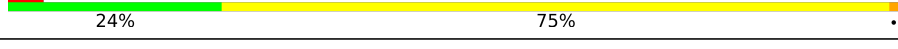
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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 53  | Lh    | 122    |    |
| 53  | lh    | 122    |    |
| 54  | Li    | 102    |    |
| 54  | li    | 102    |    |
| 55  | Lj    | 86     |    |
| 55  | lj    | 86     |    |
| 56  | Lk    | 69     |    |
| 56  | lk    | 69     |    |
| 57  | Ll    | 50     |    |
| 57  | ll    | 50     |    |
| 58  | Lm    | 52     |   |
| 58  | lm    | 52     |  |
| 59  | Ln    | 24     |  |
| 59  | ln    | 24     |  |
| 60  | Lo    | 105    |  |
| 60  | lo    | 105    |  |
| 61  | Lp    | 91     |  |
| 61  | lp    | 91     |  |
| 62  | Lr    | 125    |  |
| 62  | lr    | 125    |  |
| 63  | Lz    | 217    |  |
| 63  | lz    | 217    |  |
| 64  | SR    | 135    |  |
| 64  | sR    | 135    |  |
| 65  | SD    | 227    |  |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 65  | sD    | 227    |    |
| 66  | SF    | 189    |    |
| 66  | sF    | 189    |    |
| 67  | SK    | 98     |    |
| 67  | sK    | 98     |    |
| 68  | SP    | 121    |    |
| 68  | sP    | 121    |    |
| 69  | SQ    | 144    |    |
| 69  | sQ    | 144    |    |
| 70  | SS    | 145    |    |
| 70  | sS    | 145    |    |
| 71  | ST    | 143    |  |
| 71  | sT    | 143    |  |
| 72  | SU    | 104    |  |
| 72  | sU    | 104    |  |
| 73  | Sc    | 64     |  |
| 73  | sc    | 64     |  |
| 74  | Sd    | 55     |  |
| 74  | sd    | 55     |  |
| 75  | Sg    | 313    |  |
| 75  | sg    | 313    |  |
| 76  | SM    | 122    |  |
| 76  | sM    | 122    |  |
| 77  | SZ    | 75     |  |
| 77  | sZ    | 75     |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 78  | Sf    | 67     |                  |
| 78  | sf    | 67     |                  |
| 79  | S2    | 1740   |                  |
| 79  | s2    | 1740   |                  |
| 80  | CB    | 856    |                  |
| 80  | cB    | 856    |                  |
| 81  | AP    | 73     |                  |
| 81  | aP    | 73     |                  |
| 82  | PE    | 76     |                  |
| 82  | pE    | 76     |                  |
| 83  | Ls    | 196    |                  |
| 83  | ls    | 196    |                  |
| 84  | Lt    | 141    |                  |
| 84  | lt    | 141    |                  |
| 85  | L5    | 3740   |                  |
| 85  | l5    | 3740   |                  |
| 86  | Se    | 47     |                  |
| 87  | LW    | 124    |                  |
| 87  | IW    | 124    |                  |

## 2 Entry composition

There are 89 unique types of molecules in this entry. The entry contains 459641 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Endothelial differentiation-related factor 1.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 1   | CH    | 125      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 968   | 595 | 189 | 184 |         |       |
| 1   | cH    | 125      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 968   | 595 | 189 | 184 |         |       |

There are 8 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment   | Reference  |
|-------|---------|----------|--------|-----------|------------|
| CH    | 30      | ARG      | GLN    | conflict  | UNP O60869 |
| CH    | 32      | ALA      | ARG    | conflict  | UNP O60869 |
| CH    | 33      | ALA      | -      | insertion | UNP O60869 |
| CH    | 34      | ALA      | -      | insertion | UNP O60869 |
| cH    | 30      | ARG      | GLN    | conflict  | UNP O60869 |
| cH    | 32      | ALA      | ARG    | conflict  | UNP O60869 |
| cH    | 33      | ALA      | -      | insertion | UNP O60869 |
| cH    | 34      | ALA      | -      | insertion | UNP O60869 |

- Molecule 2 is a protein called Small ribosomal subunit protein eS4, X isoform.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 2   | sE    | 262      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2076  | 1324 | 386 | 358 | 8 |         |       |
| 2   | SE    | 262      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2076  | 1324 | 386 | 358 | 8 |         |       |

- Molecule 3 is a protein called 40S ribosomal protein S8.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 3   | sI    | 206      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1686  | 1058 | 332 | 291 | 5 |         |       |
| 3   | SI    | 206      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1686  | 1058 | 332 | 291 | 5 |         |       |

- Molecule 4 is a protein called 40S ribosomal protein S11.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 4   | sL    | 153      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1247  | 793 | 234 | 214 | 6 |         |       |
| 4   | SL    | 153      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1247  | 793 | 234 | 214 | 6 |         |       |

- Molecule 5 is a protein called 40S ribosomal protein S23.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 5   | sX    | 141      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1098  | 693 | 219 | 183 | 3 |         |       |
| 5   | SX    | 141      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1098  | 693 | 219 | 183 | 3 |         |       |

- Molecule 6 is a protein called 40S ribosomal protein S6.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 6   | sG    | 237      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1923  | 1200 | 387 | 329 | 7 |         |       |
| 6   | SG    | 237      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1923  | 1200 | 387 | 329 | 7 |         |       |

- Molecule 7 is a protein called 40S ribosomal protein S9.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 7   | sJ    | 185      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1525  | 969 | 306 | 248 | 2 |         |       |
| 7   | SJ    | 185      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1525  | 969 | 306 | 248 | 2 |         |       |

- Molecule 8 is a protein called 40S ribosomal protein S24.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 8   | sY    | 131      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1065  | 673 | 209 | 178 | 5 |         |       |
| 8   | SY    | 131      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1065  | 673 | 209 | 178 | 5 |         |       |

- Molecule 9 is a protein called Small ribosomal subunit protein eS30.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 9   | se    | 58       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 459   | 284 | 100 | 74 | 1 |         |       |

- Molecule 10 is a protein called 40S ribosomal protein SA.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 10  | sA    | 221      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1741  | 1106 | 305 | 322 | 8 |         |       |
| 10  | SA    | 221      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1741  | 1106 | 305 | 322 | 8 |         |       |

- Molecule 11 is a protein called 40S ribosomal protein S3a.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 11  | sB    | 214      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1738  | 1103 | 310 | 311 | 14 |         |       |
| 11  | SB    | 214      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1738  | 1103 | 310 | 311 | 14 |         |       |

- Molecule 12 is a protein called Small ribosomal subunit protein eS7.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 12  | sH    | 186      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1497  | 956 | 274 | 266 | 1 |         |       |
| 12  | SH    | 186      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1497  | 956 | 274 | 266 | 1 |         |       |

- Molecule 13 is a protein called 40S ribosomal protein S21.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 13  | sV    | 83       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 636   | 393 | 117 | 121 | 5 |         |       |
| 13  | SV    | 83       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 636   | 393 | 117 | 121 | 5 |         |       |

- Molecule 14 is a protein called 40S ribosomal protein S26.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 14  | sa    | 102      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 821   | 512 | 171 | 133 | 5 |         |       |
| 14  | Sa    | 102      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 821   | 512 | 171 | 133 | 5 |         |       |

- Molecule 15 is a protein called 40S ribosomal protein S2.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 15  | sC    | 222      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1725  | 1115 | 298 | 302 | 10 |         |       |
| 15  | SC    | 222      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1725  | 1115 | 298 | 302 | 10 |         |       |

- Molecule 16 is a protein called 40S ribosomal protein S13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 16  | sN    | 150      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1208  | 773 | 229 | 205 | 1 |         |       |
| 16  | SN    | 150      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1208  | 773 | 229 | 205 | 1 |         |       |

- Molecule 17 is a protein called Small ribosomal subunit protein uS11.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 17  | sO    | 140      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1049  | 642 | 204 | 197 | 6 |         |       |
| 17  | SO    | 140      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1049  | 642 | 204 | 197 | 6 |         |       |

- Molecule 18 is a protein called 40S ribosomal protein S15a.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 18  | sW    | 129      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1034  | 659 | 193 | 176 | 6 |         |       |
| 18  | SW    | 129      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1034  | 659 | 193 | 176 | 6 |         |       |

- Molecule 19 is a protein called Small ribosomal subunit protein eS27.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 19  | sb    | 83       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 651   | 408 | 121 | 115 | 7 |         |       |
| 19  | Sb    | 83       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 651   | 408 | 121 | 115 | 7 |         |       |

- Molecule 20 is a RNA chain called RNA (120-MER)5S rRNA [Homo sapiens].

| Mol | Chain | Residues | Atoms |      |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|-------|
| 20  | 17    | 120      | Total | C    | N   | O   | P   | 0       | 0     |
|     |       |          | 2561  | 1141 | 456 | 844 | 120 |         |       |
| 20  | L7    | 120      | Total | C    | N   | O   | P   | 0       | 0     |
|     |       |          | 2561  | 1141 | 456 | 844 | 120 |         |       |

- Molecule 21 is a RNA chain called RNA (156-MER)5.8S rRNA [Homo sapiens].

| Mol | Chain | Residues | Atoms |      |     |      |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|-----|---------|-------|
| 21  | 18    | 156      | Total | C    | N   | O    | P   | 0       | 0     |
|     |       |          | 3314  | 1480 | 585 | 1094 | 155 |         |       |
| 21  | L8    | 156      | Total | C    | N   | O    | P   | 0       | 0     |
|     |       |          | 3314  | 1480 | 585 | 1094 | 155 |         |       |

- Molecule 22 is a protein called 60S ribosomal protein L8.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 22  | 1A    | 248      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1898  | 1189 | 389 | 314 | 6 |         |       |
| 22  | LA    | 248      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1898  | 1189 | 389 | 314 | 6 |         |       |

- Molecule 23 is a protein called Large ribosomal subunit protein uL3.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 23  | 1B    | 402      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3238  | 2060 | 608 | 556 | 14 |         |       |
| 23  | LB    | 402      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3238  | 2060 | 608 | 556 | 14 |         |       |

- Molecule 24 is a protein called 60S ribosomal protein L4.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 24  | 1C    | 368      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2927  | 1840 | 583 | 489 | 15 |         |       |
| 24  | LC    | 368      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2927  | 1840 | 583 | 489 | 15 |         |       |

- Molecule 25 is a protein called Large ribosomal subunit protein uL18.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 25  | 1D    | 293      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2382  | 1507 | 434 | 427 | 14 |         |       |

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| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 25  | LD    | 293      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2382  | 1507 | 434 | 427 | 14 |         |       |

- Molecule 26 is a protein called Large ribosomal subunit protein eL6.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 26  | lE    | 236      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1904  | 1222 | 361 | 317 | 4 |         |       |
| 26  | LE    | 236      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1904  | 1222 | 361 | 317 | 4 |         |       |

- Molecule 27 is a protein called 60S ribosomal protein L7.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 27  | lF    | 225      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1870  | 1202 | 358 | 301 | 9 |         |       |
| 27  | LF    | 225      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1870  | 1202 | 358 | 301 | 9 |         |       |

- Molecule 28 is a protein called 60S ribosomal protein L7a.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 28  | lG    | 241      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1927  | 1228 | 371 | 324 | 4 |         |       |
| 28  | LG    | 241      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1927  | 1228 | 371 | 324 | 4 |         |       |

- Molecule 29 is a protein called 60S ribosomal protein L9.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 29  | lH    | 190      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1518  | 956 | 284 | 272 | 6 |         |       |
| 29  | LH    | 190      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1518  | 956 | 284 | 272 | 6 |         |       |

- Molecule 30 is a protein called Ribosomal protein uL16-like.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 30  | lI    | 202      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1634  | 1037 | 314 | 269 | 14 |         |       |
| 30  | LI    | 202      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1634  | 1037 | 314 | 269 | 14 |         |       |

- Molecule 31 is a protein called 60S ribosomal protein L11.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 31  | IJ    | 176      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1410  | 888 | 263 | 253 | 6 |         |       |
| 31  | LJ    | 176      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1410  | 888 | 263 | 253 | 6 |         |       |

- Molecule 32 is a protein called Large ribosomal subunit protein eL13.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 32  | IL    | 210      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1701  | 1064 | 352 | 281 | 4 |         |       |
| 32  | LL    | 210      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1701  | 1064 | 352 | 281 | 4 |         |       |

- Molecule 33 is a protein called 60S ribosomal protein L14.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 33  | IM    | 139      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1138  | 730 | 218 | 183 | 7 |         |       |
| 33  | LM    | 139      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1138  | 730 | 218 | 183 | 7 |         |       |

- Molecule 34 is a protein called 60S ribosomal protein L15.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 34  | IN    | 203      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1701  | 1072 | 359 | 266 | 4 |         |       |
| 34  | LN    | 203      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1701  | 1072 | 359 | 266 | 4 |         |       |

- Molecule 35 is a protein called 60S ribosomal protein L13a.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 35  | IO    | 201      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1650  | 1063 | 321 | 261 | 5 |         |       |
| 35  | LO    | 201      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1650  | 1063 | 321 | 261 | 5 |         |       |

- Molecule 36 is a protein called 60S ribosomal protein L17.



| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 36  | IP    | 153      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1242  | 776 | 241 | 216 | 9 |         |       |
| 36  | LP    | 153      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1242  | 776 | 241 | 216 | 9 |         |       |

- Molecule 37 is a protein called 60S ribosomal protein L18.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 37  | lQ    | 187      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1513  | 944 | 314 | 250 | 5 |         |       |
| 37  | LQ    | 187      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1513  | 944 | 314 | 250 | 5 |         |       |

- Molecule 38 is a protein called 60S ribosomal protein L19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 38  | lR    | 187      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1566  | 971 | 336 | 250 | 9 |         |       |
| 38  | LR    | 187      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1566  | 971 | 336 | 250 | 9 |         |       |

- Molecule 39 is a protein called 60S ribosomal protein L18a.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 39  | lS    | 175      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1453  | 925 | 283 | 235 | 10 |         |       |
| 39  | LS    | 175      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1453  | 925 | 283 | 235 | 10 |         |       |

- Molecule 40 is a protein called 60S ribosomal protein L21.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 40  | lT    | 159      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1298  | 823 | 252 | 217 | 6 |         |       |
| 40  | LT    | 159      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1298  | 823 | 252 | 217 | 6 |         |       |

- Molecule 41 is a protein called Heparin-binding protein HBp15.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 41  | lU    | 101      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 825   | 529 | 144 | 150 | 2 |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 41  | LU    | 101      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 825   | 529 | 144 | 150 | 2 |         |       |

- Molecule 42 is a protein called 60S ribosomal protein L23.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 42  | IV    | 131      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 979   | 618 | 184 | 172 | 5 |         |       |
| 42  | LV    | 131      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 979   | 618 | 184 | 172 | 5 |         |       |

- Molecule 43 is a protein called 60S ribosomal protein L23a.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 43  | IX    | 120      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 985   | 630 | 185 | 169 | 1 |         |       |
| 43  | LX    | 120      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 985   | 630 | 185 | 169 | 1 |         |       |

- Molecule 44 is a protein called 60S ribosomal protein L26.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 44  | IY    | 134      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1115  | 700 | 226 | 186 | 3 |         |       |
| 44  | LY    | 134      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1115  | 700 | 226 | 186 | 3 |         |       |

- Molecule 45 is a protein called 60S ribosomal protein L27.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 45  | IZ    | 135      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1107  | 714 | 208 | 182 | 3 |         |       |
| 45  | LZ    | 135      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1107  | 714 | 208 | 182 | 3 |         |       |

- Molecule 46 is a protein called 60S ribosomal protein L27a.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 46  | la    | 147      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1162  | 736 | 237 | 186 | 3 |         |       |
| 46  | La    | 147      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1162  | 736 | 237 | 186 | 3 |         |       |

- Molecule 47 is a protein called Large ribosomal subunit protein eL29.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 47  | lb    | 109      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 876   | 546 | 189 | 137 | 4 |         |       |
| 47  | Lb    | 109      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 876   | 546 | 189 | 137 | 4 |         |       |

- Molecule 48 is a protein called 60S ribosomal protein L30.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 48  | lc    | 98       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 764   | 485 | 135 | 138 | 6 |         |       |
| 48  | Lc    | 98       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 764   | 485 | 135 | 138 | 6 |         |       |

- Molecule 49 is a protein called 60S ribosomal protein L31.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 49  | ld    | 107      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 888   | 560 | 171 | 155 | 2 |         |       |
| 49  | Ld    | 107      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 888   | 560 | 171 | 155 | 2 |         |       |

- Molecule 50 is a protein called 60S ribosomal protein L32.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 50  | le    | 128      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1053  | 667 | 216 | 165 | 5 |         |       |
| 50  | Le    | 128      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1053  | 667 | 216 | 165 | 5 |         |       |

- Molecule 51 is a protein called 60S ribosomal protein L35a.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 51  | lf    | 109      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 876   | 555 | 174 | 144 | 3 |         |       |
| 51  | Lf    | 109      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 876   | 555 | 174 | 144 | 3 |         |       |

- Molecule 52 is a protein called 60S ribosomal protein L34.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 52  | lg    | 114      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 906   | 566 | 187 | 147 | 6 |         |       |
| 52  | Lg    | 114      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 906   | 566 | 187 | 147 | 6 |         |       |

- Molecule 53 is a protein called 60S ribosomal protein L35.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 53  | lh    | 122      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1015  | 641 | 205 | 168 | 1 |         |       |
| 53  | Lh    | 122      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1015  | 641 | 205 | 168 | 1 |         |       |

- Molecule 54 is a protein called 60S ribosomal protein L36.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 54  | li    | 102      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 832   | 521 | 177 | 129 | 5 |         |       |
| 54  | Li    | 102      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 832   | 521 | 177 | 129 | 5 |         |       |

- Molecule 55 is a protein called 60S ribosomal protein L37.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 55  | lj    | 86       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 705   | 434 | 155 | 111 | 5 |         |       |
| 55  | Lj    | 86       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 705   | 434 | 155 | 111 | 5 |         |       |

- Molecule 56 is a protein called 60S ribosomal protein L38.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 56  | lk    | 69       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 569   | 366 | 103 | 99 | 1 |         |       |
| 56  | Lk    | 69       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 569   | 366 | 103 | 99 | 1 |         |       |

- Molecule 57 is a protein called 60S ribosomal protein L39.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 57  | ll    | 50       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 444   | 281 | 98 | 64 | 1 |         |       |

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| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 57  | Ll    | 50       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 444   | 281 | 98 | 64 | 1 |         |       |

- Molecule 58 is a protein called Large ribosomal subunit protein eL40.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 58  | lm    | 52       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 429   | 266 | 90 | 67 | 6 |         |       |
| 58  | Lm    | 52       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 429   | 266 | 90 | 67 | 6 |         |       |

- Molecule 59 is a protein called 60S ribosomal protein L41.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 59  | ln    | 24       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 230   | 139 | 62 | 26 | 3 |         |       |
| 59  | Ln    | 24       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 230   | 139 | 62 | 26 | 3 |         |       |

- Molecule 60 is a protein called 60S ribosomal protein L36a.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 60  | lo    | 105      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 862   | 542 | 175 | 139 | 6 |         |       |
| 60  | Lo    | 105      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 862   | 542 | 175 | 139 | 6 |         |       |

- Molecule 61 is a protein called 60S ribosomal protein L37a.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 61  | lp    | 91       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 708   | 445 | 136 | 120 | 7 |         |       |
| 61  | Lp    | 91       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 708   | 445 | 136 | 120 | 7 |         |       |

- Molecule 62 is a protein called 60S ribosomal protein L28.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 62  | lr    | 125      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1002  | 622 | 207 | 168 | 5 |         |       |
| 62  | Lr    | 125      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1002  | 622 | 207 | 168 | 5 |         |       |

- Molecule 63 is a protein called 60S ribosomal protein L10a.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 63  | lz    | 217      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1741  | 1113 | 312 | 307 | 9 |         |       |
| 63  | Lz    | 217      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1741  | 1113 | 312 | 307 | 9 |         |       |

- Molecule 64 is a protein called 40S ribosomal protein S17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 64  | sR    | 135      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1090  | 685 | 202 | 198 | 5 |         |       |
| 64  | SR    | 135      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1090  | 685 | 202 | 198 | 5 |         |       |

- Molecule 65 is a protein called Small ribosomal subunit protein uS3.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 65  | sD    | 227      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1765  | 1125 | 317 | 315 | 8 |         |       |
| 65  | SD    | 227      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1765  | 1125 | 317 | 315 | 8 |         |       |

- Molecule 66 is a protein called 40S ribosomal protein S5.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 66  | sF    | 189      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1495  | 934 | 284 | 270 | 7 |         |       |
| 66  | SF    | 189      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1495  | 934 | 284 | 270 | 7 |         |       |

- Molecule 67 is a protein called 40S ribosomal protein S10.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 67  | sK    | 98       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 827   | 539 | 148 | 134 | 6 |         |       |
| 67  | SK    | 98       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 827   | 539 | 148 | 134 | 6 |         |       |

- Molecule 68 is a protein called Small ribosomal subunit protein uS19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 68  | sP    | 121      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 985   | 623 | 185 | 170 | 7 |         |       |
| 68  | SP    | 121      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 985   | 623 | 185 | 170 | 7 |         |       |

- Molecule 69 is a protein called Small ribosomal subunit protein uS9.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 69  | sQ    | 144      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1142  | 726 | 216 | 197 | 3 |         |       |
| 69  | SQ    | 144      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1142  | 726 | 216 | 197 | 3 |         |       |

- Molecule 70 is a protein called 40S ribosomal protein S18.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 70  | sS    | 145      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1198  | 751 | 242 | 203 | 2 |         |       |
| 70  | SS    | 145      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1198  | 751 | 242 | 203 | 2 |         |       |

- Molecule 71 is a protein called 40S ribosomal protein S19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 71  | sT    | 143      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1112  | 697 | 214 | 198 | 3 |         |       |
| 71  | ST    | 143      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1112  | 697 | 214 | 198 | 3 |         |       |

- Molecule 72 is a protein called 40S ribosomal protein S20.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 72  | sU    | 104      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 821   | 514 | 155 | 148 | 4 |         |       |
| 72  | SU    | 104      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 821   | 514 | 155 | 148 | 4 |         |       |

- Molecule 73 is a protein called 40S ribosomal protein S28.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 73  | sc    | 64       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 506   | 308 | 102 | 94 | 2 |         |       |

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| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 73  | Sc    | 64       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 506   | 308 | 102 | 94 | 2 |         |       |

- Molecule 74 is a protein called 40S ribosomal protein S29.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 74  | sd    | 55       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 459   | 286 | 94 | 74 | 5 |         |       |
| 74  | Sd    | 55       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 459   | 286 | 94 | 74 | 5 |         |       |

- Molecule 75 is a protein called Receptor of activated protein C kinase 1.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 75  | sg    | 313      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2436  | 1535 | 424 | 465 | 12 |         |       |
| 75  | Sg    | 313      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2436  | 1535 | 424 | 465 | 12 |         |       |

- Molecule 76 is a protein called Small ribosomal subunit protein eS12.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 76  | sM    | 122      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 940   | 590 | 164 | 177 | 9 |         |       |
| 76  | SM    | 122      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 940   | 590 | 164 | 177 | 9 |         |       |

- Molecule 77 is a protein called Small ribosomal subunit protein eS25.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 77  | sZ    | 75       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 598   | 382 | 111 | 104 | 1 |         |       |
| 77  | SZ    | 75       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 598   | 382 | 111 | 104 | 1 |         |       |

- Molecule 78 is a protein called Ubiquitin-40S ribosomal protein S27a.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 78  | sf    | 67       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 548   | 346 | 102 | 93 | 7 |         |       |
| 78  | Sf    | 67       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 548   | 346 | 102 | 93 | 7 |         |       |



- Molecule 79 is a RNA chain called 18S rRNA [Homo sapiens].

| Mol | Chain | Residues | Atoms |       |      |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|-------|
| 79  | s2    | 1740     | Total | C     | N    | O     | P    | 0       | 0     |
|     |       |          | 36898 | 16459 | 6599 | 12101 | 1739 |         |       |
| 79  | S2    | 1740     | Total | C     | N    | O     | P    | 0       | 0     |
|     |       |          | 36898 | 16459 | 6599 | 12101 | 1739 |         |       |

- Molecule 80 is a protein called Elongation factor 2.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 80  | cB    | 846      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 6605  | 4193 | 1136 | 1232 | 44 |         |       |
| 80  | CB    | 846      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 6605  | 4193 | 1136 | 1232 | 44 |         |       |

- Molecule 81 is a RNA chain called A/P site tRNA [Homo sapiens].

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 81  | aP    | 71       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 1514  | 677 | 275 | 492 | 70 |         |       |
| 81  | AP    | 71       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 1514  | 677 | 275 | 492 | 70 |         |       |

- Molecule 82 is a RNA chain called P/E site tRNA [Homo sapiens].

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 82  | pE    | 75       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 1593  | 712 | 281 | 526 | 74 |         |       |
| 82  | PE    | 75       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 1593  | 712 | 281 | 526 | 74 |         |       |

- Molecule 83 is a protein called 60S acidic ribosomal protein P0.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 83  | ls    | 196      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1496  | 952 | 259 | 276 | 9 |         |       |
| 83  | Ls    | 196      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1496  | 952 | 259 | 276 | 9 |         |       |

- Molecule 84 is a protein called 60S ribosomal protein L12 [Homo sapiens].

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 84  | lt    | 141      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1046  | 652 | 191 | 199 | 4 |         |       |
| 84  | Lt    | 141      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1046  | 652 | 191 | 199 | 4 |         |       |

- Molecule 85 is a RNA chain called 28S rRNA [Homo sapiens].

| Mol | Chain | Residues | Atoms |       |       |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|-------|
| 85  | l5    | 3708     | Total | C     | N     | O     | P    | 0       | 0     |
|     |       |          | 79496 | 35401 | 14553 | 25835 | 3707 |         |       |
| 85  | L5    | 3708     | Total | C     | N     | O     | P    | 0       | 0     |
|     |       |          | 79496 | 35401 | 14553 | 25835 | 3707 |         |       |

- Molecule 86 is a protein called Small ribosomal subunit protein eS30.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 86  | Se    | 47       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 378   | 234 | 84 | 59 | 1 |         |       |

- Molecule 87 is a protein called Ribosomal protein L24.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 87  | lW    | 118      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 965   | 604 | 199 | 158 | 4 |         |       |
| 87  | LW    | 118      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 965   | 604 | 199 | 158 | 4 |         |       |

- Molecule 88 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 88  | sa    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 88  | lg    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 88  | lj    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 88  | lm    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 88  | lo    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 88  | lp    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |

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| Mol | Chain | Residues | Atoms      |         | AltConf |
|-----|-------|----------|------------|---------|---------|
| 88  | Sa    | 1        | Total<br>1 | Zn<br>1 | 0       |
| 88  | Lg    | 1        | Total<br>1 | Zn<br>1 | 0       |
| 88  | Lj    | 1        | Total<br>1 | Zn<br>1 | 0       |
| 88  | Lm    | 1        | Total<br>1 | Zn<br>1 | 0       |
| 88  | Lo    | 1        | Total<br>1 | Zn<br>1 | 0       |
| 88  | Lp    | 1        | Total<br>1 | Zn<br>1 | 0       |

- Molecule 89 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

| Mol | Chain | Residues | Atoms        |           | AltConf |
|-----|-------|----------|--------------|-----------|---------|
| 89  | l7    | 3        | Total<br>3   | Mg<br>3   | 0       |
| 89  | l8    | 5        | Total<br>5   | Mg<br>5   | 0       |
| 89  | lA    | 1        | Total<br>1   | Mg<br>1   | 0       |
| 89  | lB    | 1        | Total<br>1   | Mg<br>1   | 0       |
| 89  | le    | 2        | Total<br>2   | Mg<br>2   | 0       |
| 89  | lg    | 1        | Total<br>1   | Mg<br>1   | 0       |
| 89  | lj    | 1        | Total<br>1   | Mg<br>1   | 0       |
| 89  | s2    | 29       | Total<br>29  | Mg<br>29  | 0       |
| 89  | l5    | 212      | Total<br>212 | Mg<br>212 | 0       |
| 89  | L5    | 213      | Total<br>213 | Mg<br>213 | 0       |
| 89  | L7    | 3        | Total<br>3   | Mg<br>3   | 0       |
| 89  | L8    | 5        | Total<br>5   | Mg<br>5   | 0       |
| 89  | LA    | 1        | Total<br>1   | Mg<br>1   | 0       |

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| Mol | Chain | Residues | Atoms       |          | AltConf |
|-----|-------|----------|-------------|----------|---------|
| 89  | LP    | 1        | Total<br>1  | Mg<br>1  | 0       |
| 89  | LV    | 1        | Total<br>1  | Mg<br>1  | 0       |
| 89  | Le    | 1        | Total<br>1  | Mg<br>1  | 0       |
| 89  | Lj    | 1        | Total<br>1  | Mg<br>1  | 0       |
| 89  | S2    | 29       | Total<br>29 | Mg<br>29 | 0       |

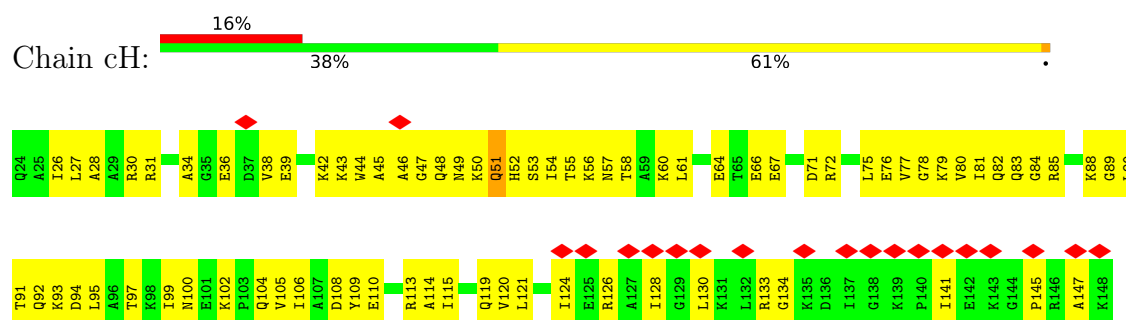
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

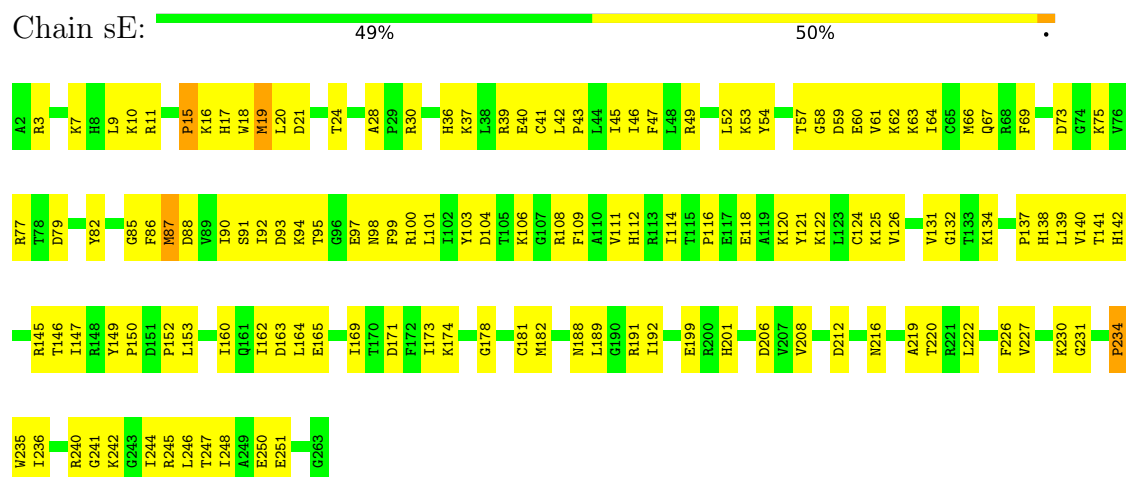
- Molecule 1: Endothelial differentiation-related factor 1



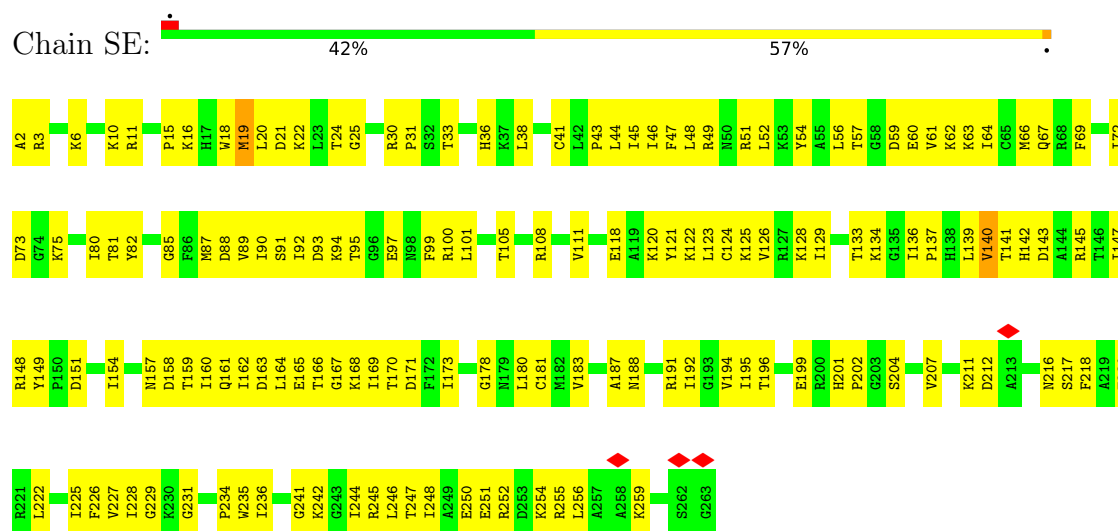
- Molecule 1: Endothelial differentiation-related factor 1



- Molecule 2: Small ribosomal subunit protein eS4, X isoform



- Molecule 2: Small ribosomal subunit protein eS4, X isoform



- Molecule 3: 40S ribosomal protein S8

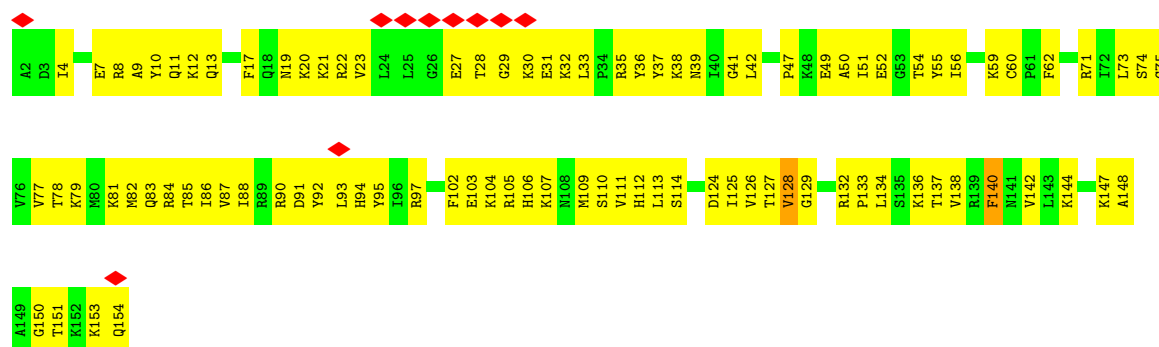


- Molecule 3: 40S ribosomal protein S8

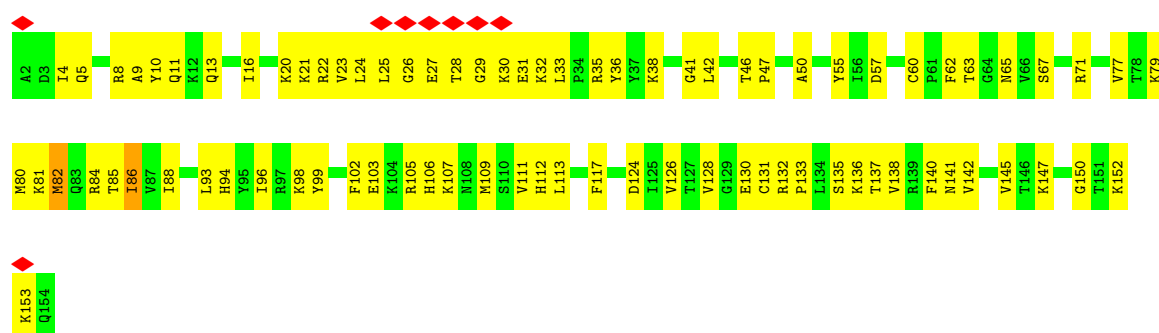


- Molecule 4: 40S ribosomal protein S11

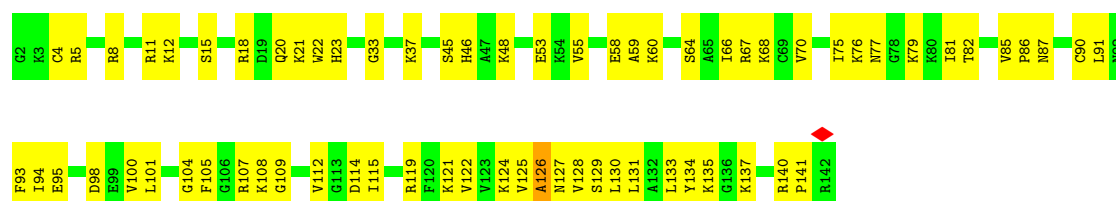




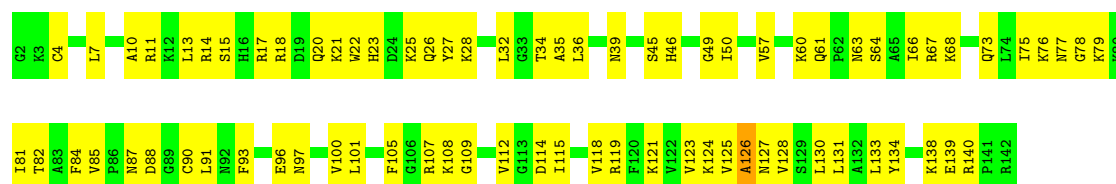
• Molecule 4: 40S ribosomal protein S11



• Molecule 5: 40S ribosomal protein S23

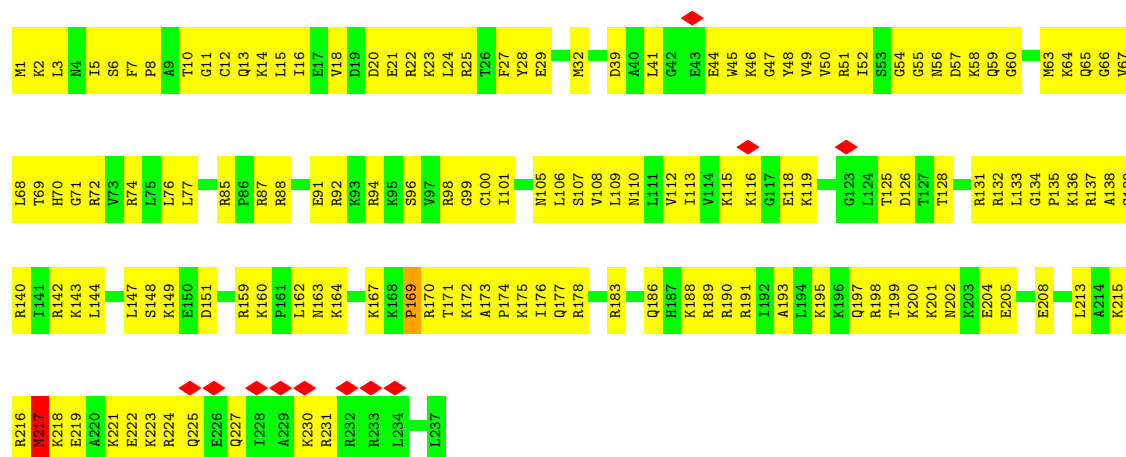


• Molecule 5: 40S ribosomal protein S23

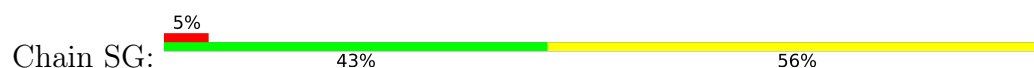


• Molecule 6: 40S ribosomal protein S6

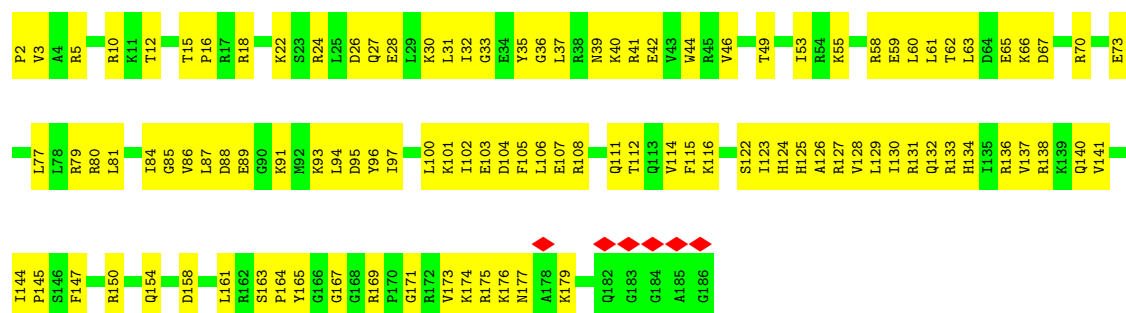




• Molecule 6: 40S ribosomal protein S6



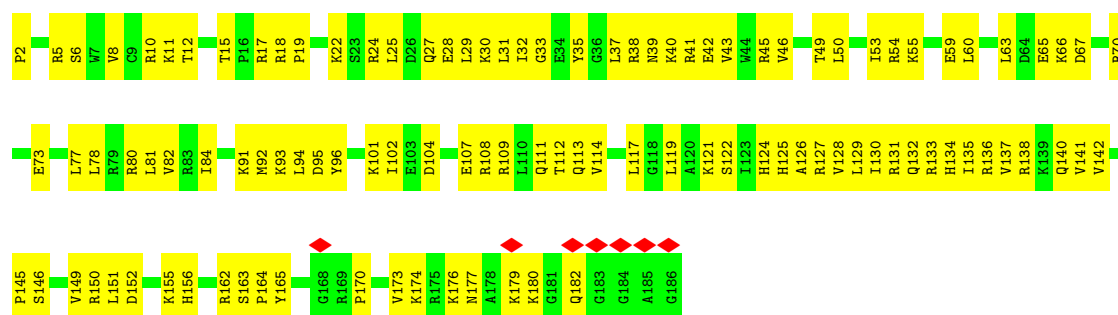
• Molecule 7: 40S ribosomal protein S9



• Molecule 7: 40S ribosomal protein S9



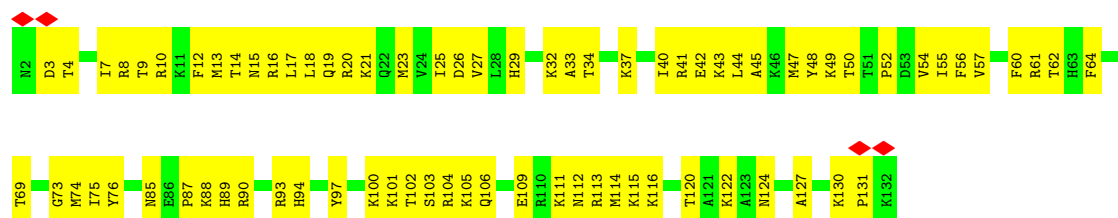




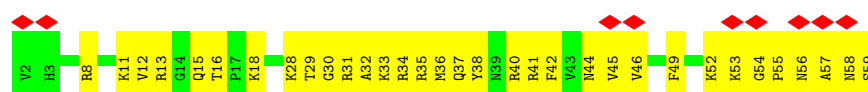
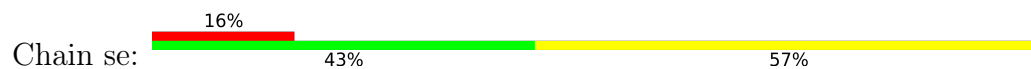
• Molecule 8: 40S ribosomal protein S24



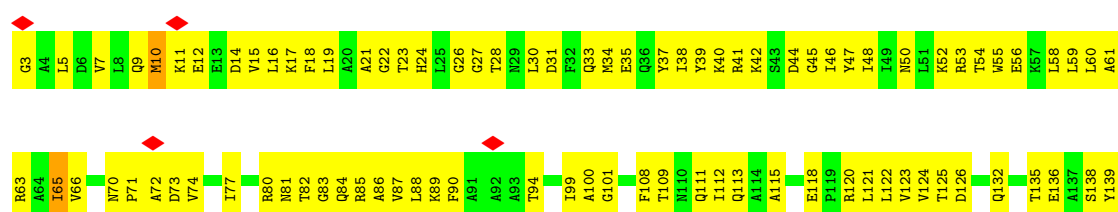
• Molecule 8: 40S ribosomal protein S24

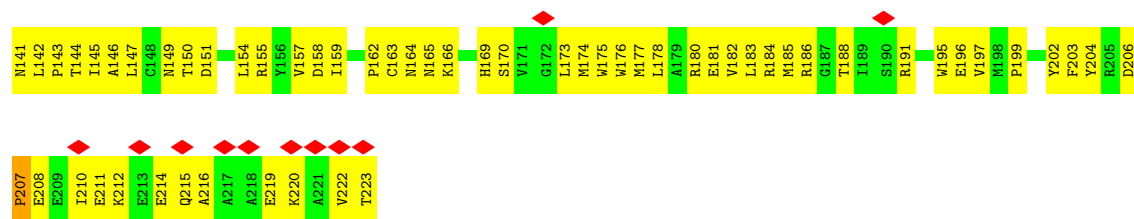


• Molecule 9: Small ribosomal subunit protein eS30

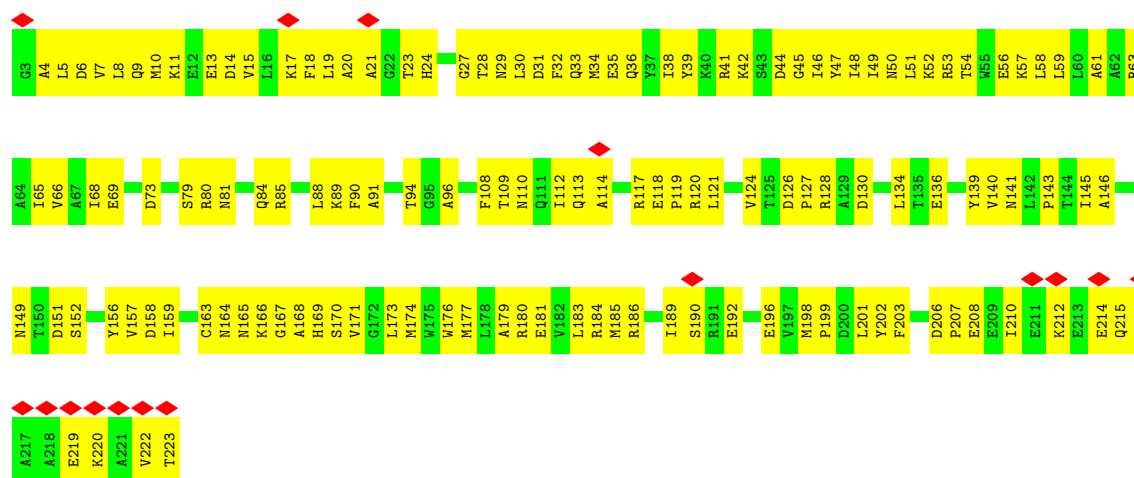


• Molecule 10: 40S ribosomal protein SA

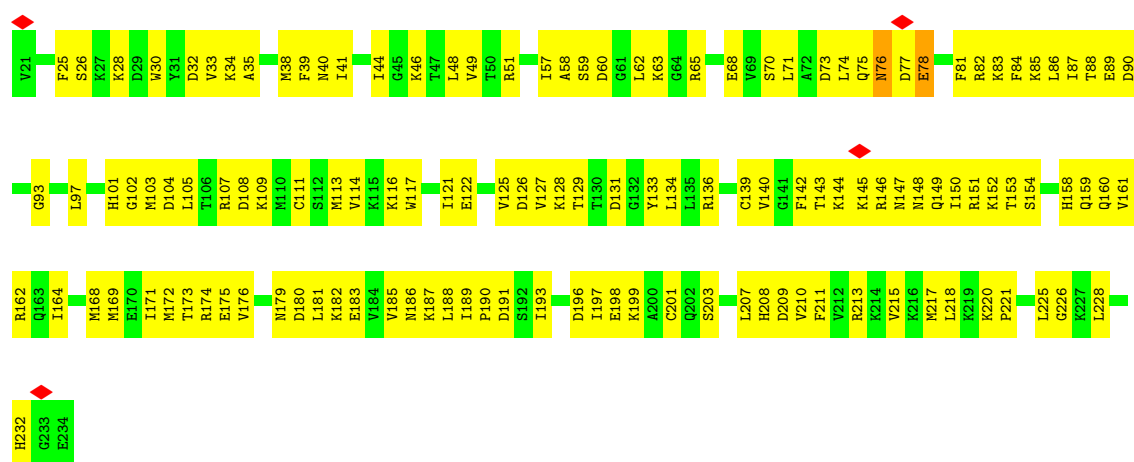




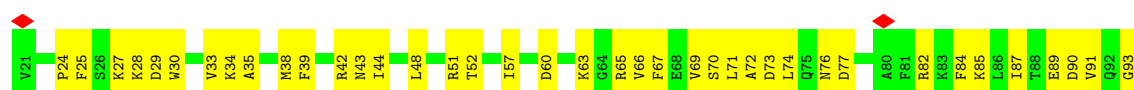
• Molecule 10: 40S ribosomal protein SA

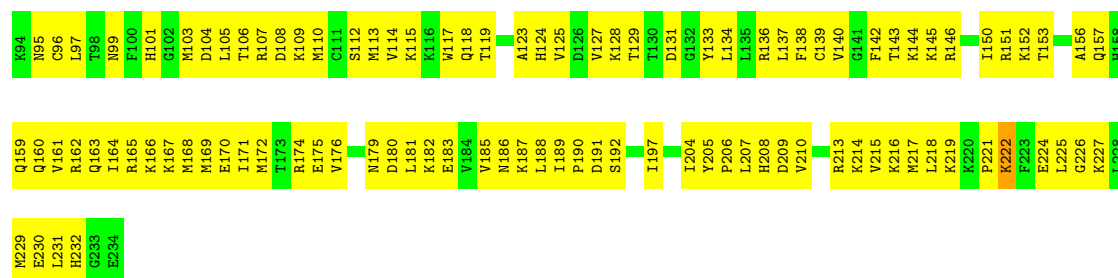


• Molecule 11: 40S ribosomal protein S3a

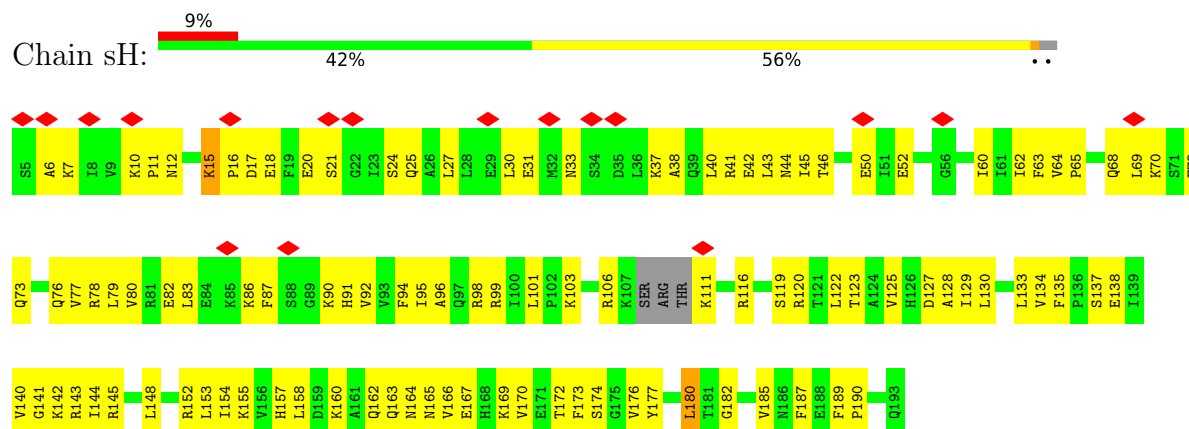


• Molecule 11: 40S ribosomal protein S3a

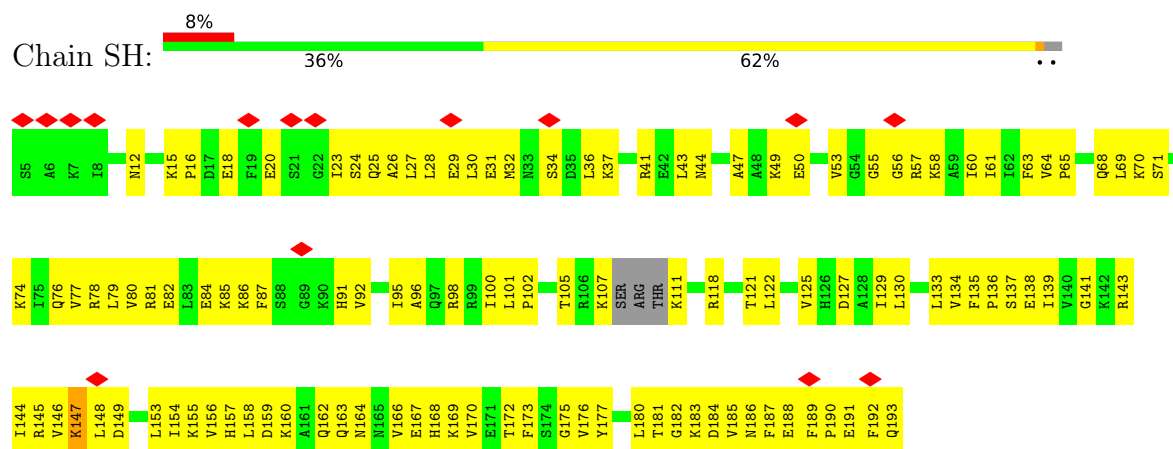




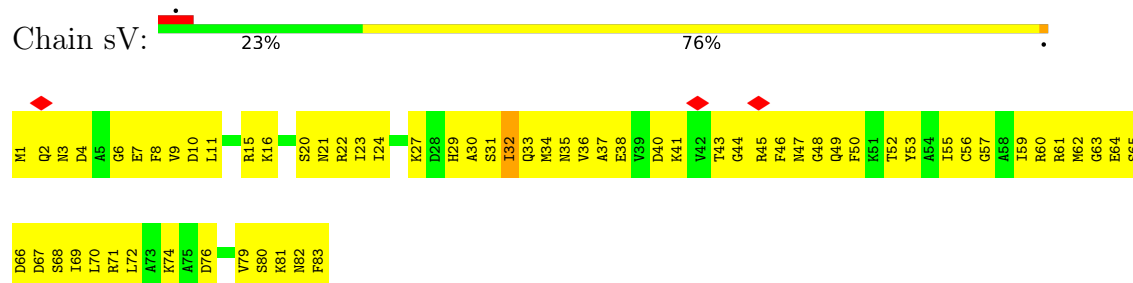
- Molecule 12: Small ribosomal subunit protein eS7



- Molecule 12: Small ribosomal subunit protein eS7

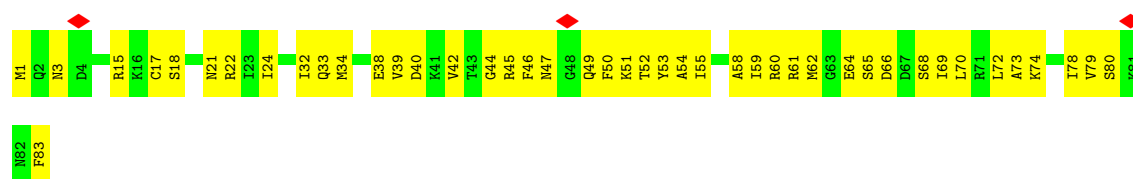


- Molecule 13: 40S ribosomal protein S21



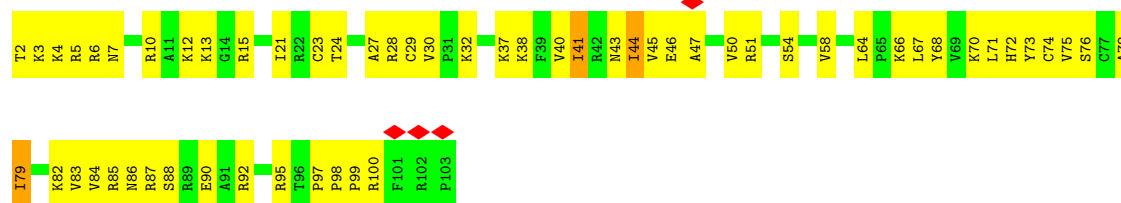
- Molecule 13: 40S ribosomal protein S21

Chain SV:  47% 53%



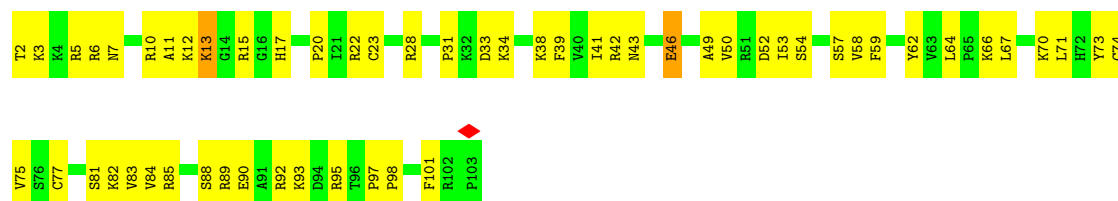
- Molecule 14: 40S ribosomal protein S26

Chain sa:  43% 54%



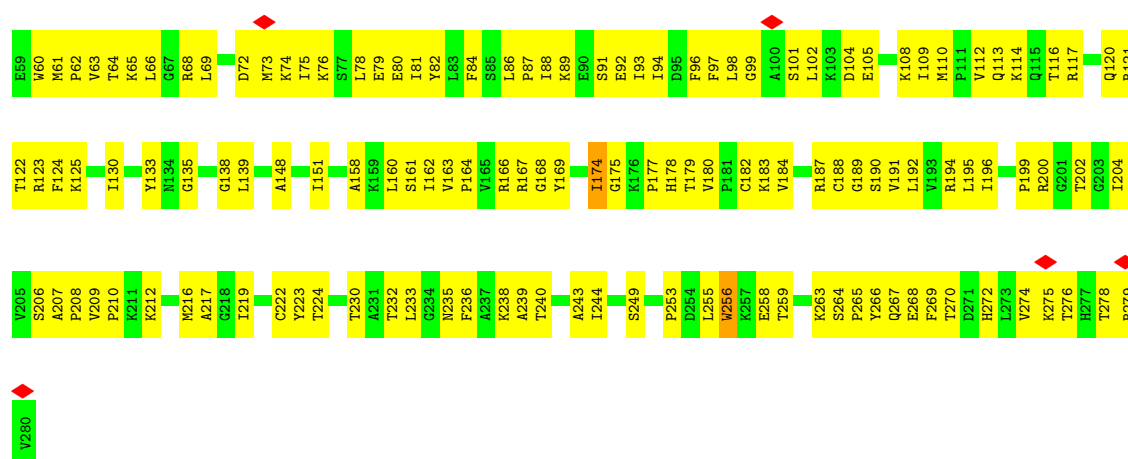
- Molecule 14: 40S ribosomal protein S26

Chain Sa:  45% 53%

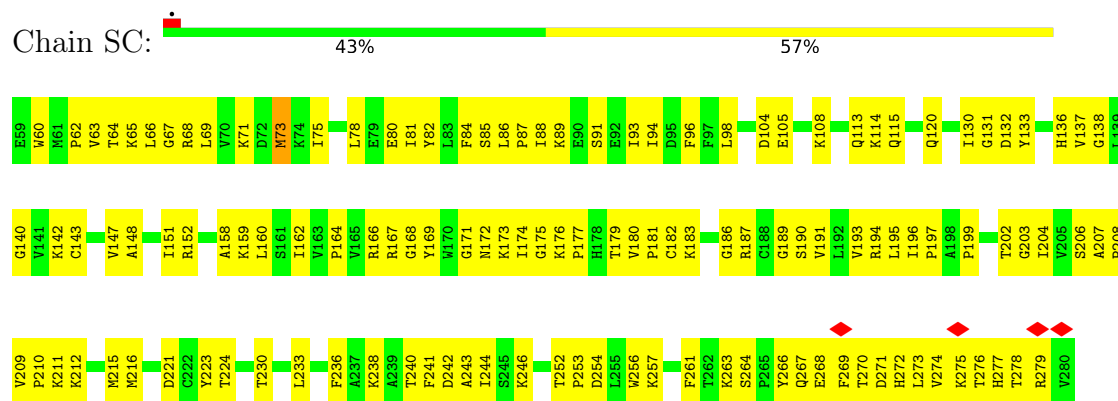


- Molecule 15: 40S ribosomal protein S2

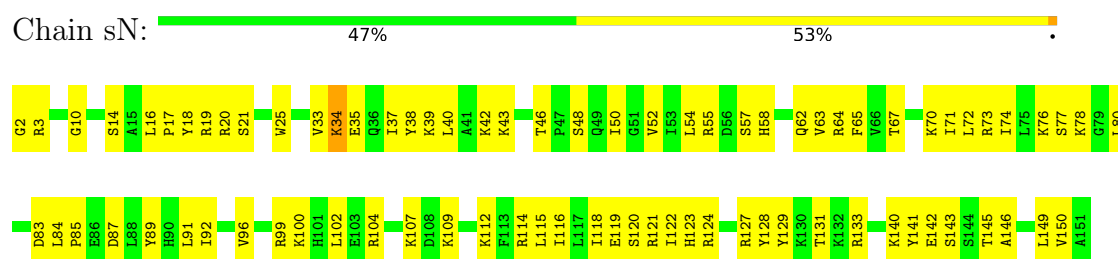
Chain sC:  41% 58%



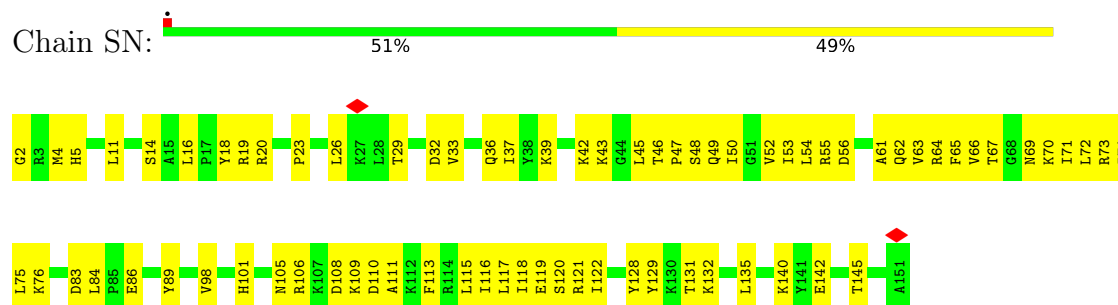
- Molecule 15: 40S ribosomal protein S2



• Molecule 16: 40S ribosomal protein S13



• Molecule 16: 40S ribosomal protein S13

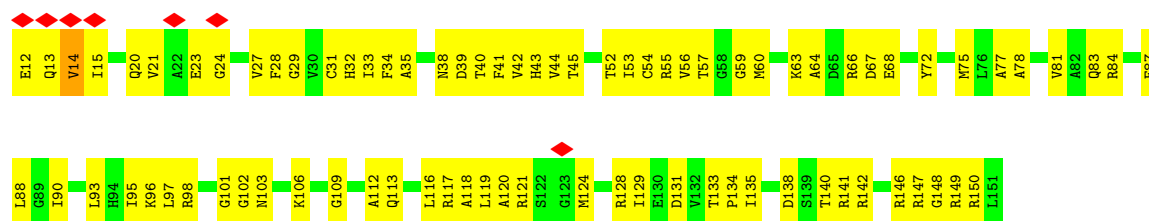


• Molecule 17: Small ribosomal subunit protein uS11



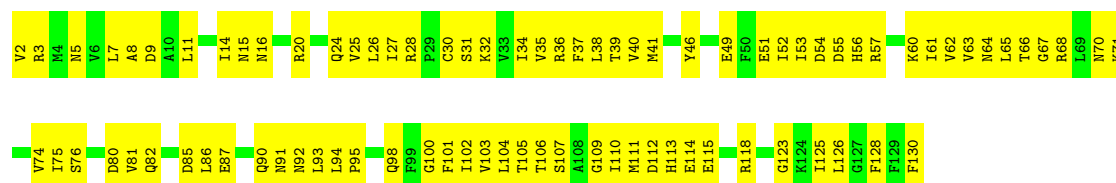
• Molecule 17: Small ribosomal subunit protein uS11





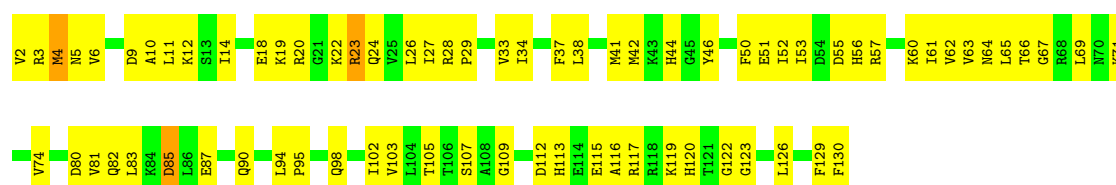
- Molecule 18: 40S ribosomal protein S15a

Chain sW: 35% 65%



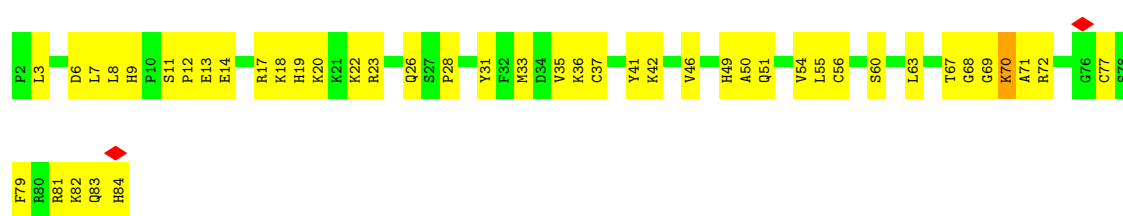
- Molecule 18: 40S ribosomal protein S15a

Chain SW: 43% 54%



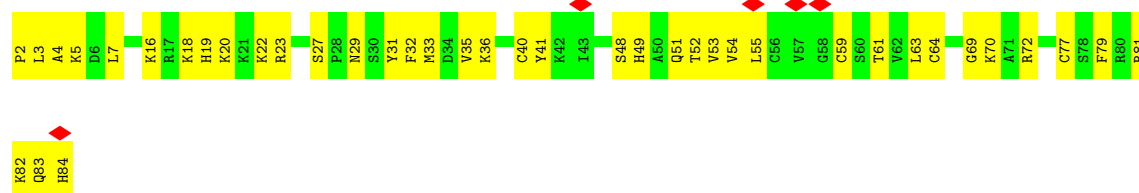
- Molecule 19: Small ribosomal subunit protein eS27

Chain sb: 46% 53%



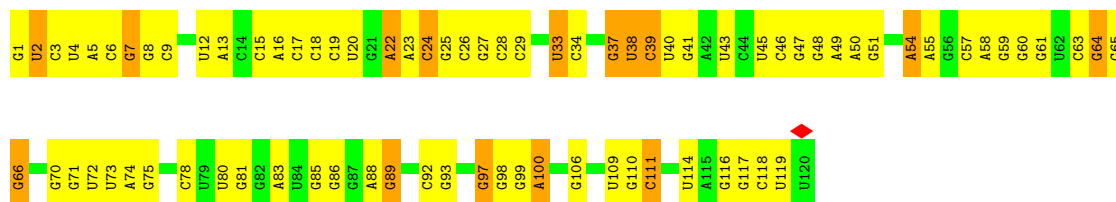
- Molecule 19: Small ribosomal subunit protein eS27

Chain Sb: 6% 52% 48%



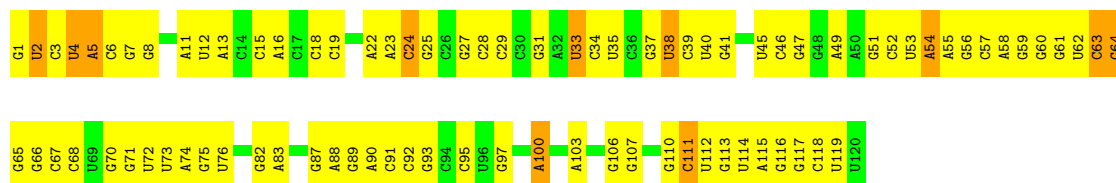
- Molecule 20: RNA (120-MER)5S rRNA [Homo sapiens]

Chain 17:  33% 54% 12%



- Molecule 20: RNA (120-MER)5S rRNA [Homo sapiens]

Chain L7:  29% 62% 9%



- Molecule 21: RNA (156-MER)5.8S rRNA [Homo sapiens]

Chain 18:  21% 66% 13%



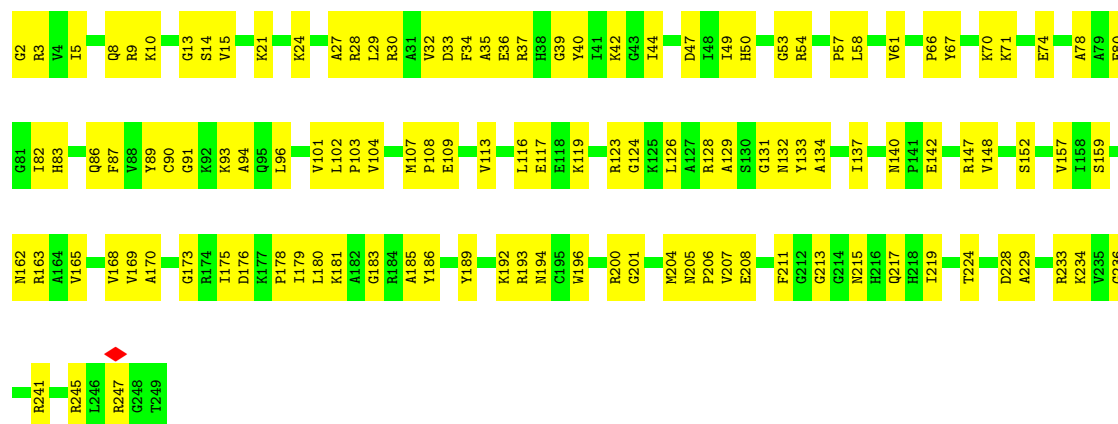
- Molecule 21: RNA (156-MER)5.8S rRNA [Homo sapiens]

Chain L8:  22% 67% 11%



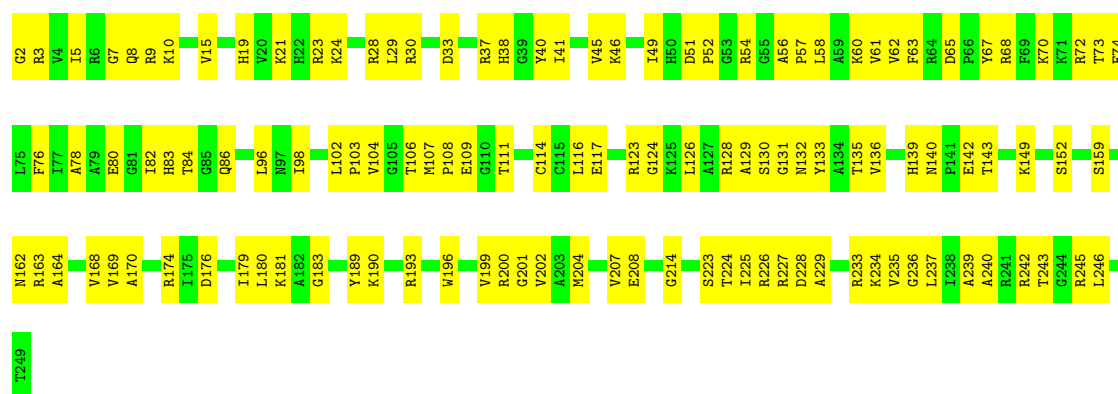
- Molecule 22: 60S ribosomal protein L8

Chain 1A:  52% 48%



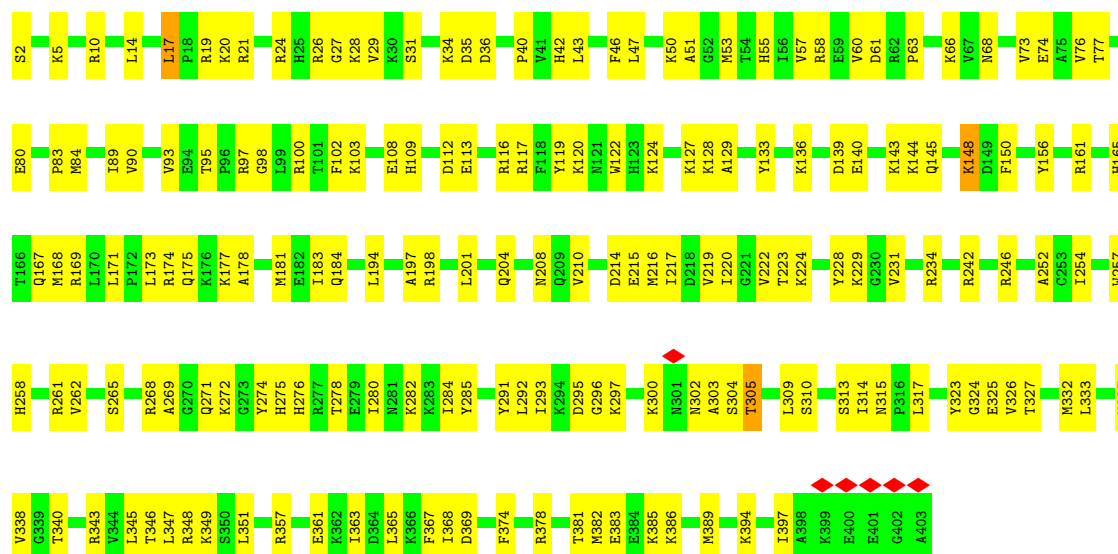
• Molecule 22: 60S ribosomal protein L8

Chain LA: 52% 48%



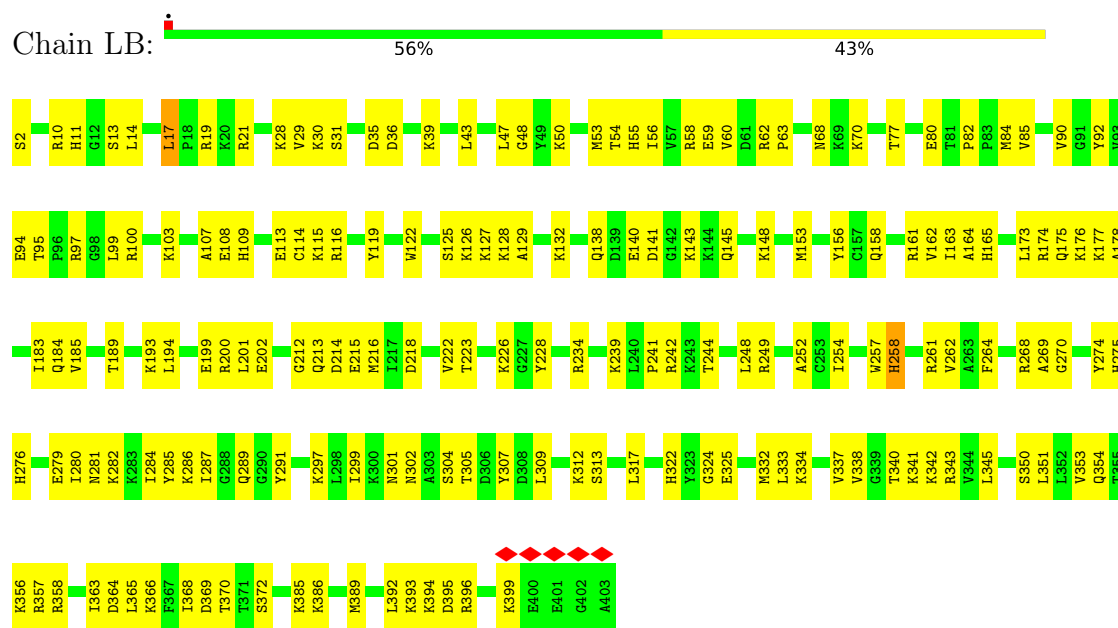
• Molecule 23: Large ribosomal subunit protein uL3

Chain LB: 56% 44%

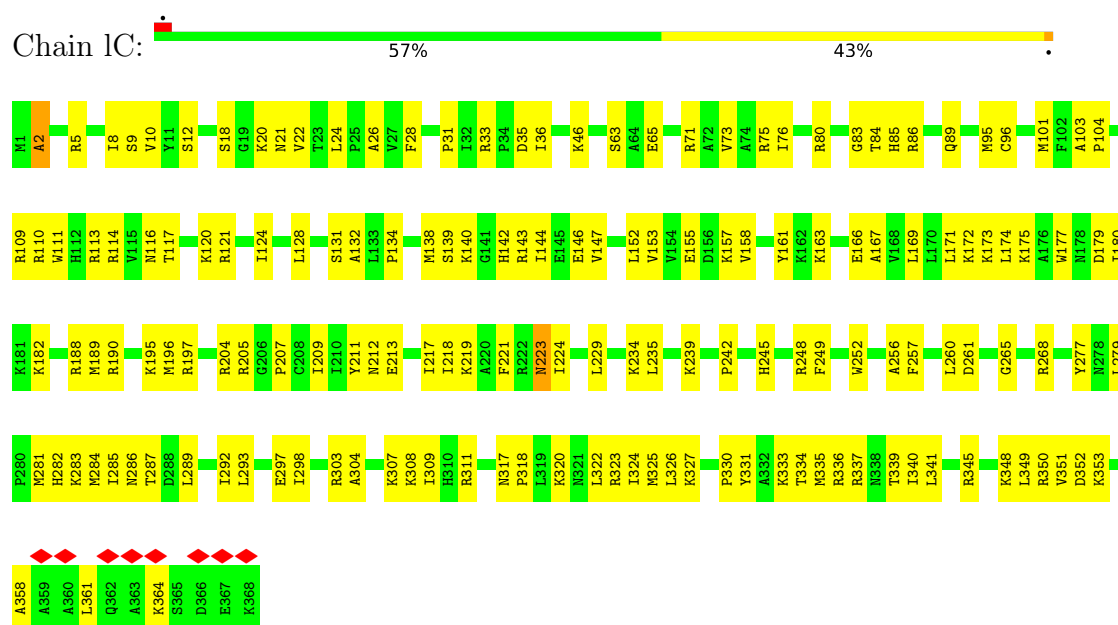




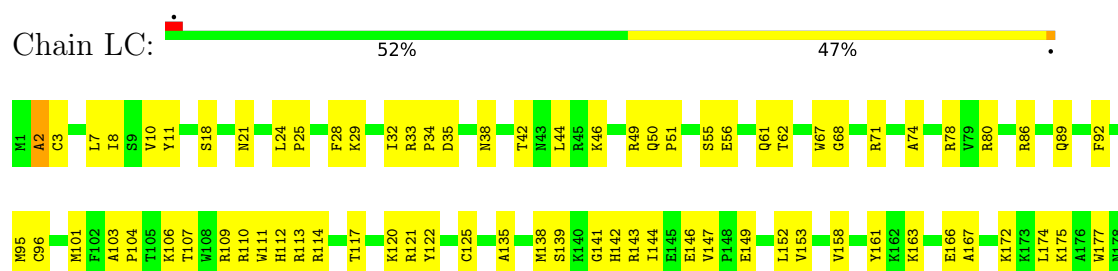
- Molecule 23: Large ribosomal subunit protein uL3

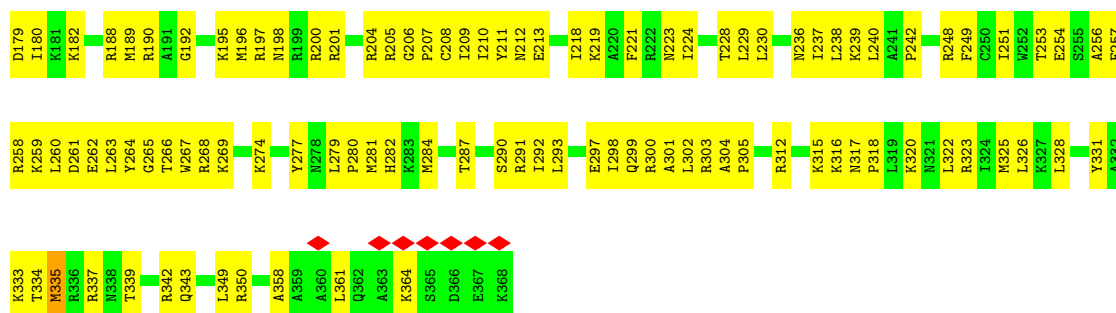


- Molecule 24: 60S ribosomal protein L4

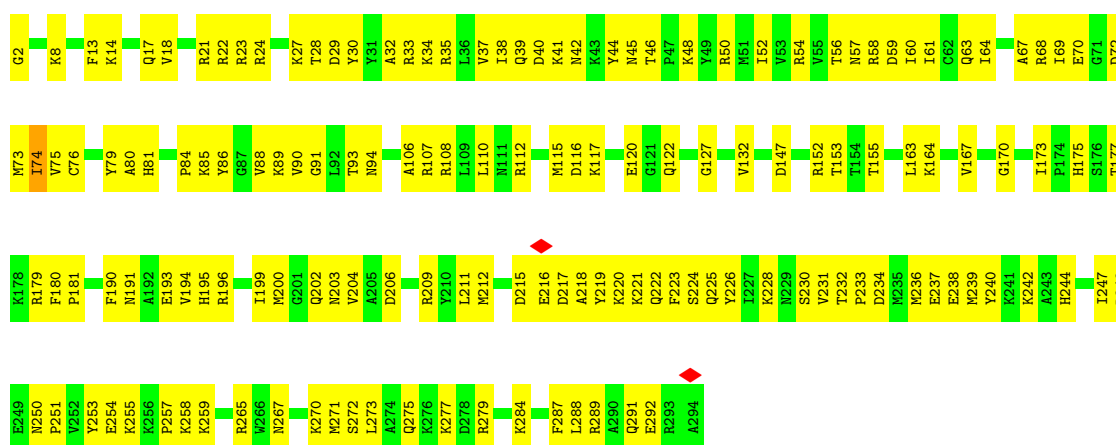


- Molecule 24: 60S ribosomal protein L4

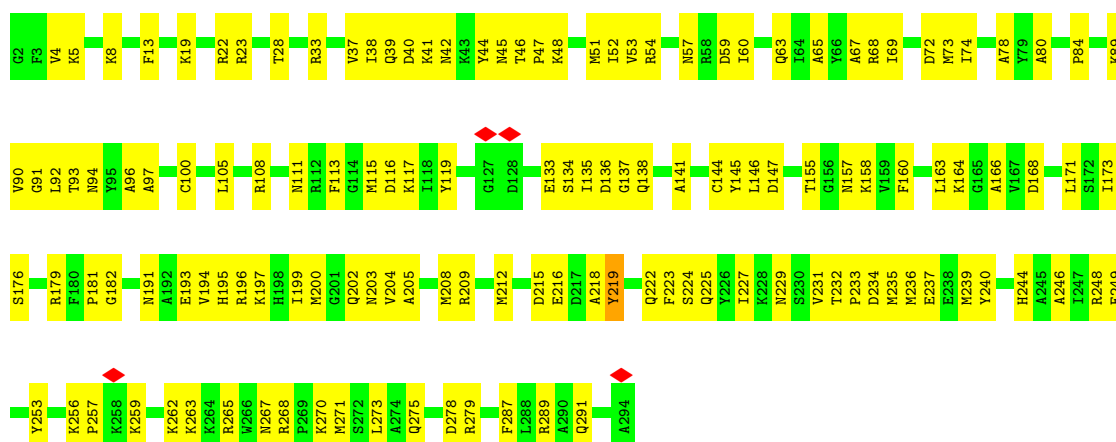




- Molecule 25: Large ribosomal subunit protein uL18

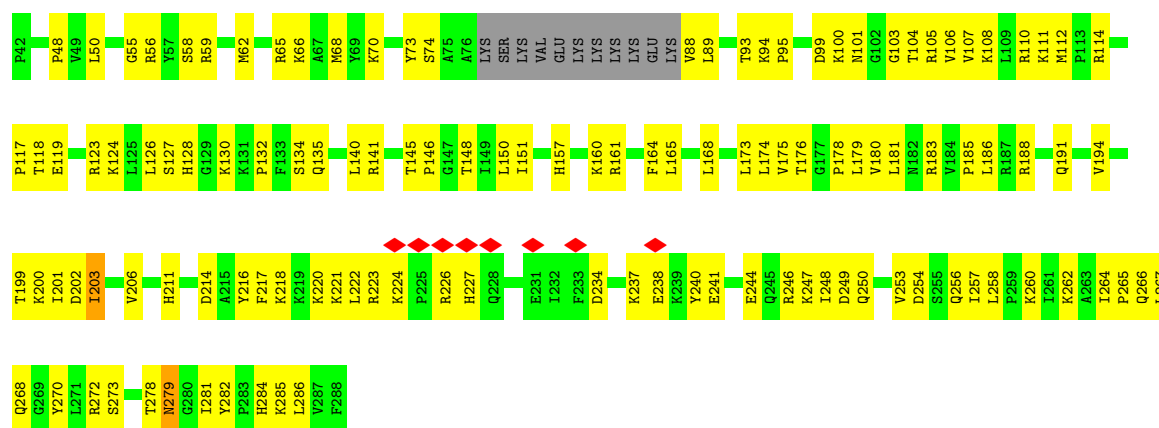


- Molecule 25: Large ribosomal subunit protein uL18

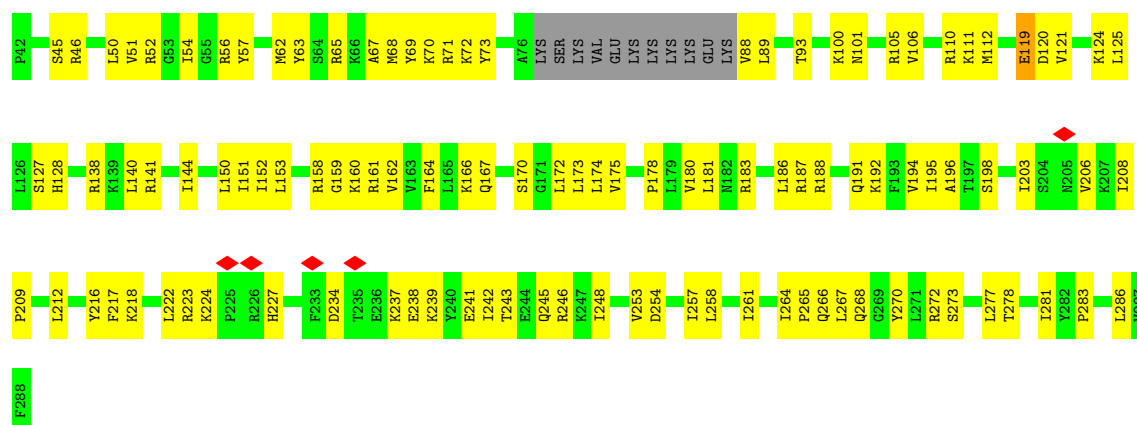


- Molecule 26: Large ribosomal subunit protein eL6

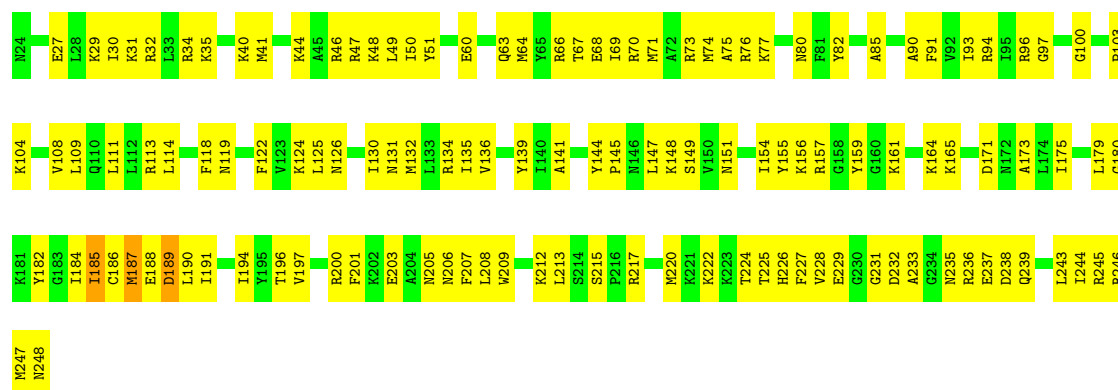




• Molecule 26: Large ribosomal subunit protein eL6

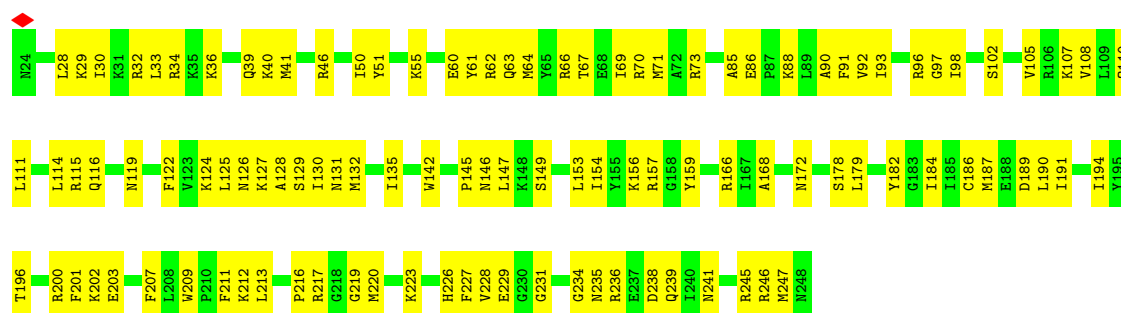


• Molecule 27: 60S ribosomal protein L7

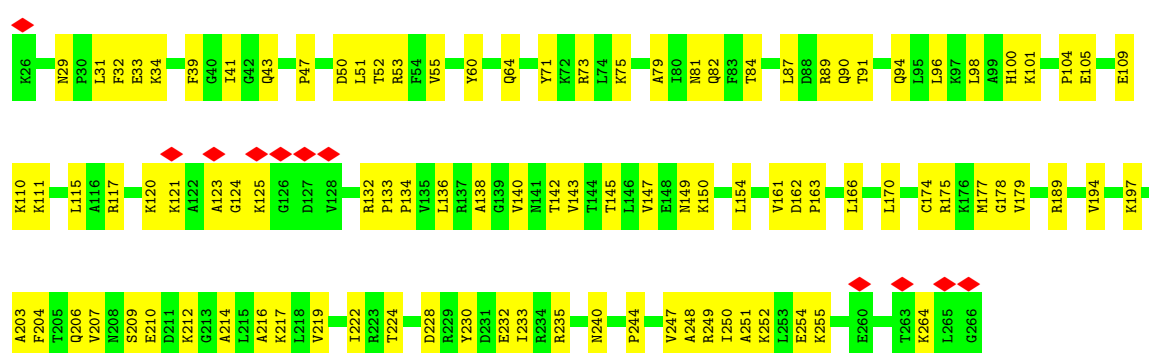


• Molecule 27: 60S ribosomal protein L7

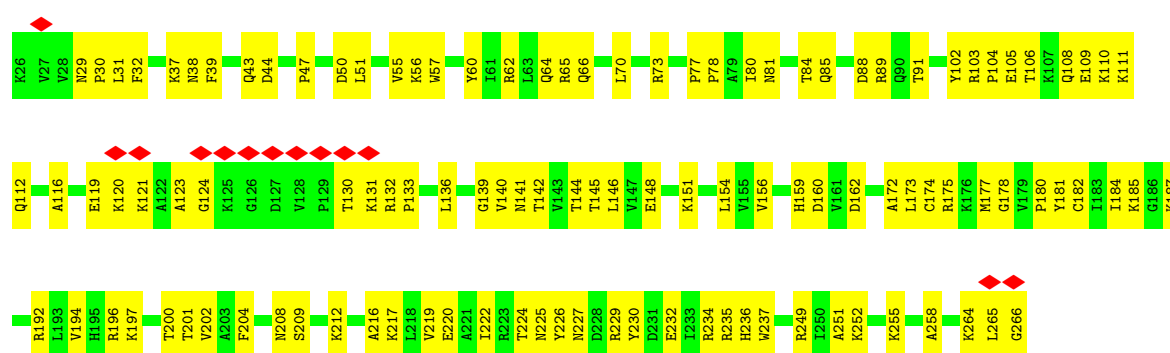




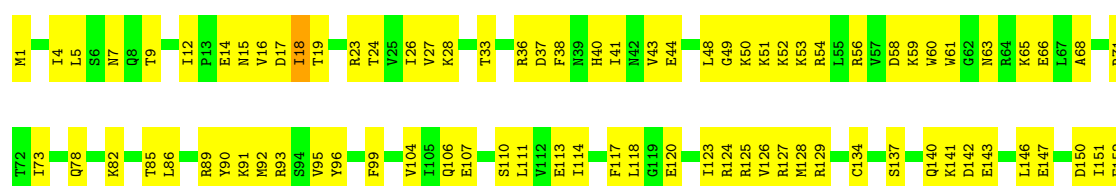
• Molecule 28: 60S ribosomal protein L7a



• Molecule 28: 60S ribosomal protein L7a

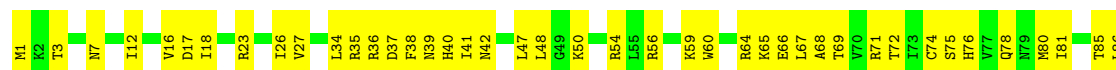


• Molecule 29: 60S ribosomal protein L9

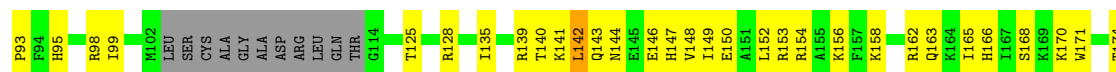
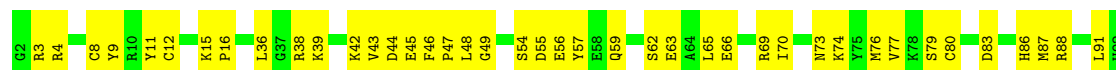




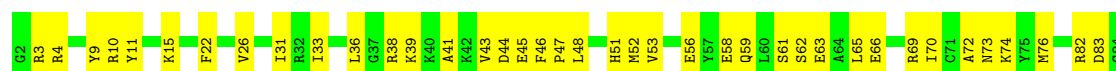
- Molecule 29: 60S ribosomal protein L9



- Molecule 30: Ribosomal protein uL16-like

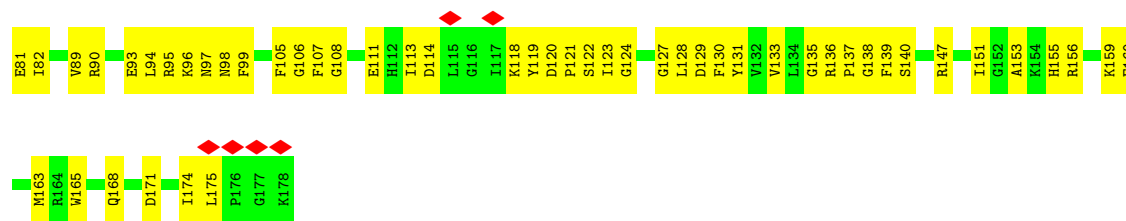


- Molecule 30: Ribosomal protein uL16-like

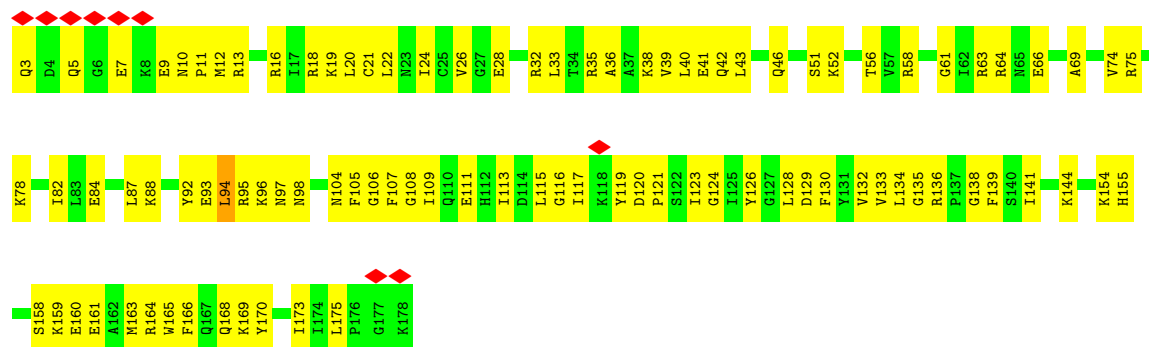


- Molecule 31: 60S ribosomal protein L11

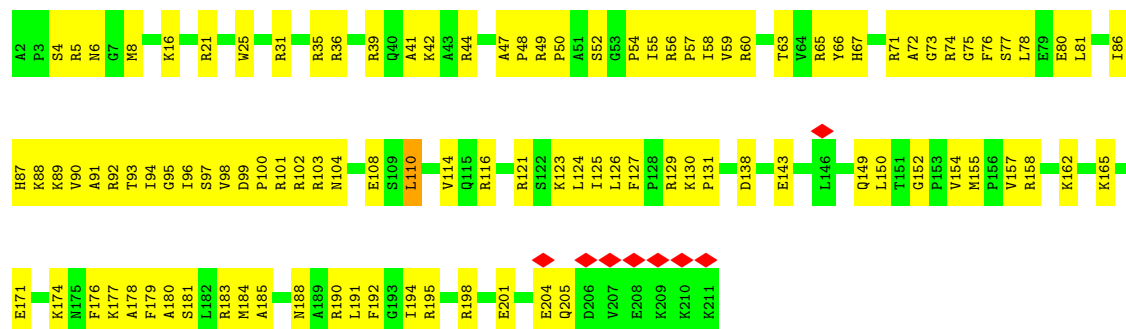




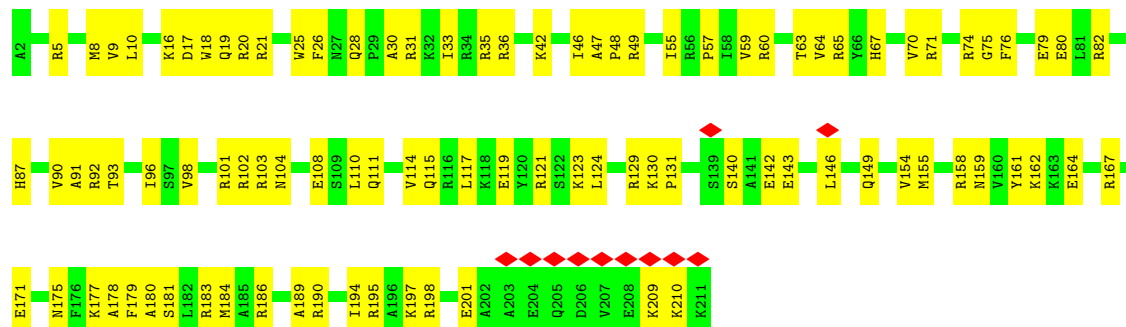
• Molecule 31: 60S ribosomal protein L11



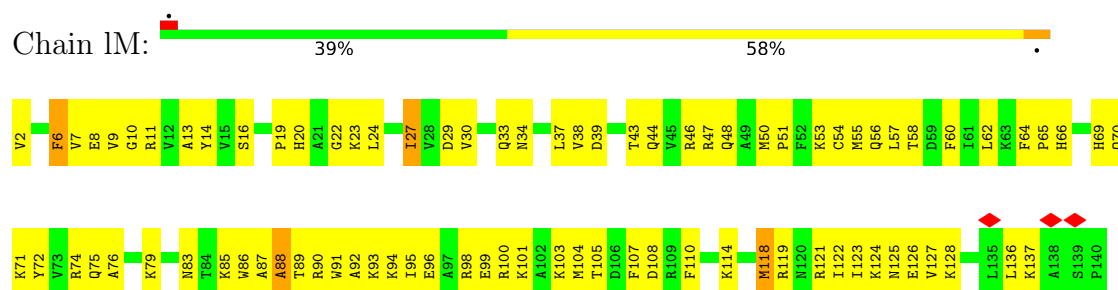
• Molecule 32: Large ribosomal subunit protein eL13



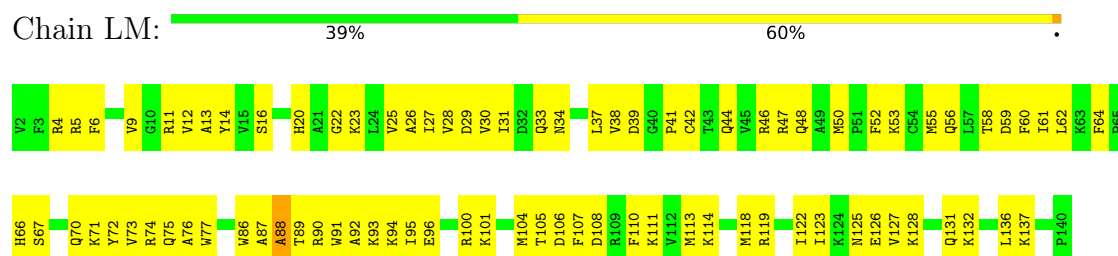
• Molecule 32: Large ribosomal subunit protein eL13



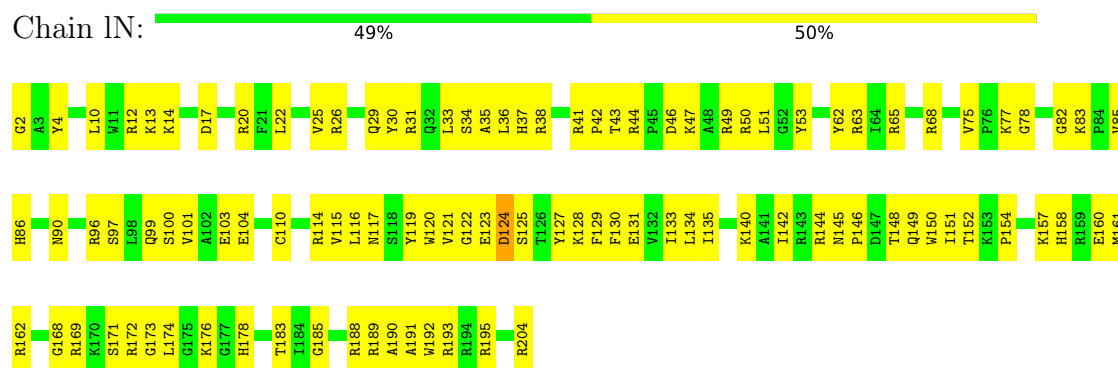
- Molecule 33: 60S ribosomal protein L14



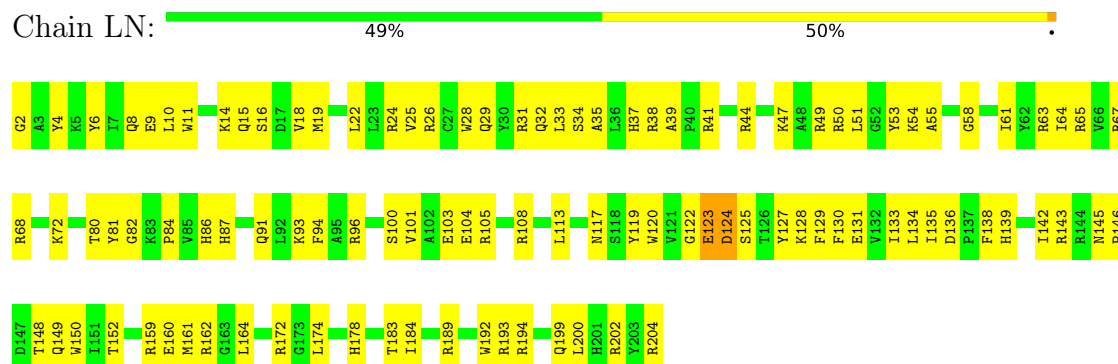
- Molecule 33: 60S ribosomal protein L14



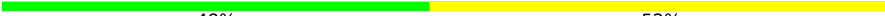
- Molecule 34: 60S ribosomal protein L15

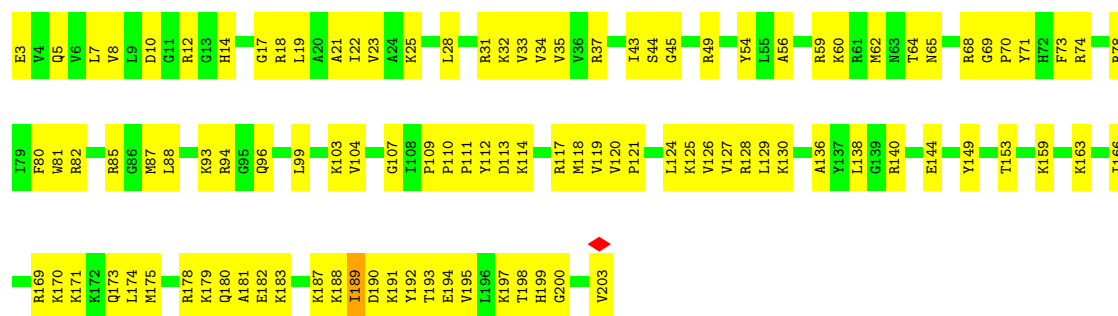


- Molecule 34: 60S ribosomal protein L15



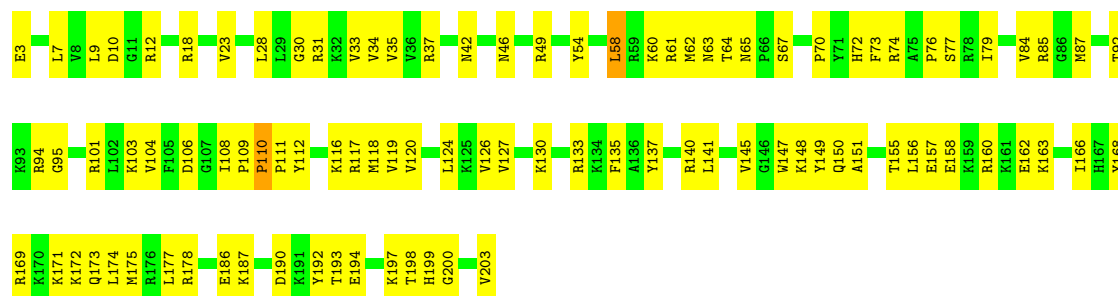
- Molecule 35: 60S ribosomal protein L13a

Chain IO:  48% 52%



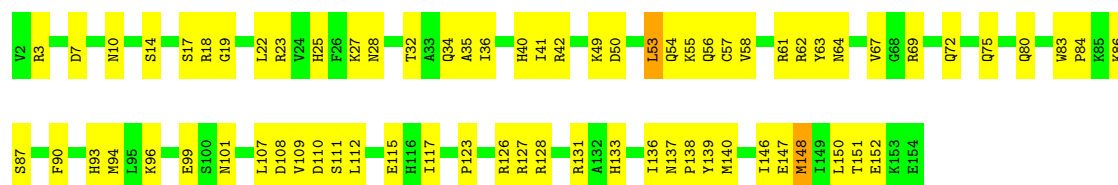
- Molecule 35: 60S ribosomal protein L13a

Chain LO:  52% 47%



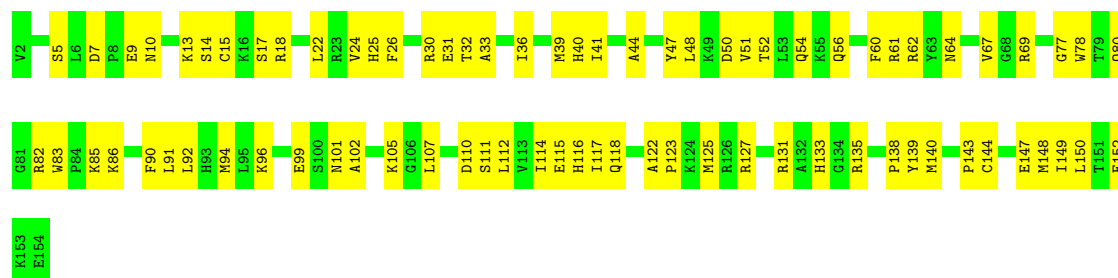
- Molecule 36: 60S ribosomal protein L17

Chain IP:  54% 45%



- Molecule 36: 60S ribosomal protein L17

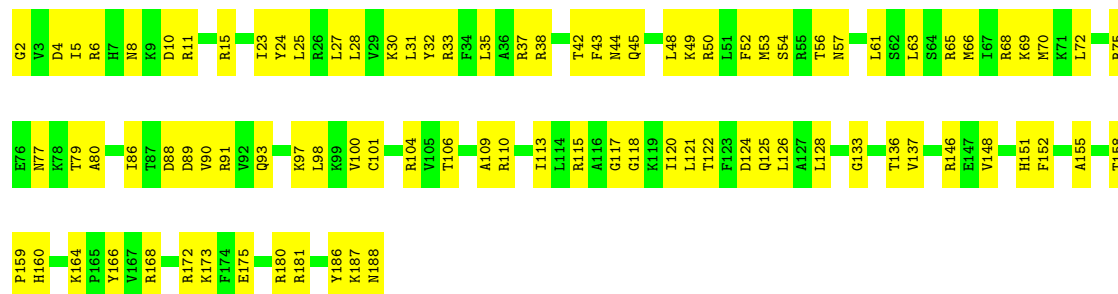
Chain LP:  50% 50%



- Molecule 37: 60S ribosomal protein L18

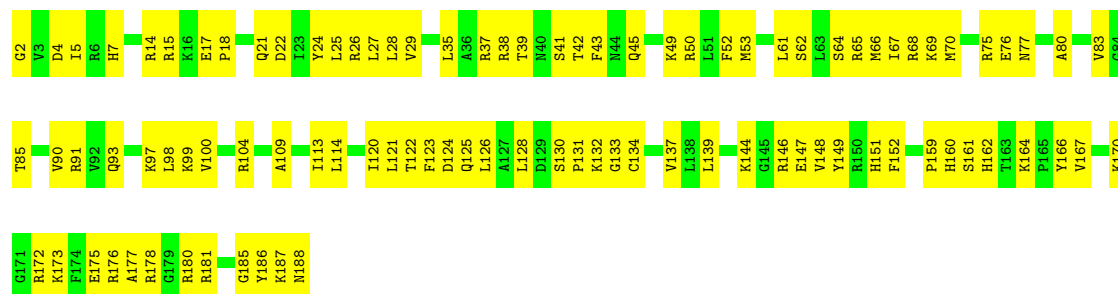


Chain IQ:  51% 49%



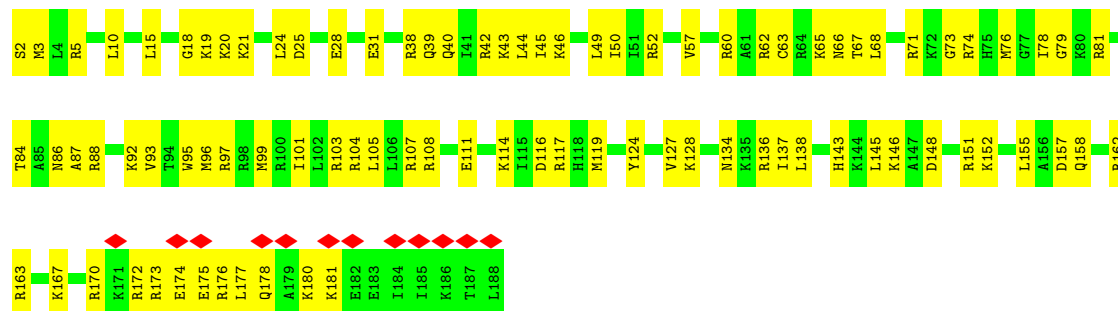
- Molecule 37: 60S ribosomal protein L18

Chain LQ:  49% 51%



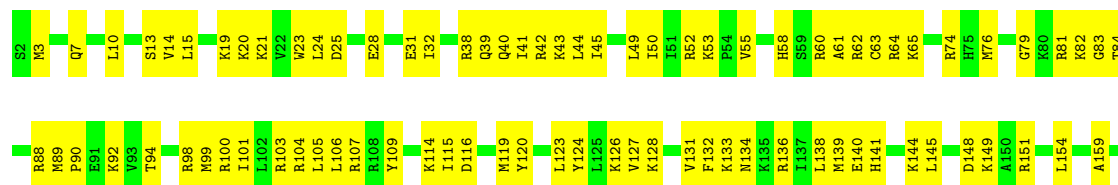
- Molecule 38: 60S ribosomal protein L19

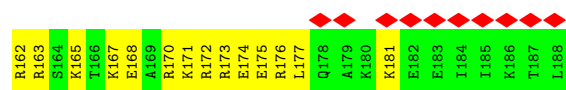
Chain IR:  6% 52% 48%



- Molecule 38: 60S ribosomal protein L19

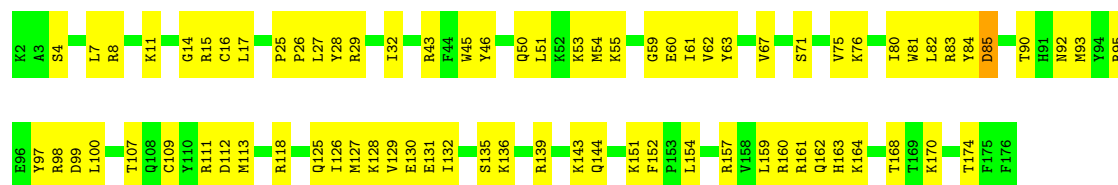
Chain LR:  5% 48% 52%





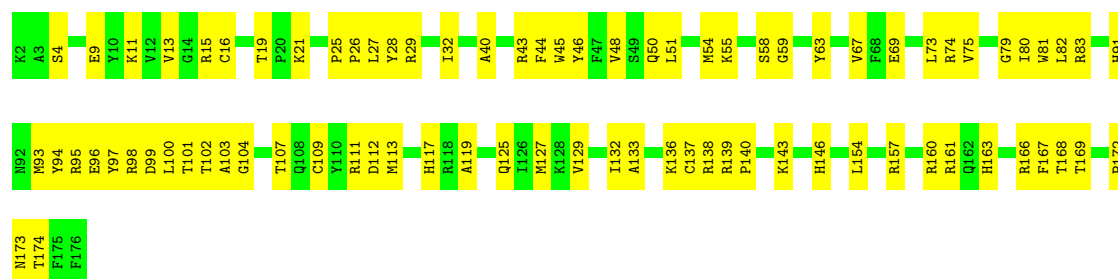
• Molecule 39: 60S ribosomal protein L18a

Chain IS: 56% 43%



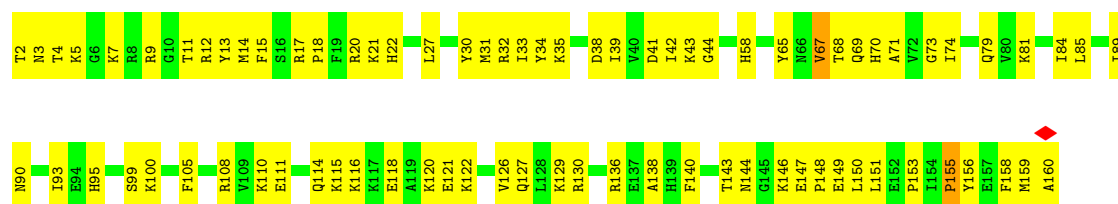
• Molecule 39: 60S ribosomal protein L18a

Chain LS: 54% 46%



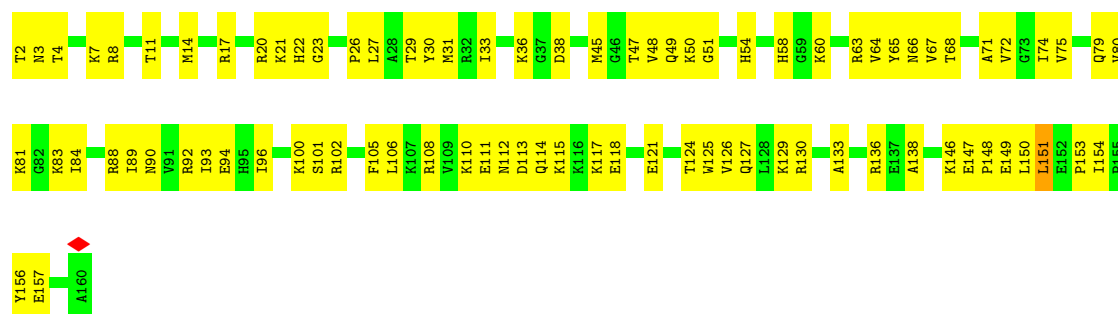
• Molecule 40: 60S ribosomal protein L21

Chain IT: 50% 49%

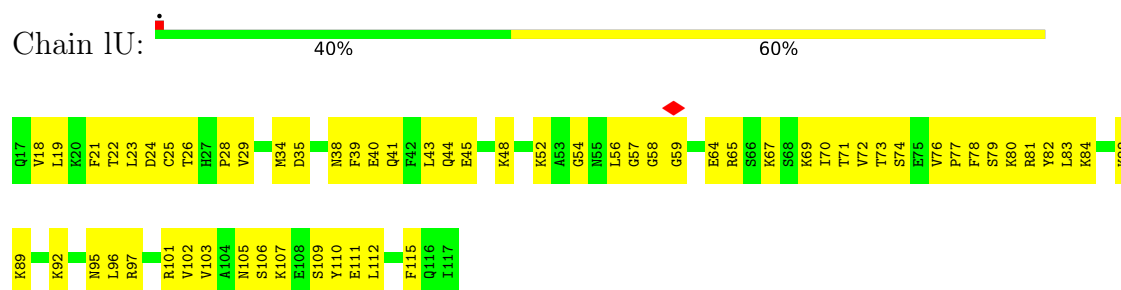


• Molecule 40: 60S ribosomal protein L21

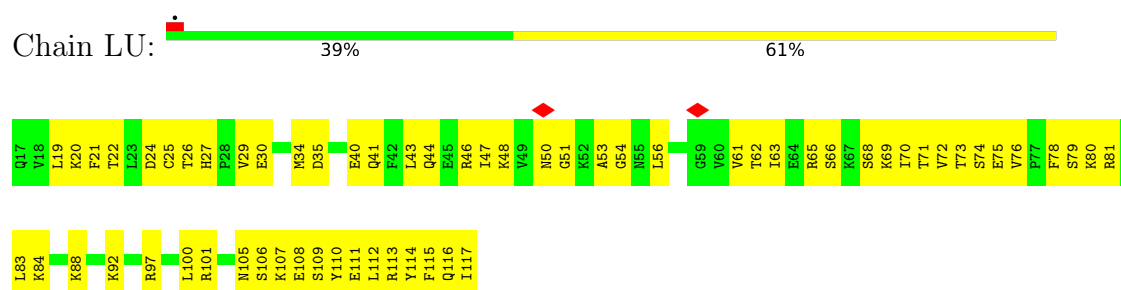
Chain LT: 47% 53%



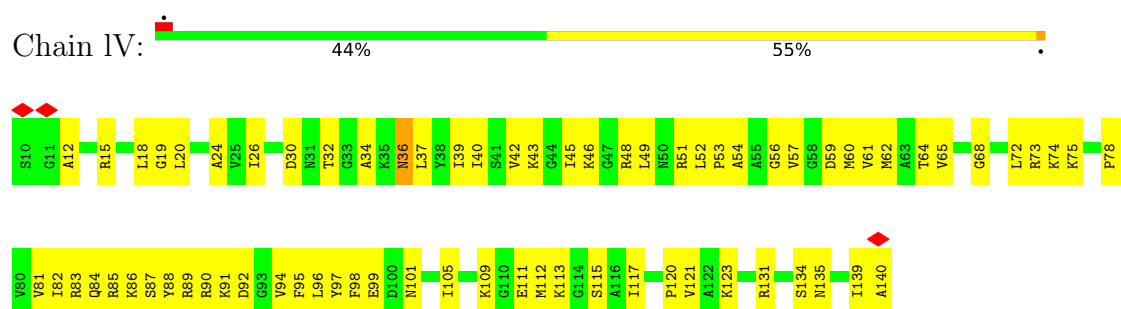
- Molecule 41: Heparin-binding protein HBp15



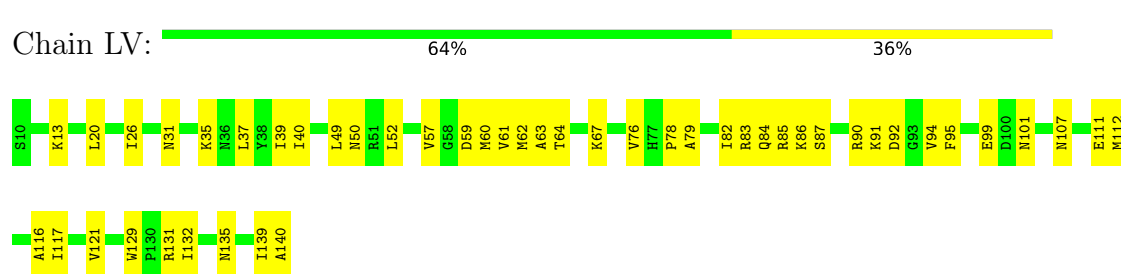
- Molecule 41: Heparin-binding protein HBp15



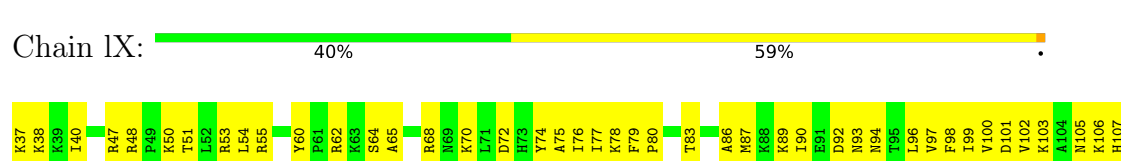
- Molecule 42: 60S ribosomal protein L23



- Molecule 42: 60S ribosomal protein L23



- Molecule 43: 60S ribosomal protein L23a

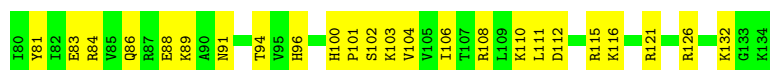




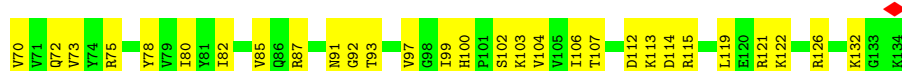
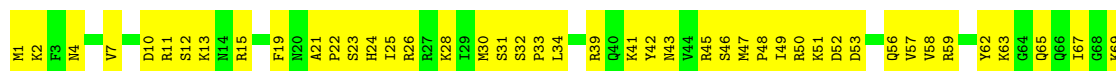
- Molecule 43: 60S ribosomal protein L23a



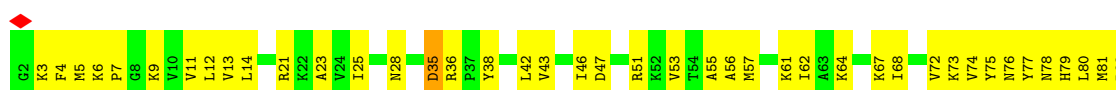
- Molecule 44: 60S ribosomal protein L26



- Molecule 44: 60S ribosomal protein L26

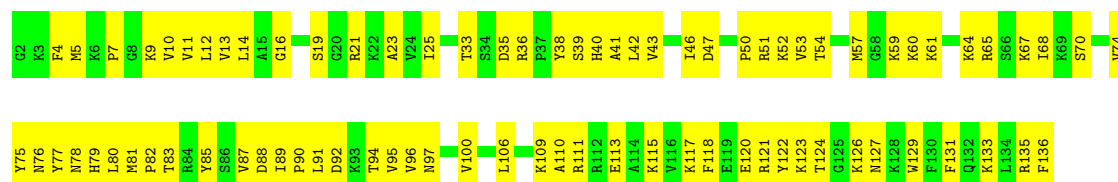


- Molecule 45: 60S ribosomal protein L27



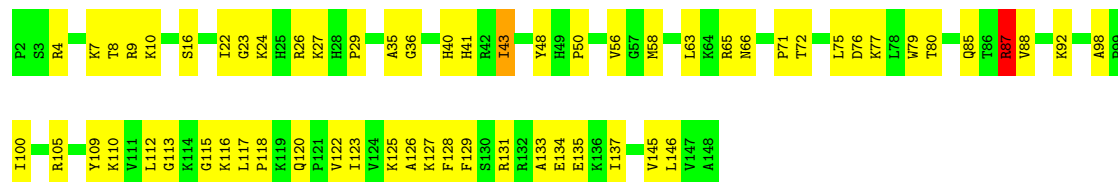
- Molecule 45: 60S ribosomal protein L27





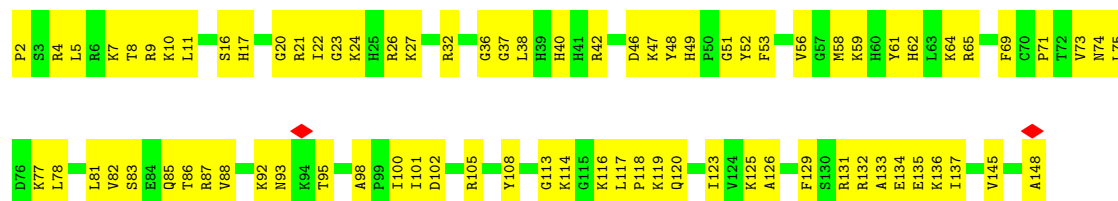
• Molecule 46: 60S ribosomal protein L27a

Chain la: 59% 40% ..



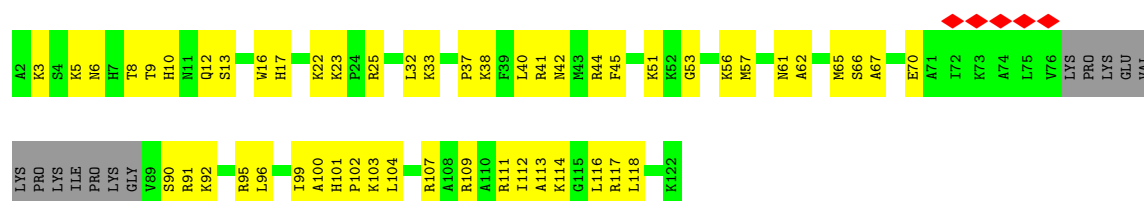
• Molecule 46: 60S ribosomal protein L27a

Chain La: 46% 54%



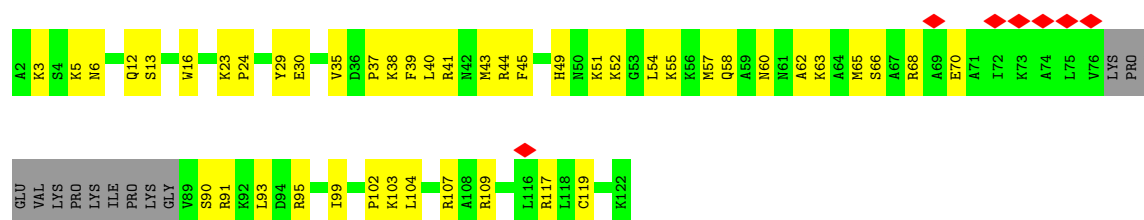
• Molecule 47: Large ribosomal subunit protein eL29

Chain lb: 47% 43% 10%



• Molecule 47: Large ribosomal subunit protein eL29

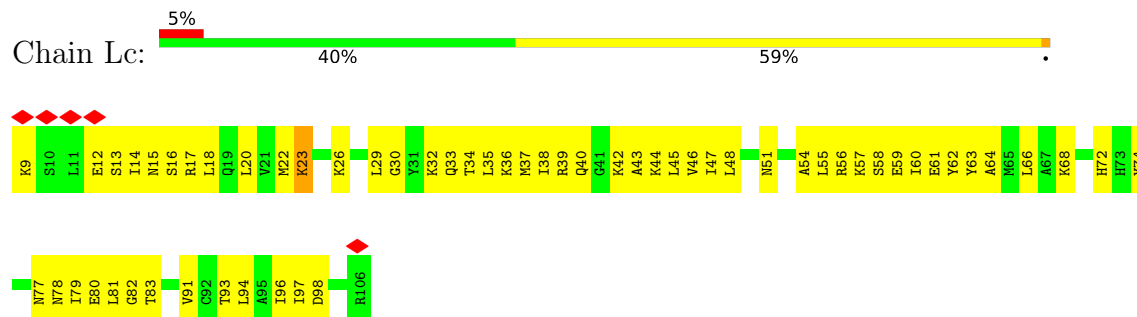
Chain Lb: 6% 53% 37% 10%



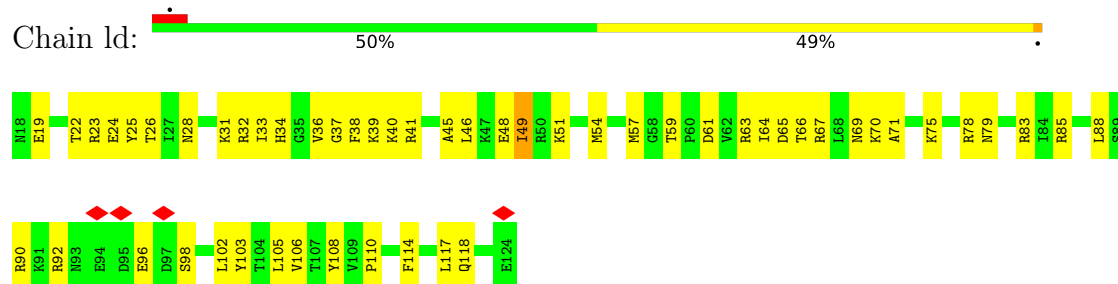
• Molecule 48: 60S ribosomal protein L30



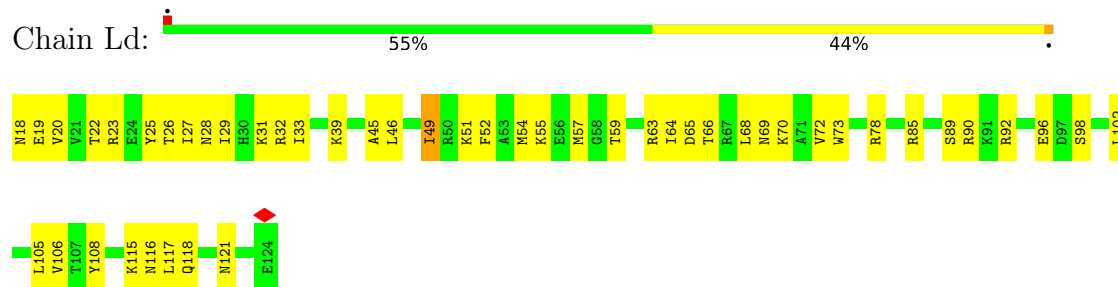
- Molecule 48: 60S ribosomal protein L30



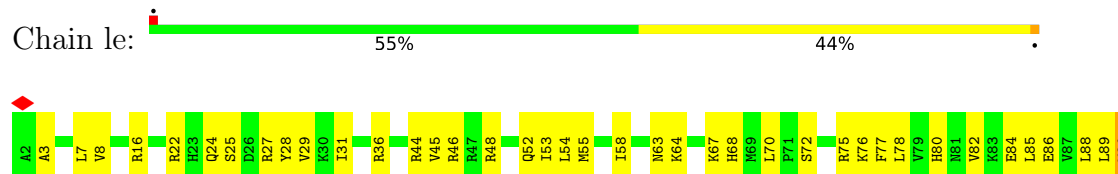
- Molecule 49: 60S ribosomal protein L31



- Molecule 49: 60S ribosomal protein L31



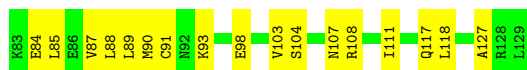
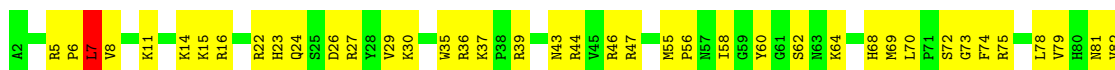
- Molecule 50: 60S ribosomal protein L32





- Molecule 50: 60S ribosomal protein L32

Chain Le: 55% 44%



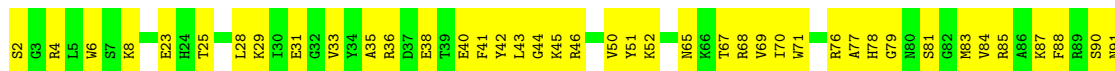
- Molecule 51: 60S ribosomal protein L35a

Chain lf: 53% 46%



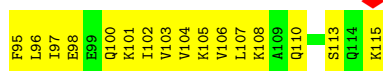
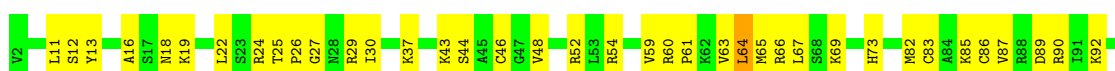
- Molecule 51: 60S ribosomal protein L35a

Chain Lf: 54% 45%



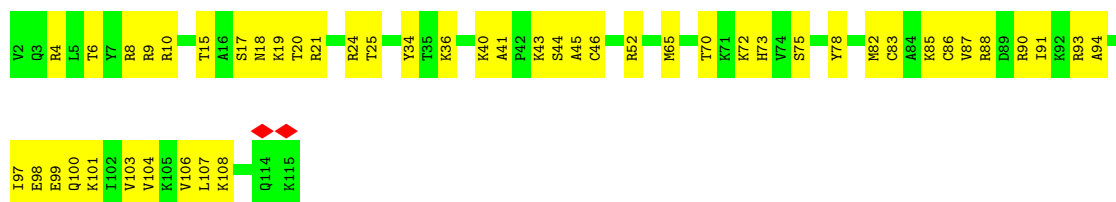
- Molecule 52: 60S ribosomal protein L34

Chain lg: 53% 46%



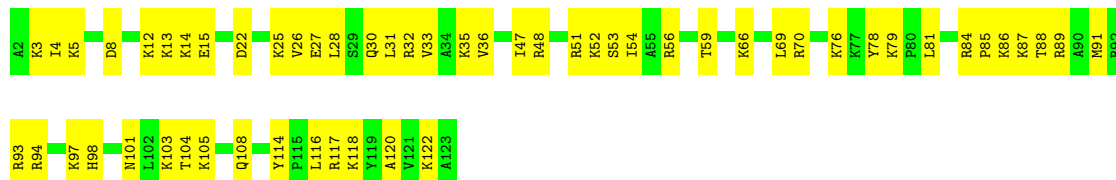
- Molecule 52: 60S ribosomal protein L34

Chain Lg: 58% 42%



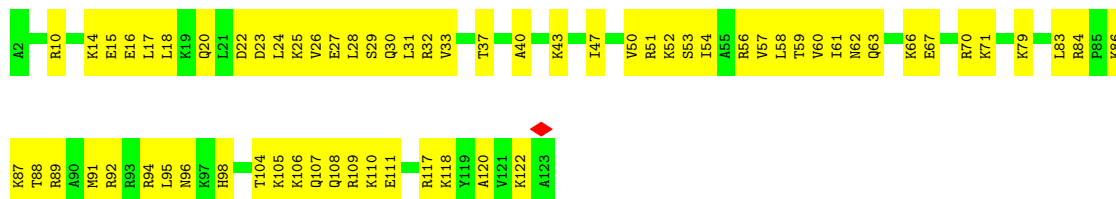
• Molecule 53: 60S ribosomal protein L35

Chain lh:



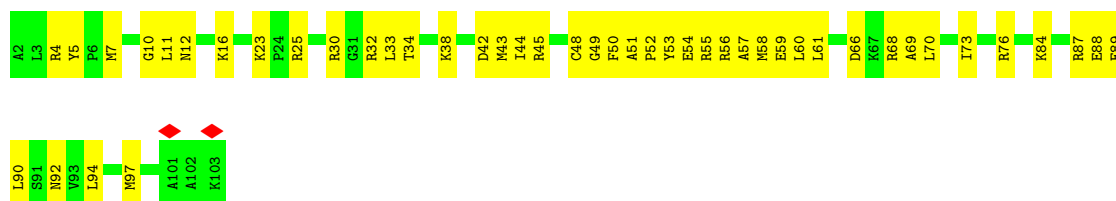
• Molecule 53: 60S ribosomal protein L35

Chain Lh:



• Molecule 54: 60S ribosomal protein L36

Chain li:



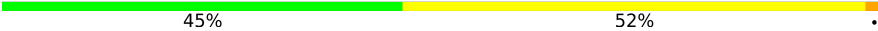
• Molecule 54: 60S ribosomal protein L36

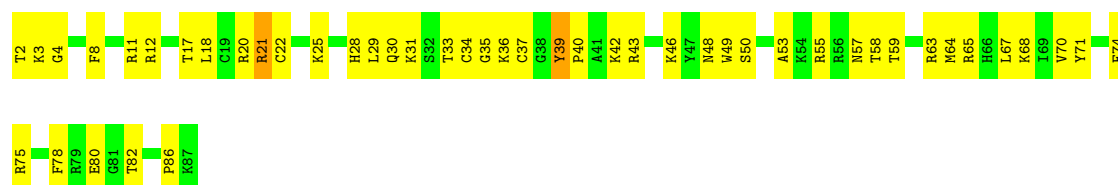
Chain Li:



• Molecule 55: 60S ribosomal protein L37

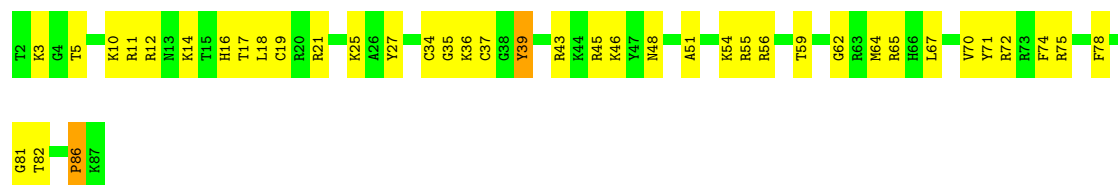


Chain lj: 

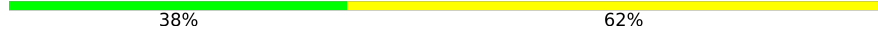


- Molecule 55: 60S ribosomal protein L37

Chain Lj: 

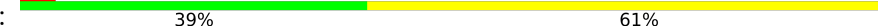


- Molecule 56: 60S ribosomal protein L38

Chain lk: 



- Molecule 56: 60S ribosomal protein L38

Chain Lk: 



- Molecule 57: 60S ribosomal protein L39

Chain ll: 



- Molecule 57: 60S ribosomal protein L39

Chain Ll: 



- Molecule 58: Large ribosomal subunit protein eL40



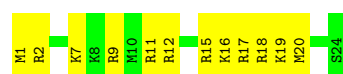
- Molecule 58: Large ribosomal subunit protein eL40



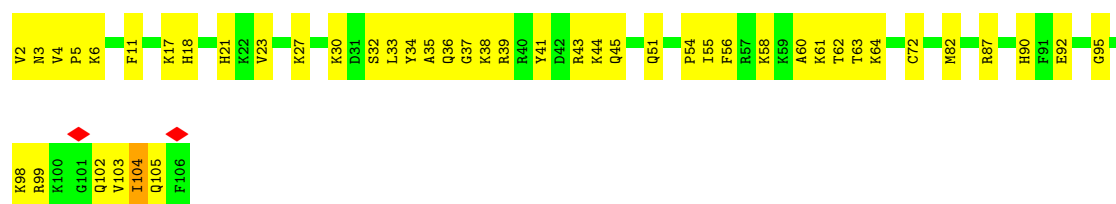
- Molecule 59: 60S ribosomal protein L41



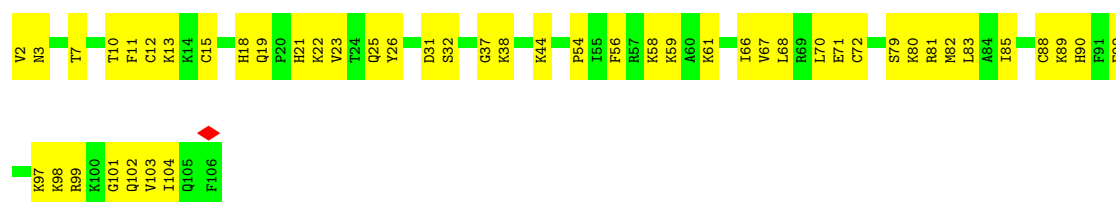
- Molecule 59: 60S ribosomal protein L41



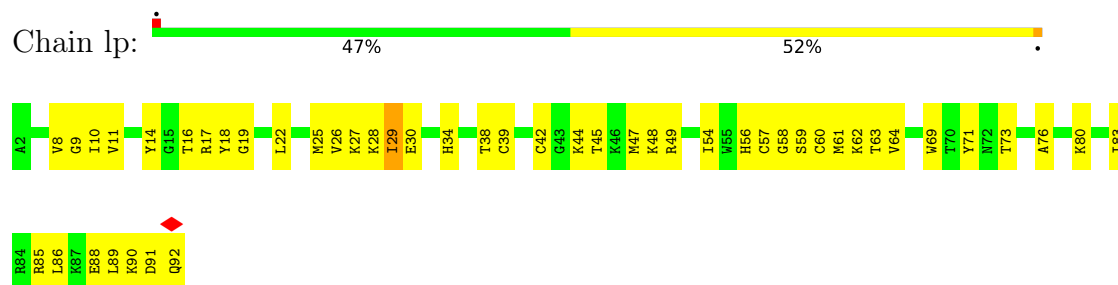
- Molecule 60: 60S ribosomal protein L36a



- Molecule 60: 60S ribosomal protein L36a



- Molecule 61: 60S ribosomal protein L37a



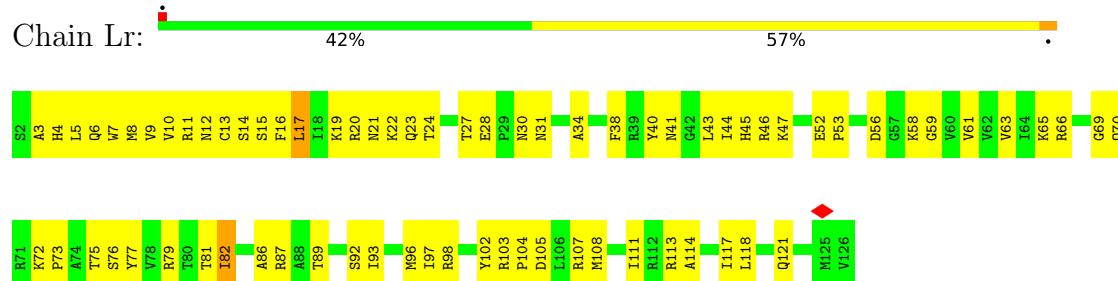
- Molecule 61: 60S ribosomal protein L37a



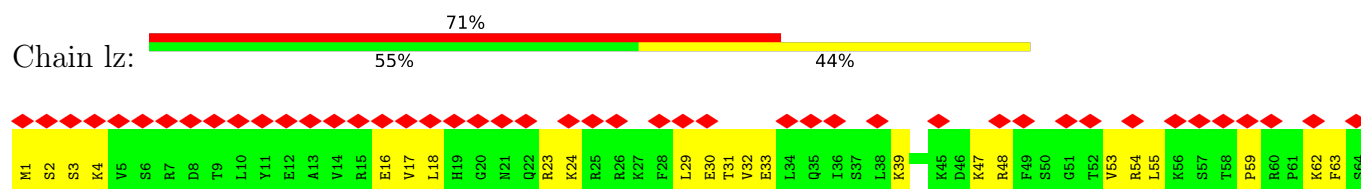
- Molecule 62: 60S ribosomal protein L28

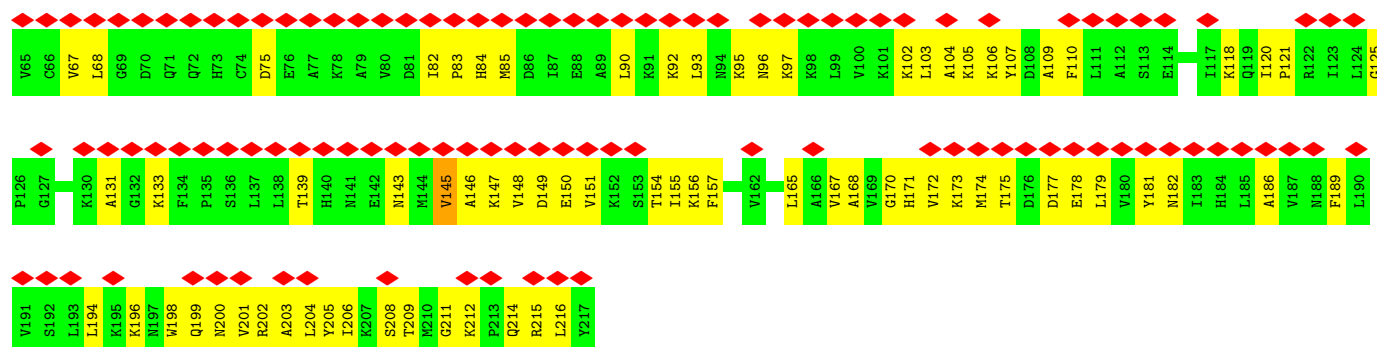


- Molecule 62: 60S ribosomal protein L28

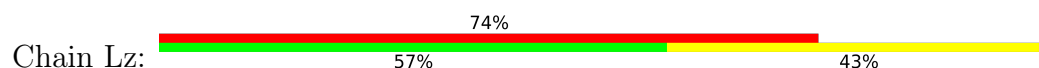


- Molecule 63: 60S ribosomal protein L10a





• Molecule 63: 60S ribosomal protein L10a

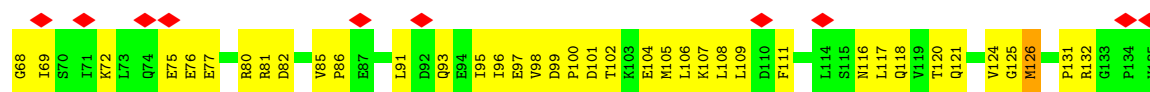


• Molecule 64: 40S ribosomal protein S17

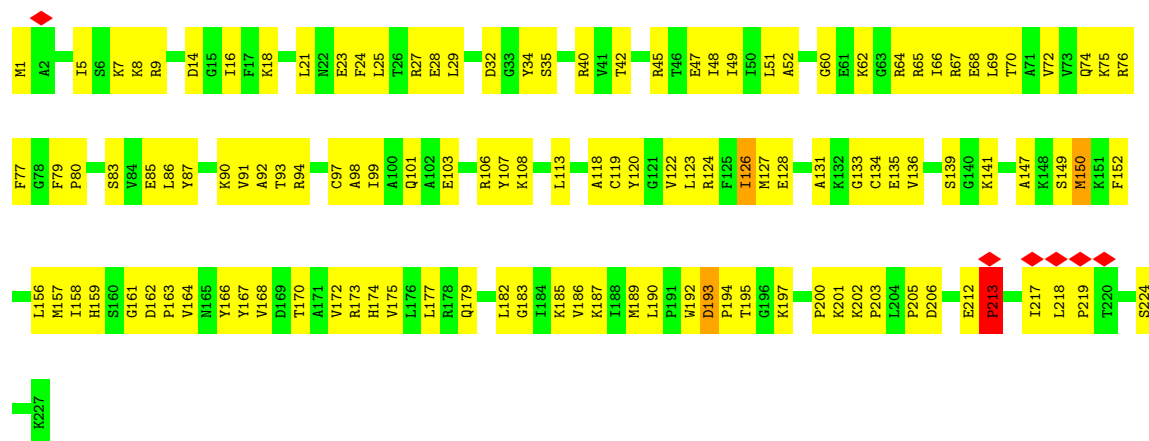


• Molecule 64: 40S ribosomal protein S17

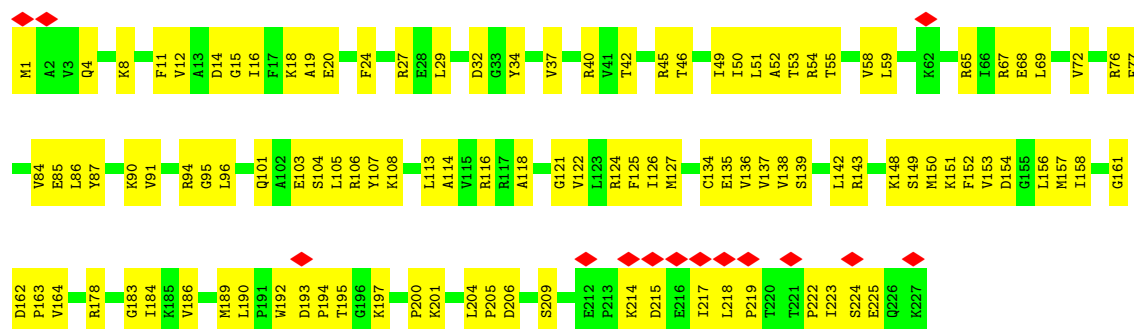




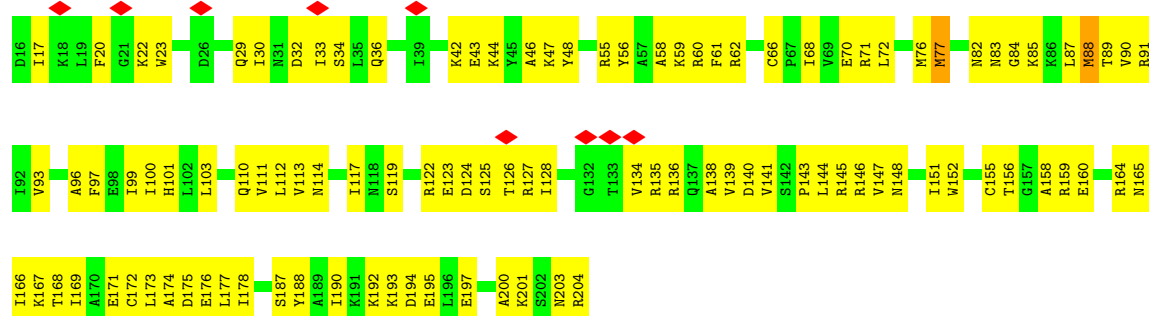
- Molecule 65: Small ribosomal subunit protein uS3



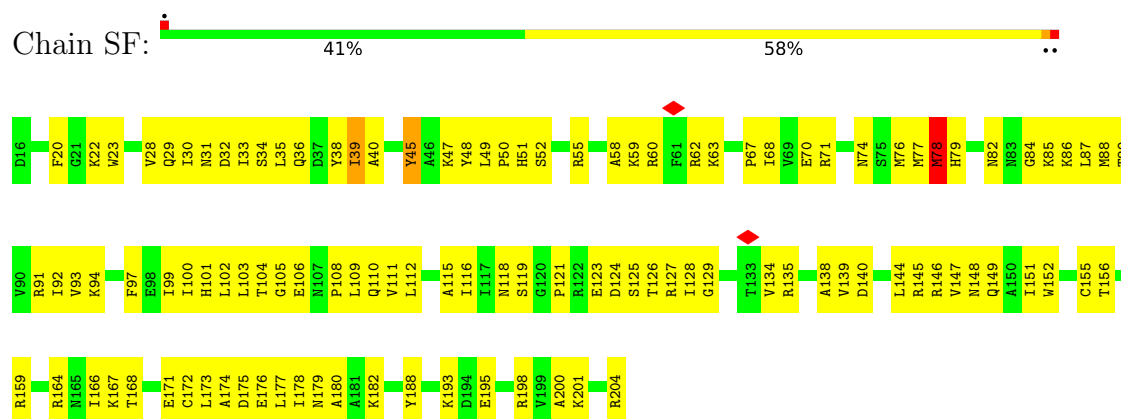
- Molecule 65: Small ribosomal subunit protein uS3



- Molecule 66: 40S ribosomal protein S5



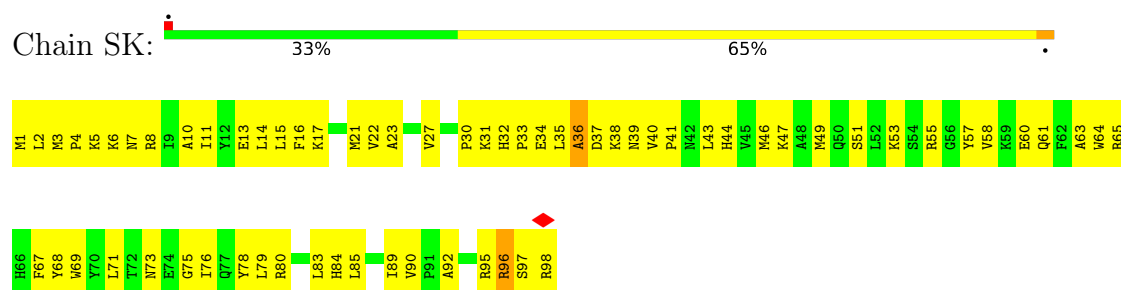
- Molecule 66: 40S ribosomal protein S5



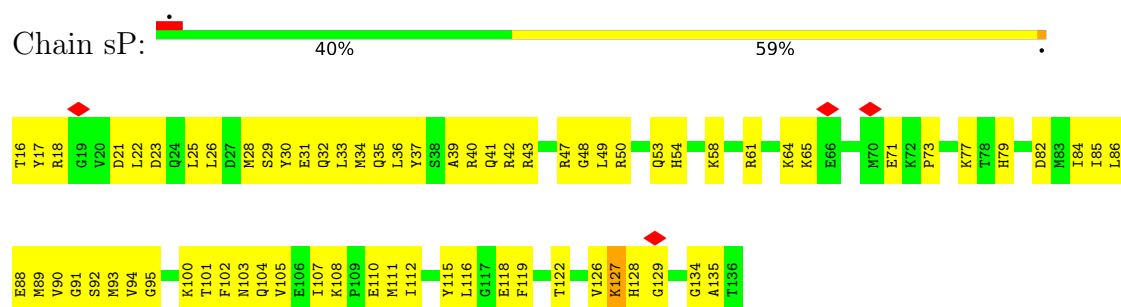
- Molecule 67: 40S ribosomal protein S10



- Molecule 67: 40S ribosomal protein S10

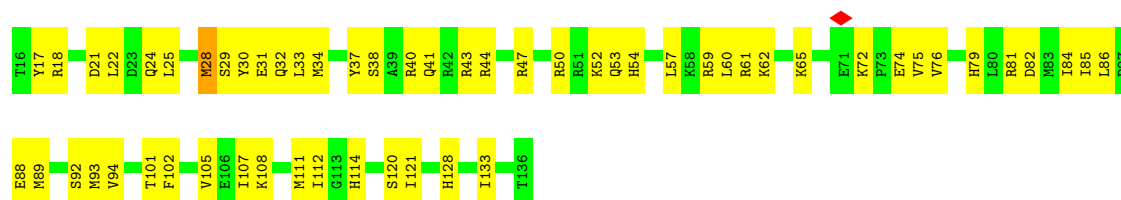


- Molecule 68: Small ribosomal subunit protein uS19



- Molecule 68: Small ribosomal subunit protein uS19

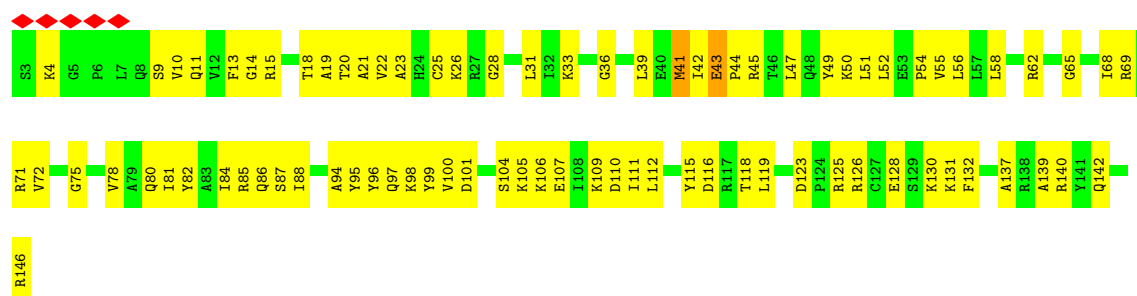




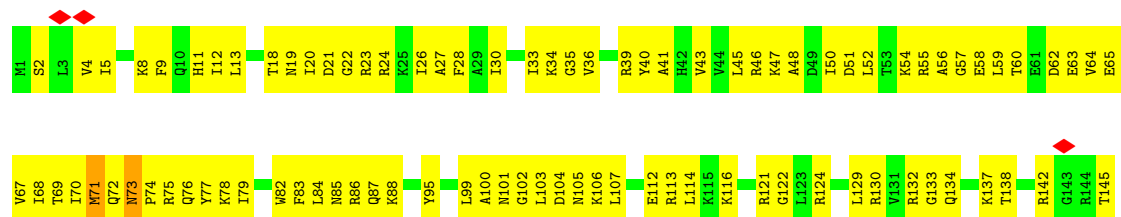
• Molecule 69: Small ribosomal subunit protein uS9



• Molecule 69: Small ribosomal subunit protein uS9

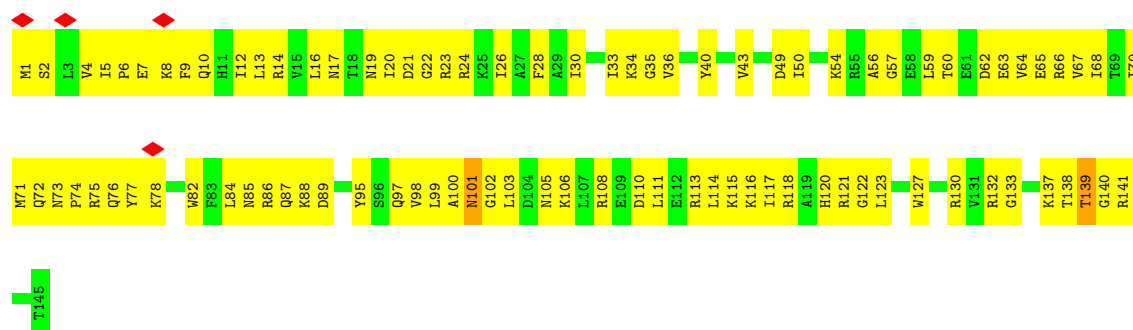


• Molecule 70: 40S ribosomal protein S18

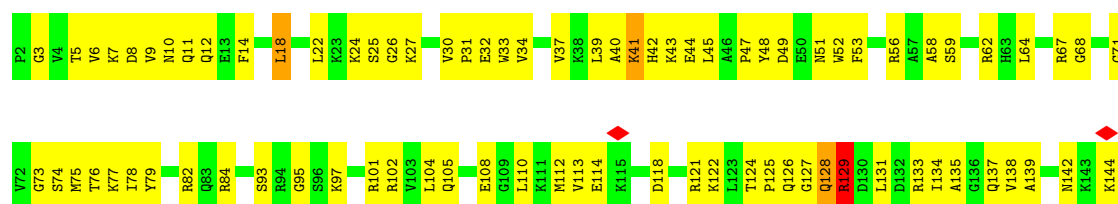


• Molecule 70: 40S ribosomal protein S18

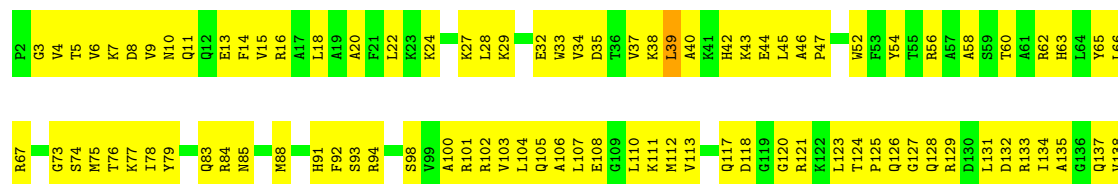




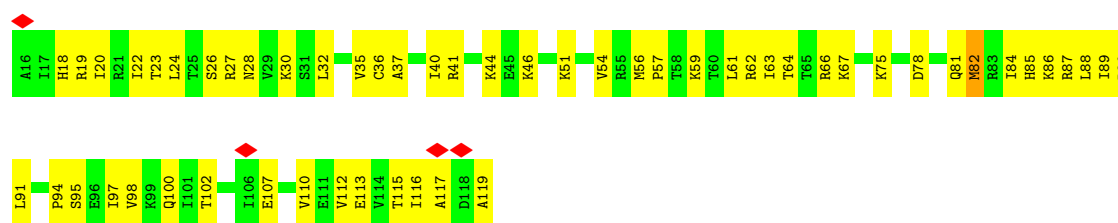
- Molecule 71: 40S ribosomal protein S19



- Molecule 71: 40S ribosomal protein S19



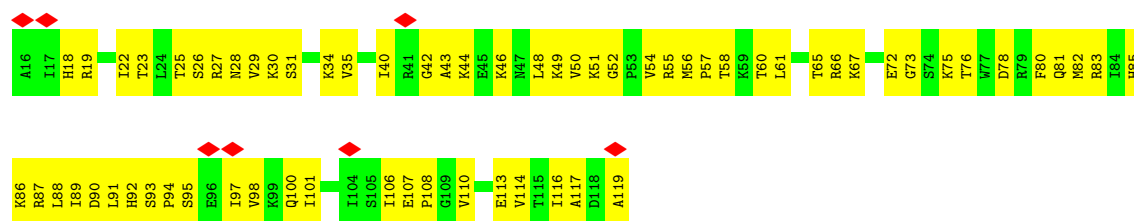
- Molecule 72: 40S ribosomal protein S20



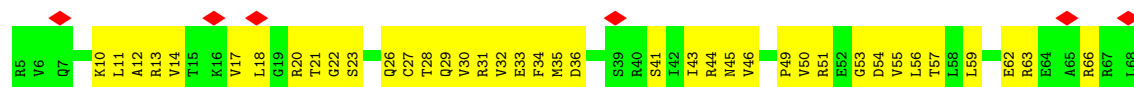
- Molecule 72: 40S ribosomal protein S20



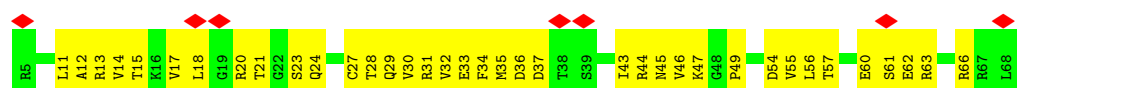




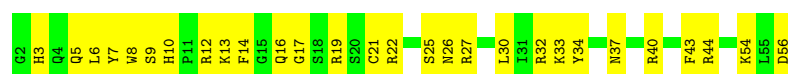
- Molecule 73: 40S ribosomal protein S28



- Molecule 73: 40S ribosomal protein S28



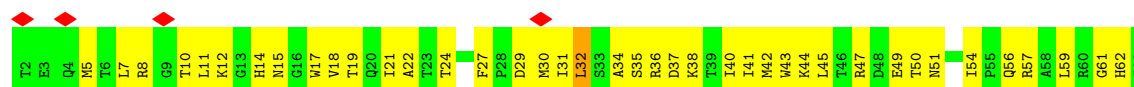
- Molecule 74: 40S ribosomal protein S29

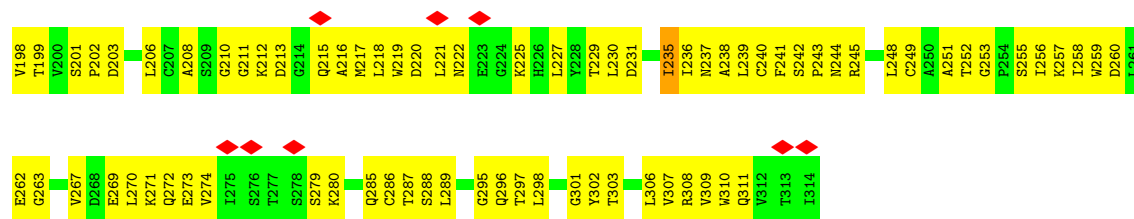


- Molecule 74: 40S ribosomal protein S29

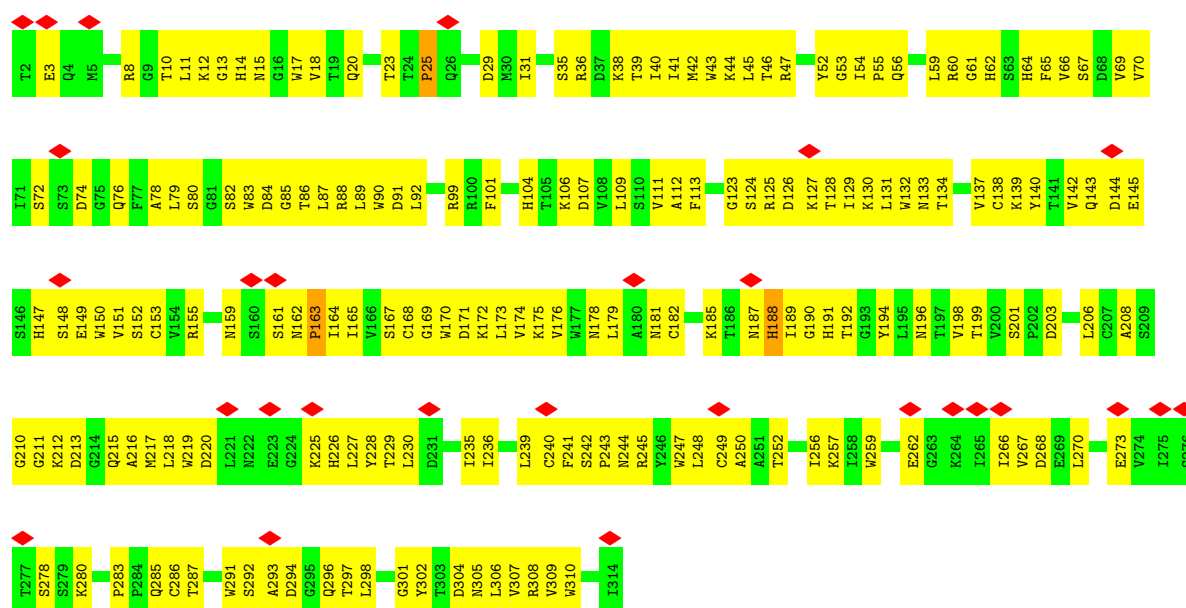


- Molecule 75: Receptor of activated protein C kinase 1

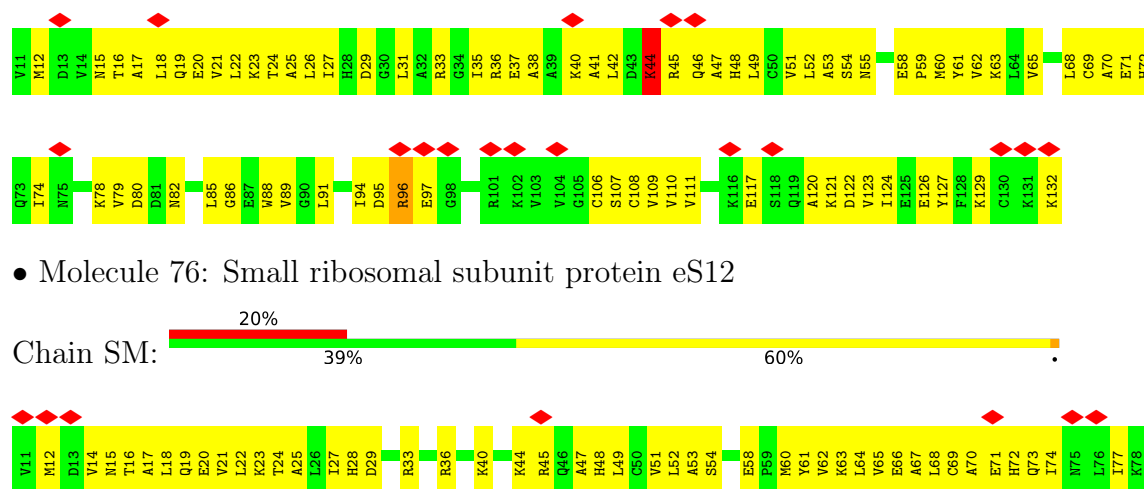




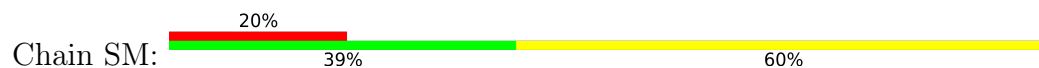
• Molecule 75: Receptor of activated protein C kinase 1

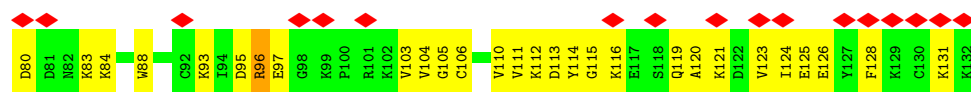


• Molecule 76: Small ribosomal subunit protein eS12

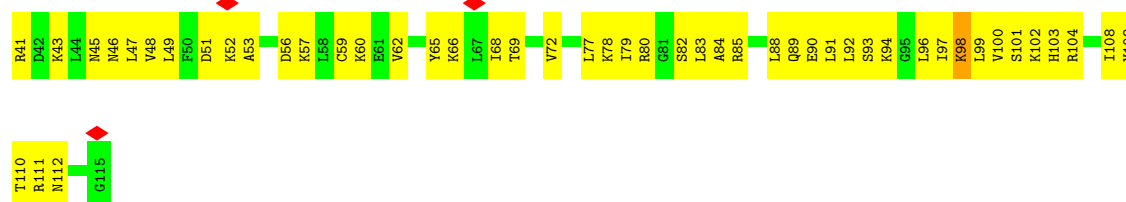
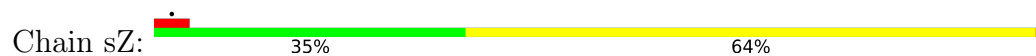


• Molecule 76: Small ribosomal subunit protein eS12

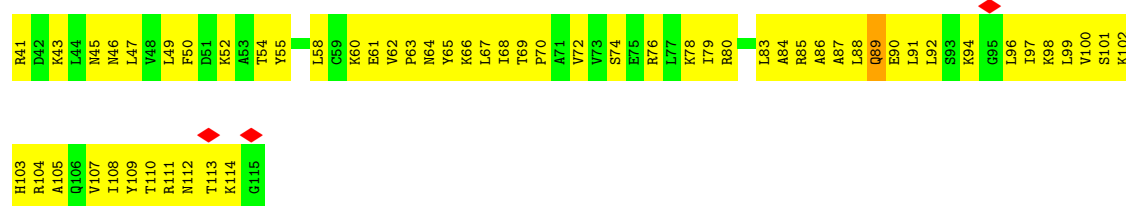




- Molecule 77: Small ribosomal subunit protein eS25



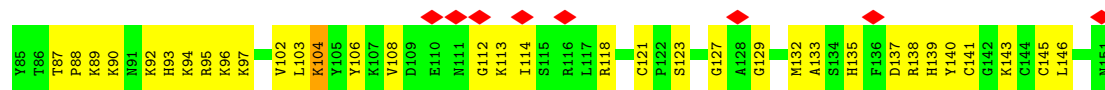
- Molecule 77: Small ribosomal subunit protein eS25



- Molecule 78: Ubiquitin-40S ribosomal protein S27a



- Molecule 78: Ubiquitin-40S ribosomal protein S27a

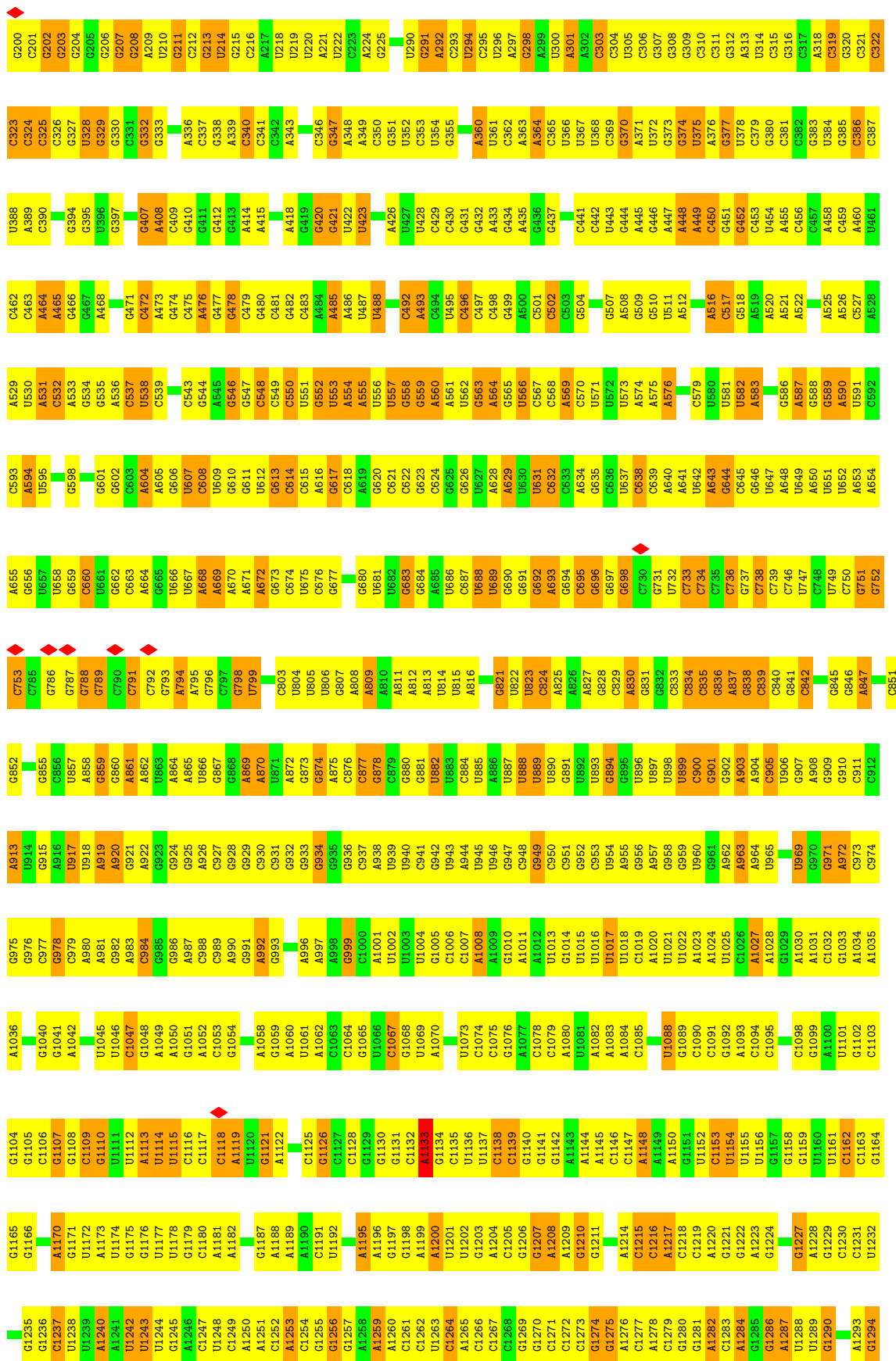


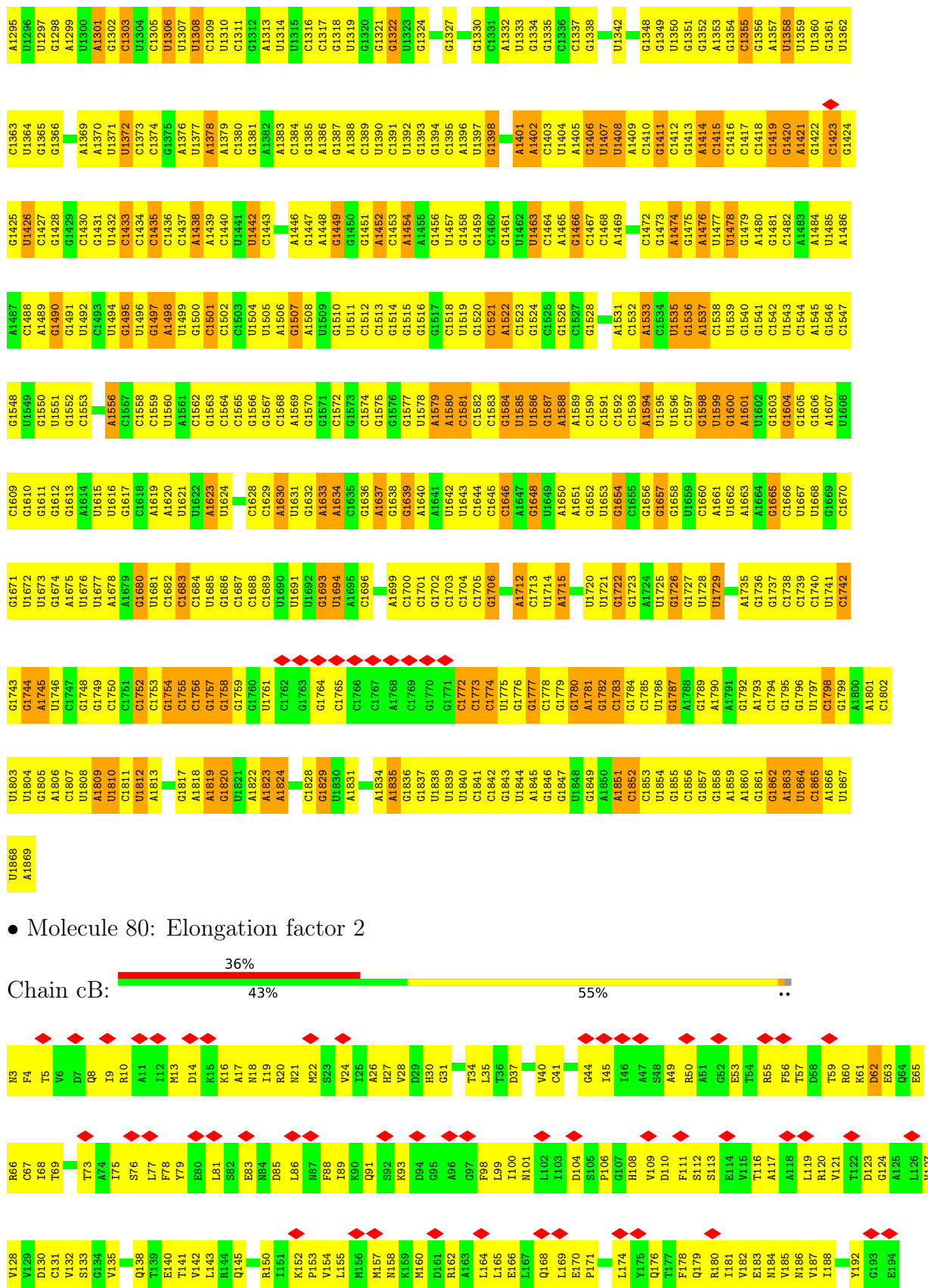
- Molecule 79: 18S rRNA [Homo sapiens]

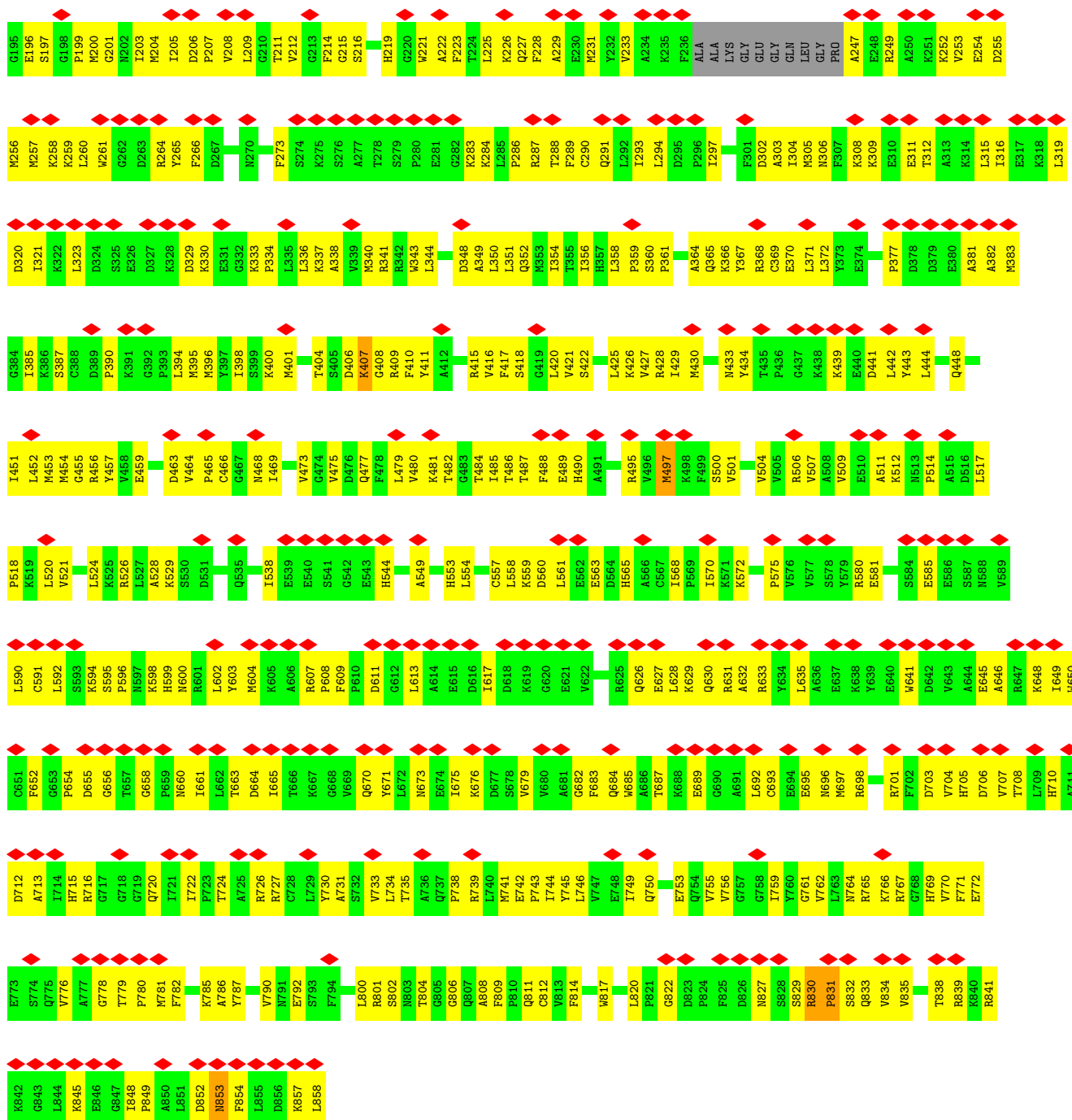


|       |       |       |      |      |      |      |      |      |      |      |      |      |      |      |
|-------|-------|-------|------|------|------|------|------|------|------|------|------|------|------|------|
| U1154 | C1094 | G1026 | A963 | G902 | C840 | C738 | A643 | U580 | A520 | C390 | C325 | G203 | A141 | A68  |
| U1155 | C1095 | A1027 | A964 | A903 | G841 | C739 | G644 | U581 | A521 | C391 | C326 | G204 | C142 |      |
| U1156 | G1096 |       | U965 | A904 | C842 | C746 | C645 | U582 | A522 | A392 | G327 | G205 | G71  | G71  |
| U1157 | G1097 | G1033 |      | C905 | C843 | U747 | G646 | U583 | A523 | A393 | U328 | G206 | U143 |      |
| U1158 | G1098 | A1034 | U969 | U906 | U844 | C748 | U647 | U584 | A524 | G394 | G329 | G207 | U144 | C72  |
| U1159 | G1099 | A1035 | G970 | G907 | U845 | C749 | A648 | C585 | U525 | G395 | G330 | G208 | G145 | C73  |
| U1160 | A1100 | A1036 | G971 | A908 | G846 | C750 | U649 | G586 | A526 | U396 | C331 | A209 | G146 | G74  |
| U1161 | G1101 | G1037 | A972 | G909 | A847 | G751 | U650 | A587 | C527 | G397 | G332 | U210 | A147 | C75  |
| G1162 | C1102 | U1038 | C973 | G910 | U848 | G752 | U651 | U588 | C528 | A403 | G333 | G211 | U148 | U76  |
| C1103 | C1103 | C1039 | C974 | A849 | U849 | C753 | U652 | G589 | A529 | A398 | G334 | G212 | A149 | A77  |
| G1104 | C912  | C850  | U653 | C850 | A653 | C754 | A653 | A590 | U530 | C399 |      | G213 | A150 | C78  |
| G1105 | A913  | C851  | G795 | U591 | A654 | C755 | A654 | A591 | A531 | C402 | G338 | U214 | C151 | A79  |
| G1106 | U914  | G852  | G796 | C592 | A655 | C756 | A655 | C592 | C532 | G403 | A339 | G215 | U152 | G80  |
| G1107 | G915  | C853  | G797 | C593 | G656 | G757 | G656 | C593 | A533 | G404 | C340 | C216 | G153 | U81  |
|       |       | A854  | G798 | U594 | U657 |      |      | A594 | G534 |      | C341 | A217 | U154 | G82  |
|       |       | G855  |      | U595 | U658 |      |      | G535 | C475 | G407 | C342 | U218 | G155 | A83  |
|       |       | C856  |      | U596 | U659 |      |      | A536 | A476 | G408 | A343 | U219 | G156 | A84  |
|       |       | A858  |      | U597 | U660 |      |      | C537 | G477 | G409 | U344 | U220 | U157 | A85  |
|       |       | G859  |      | G600 | U661 |      |      | U538 | G478 |      | U345 | A221 | A158 | C86  |
|       |       | A860  |      | G601 | G682 |      |      | C539 | C479 | A414 | C346 | U222 | U159 | U87  |
|       |       | A861  |      | G602 |      |      |      | U540 | C480 | A415 | G347 | U223 | U160 | C88  |
|       |       | A862  |      | C603 | U666 |      |      | U541 | C481 | A416 | A348 | A224 | U161 | C89  |
|       |       | U863  |      | A604 | U667 |      |      | U542 | C482 | C417 | A349 | G225 | C162 | G90  |
|       |       | A864  |      | A605 | A668 |      |      | C543 | C483 | A418 | C350 |      | U163 | A91  |
|       |       |       |      | G506 | A669 |      |      | G544 | A484 | G419 | G351 | G289 | A164 | A92  |
|       |       |       |      | U607 | A670 |      |      | A545 | A485 | G420 | U352 | U290 | G165 | U93  |
|       |       |       |      | C608 | A671 |      |      | G546 | A486 | G421 | U353 | G291 | A166 | G94  |
|       |       |       |      | U609 | A672 |      |      | C548 | U487 |      | U354 | G292 | G167 | G95  |
|       |       |       |      | G610 | C673 |      |      | C549 | U488 | A426 | G355 | U293 | C168 |      |
|       |       |       |      | G611 | C674 |      |      | C550 | U489 | A427 | U356 | U294 | U169 | U97  |
|       |       |       |      | U612 | U805 |      |      | C551 | C490 | U428 | C356 | C295 | A170 | C98  |
|       |       |       |      | G613 | C676 |      |      | U551 | C491 | C429 |      | U296 | A171 | A99  |
|       |       |       |      | C614 | G677 |      |      | G552 | C492 | C430 | U359 | A297 | U172 |      |
|       |       |       |      | G615 | U808 |      |      | U553 | A493 | G431 | A360 | G298 | A173 | A103 |
|       |       |       |      | A616 | A679 |      |      | A554 | C494 | G432 | U361 | A299 | C174 | C106 |
|       |       |       |      | G617 | G680 |      |      | U555 | U495 | A433 | C362 | U300 | U176 | A107 |
|       |       |       |      | C618 | U681 |      |      | U556 | C496 | G434 | A363 | A301 | G177 | G108 |
|       |       |       |      | A619 | U682 |      |      | U557 | C497 |      | A364 | A302 | G178 | U109 |
|       |       |       |      | G620 | G683 |      |      | G558 | C498 | G437 |      | G303 | C179 | U110 |
|       |       |       |      | C621 | G684 |      |      | G559 | C499 |      | U368 | C304 | G180 |      |
|       |       |       |      | G622 |      |      |      | A560 | A500 | G440 | C369 | U305 | A181 | G113 |
|       |       |       |      | G623 |      |      |      | A561 | C501 | C441 | G370 | C306 | G182 | G114 |
|       |       |       |      | G624 |      |      |      | U562 | C502 | U442 | U372 | G307 | G183 | U115 |
|       |       |       |      | G625 |      |      |      | G563 | C503 | U443 | G373 | G308 | U116 | U116 |
|       |       |       |      | G626 |      |      |      | A564 | G504 | G444 | G374 | G309 | G185 | C117 |
|       |       |       |      | U627 |      |      |      | G565 | G505 | A445 | U375 | C310 | G186 | C118 |
|       |       |       |      | A628 |      |      |      | U566 | G506 | G446 | A376 | G311 | G187 | G122 |
|       |       |       |      | A629 |      |      |      | C567 | G507 | A447 | G377 | G312 | C188 | G123 |
|       |       |       |      | U630 |      |      |      | C568 | A508 | U448 | U378 | G313 | U189 | U124 |
|       |       |       |      | U631 |      |      |      | A569 | G509 | A449 | C379 | U314 | G190 | U124 |
|       |       |       |      |      |      |      |      | C570 | G510 | C450 | G380 | C315 | A191 | C125 |
|       |       |       |      | A634 |      |      |      | U571 | U511 | G451 | C381 | G316 | C127 | G126 |
|       |       |       |      | G635 |      |      |      | U572 | A512 | G452 | C382 | C317 |      | C127 |
|       |       |       |      | C636 |      |      |      | U573 | G513 | C453 | G383 | A318 | C196 | G130 |
|       |       |       |      | U637 |      |      |      | A574 | U514 | U454 | U384 | G319 | U197 | G130 |
|       |       |       |      | C638 |      |      |      | A575 | G515 | A455 | G385 | C320 | U198 | C131 |
|       |       |       |      | G639 |      |      |      | A576 | A516 | C456 | C386 | C321 | U199 | G131 |
|       |       |       |      | A640 |      |      |      | U577 | C517 | C457 | C387 | C322 | G200 | C138 |
|       |       |       |      | C641 |      |      |      | C578 | G518 | A458 | U388 | C323 | C201 | C139 |
|       |       |       |      | U642 |      |      |      | C579 | A519 | C459 | A389 | C324 | G202 | C140 |

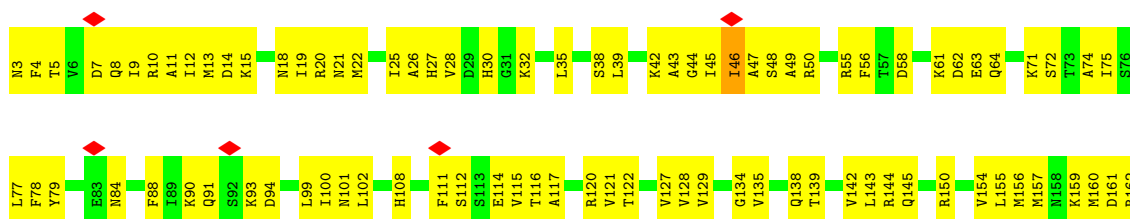




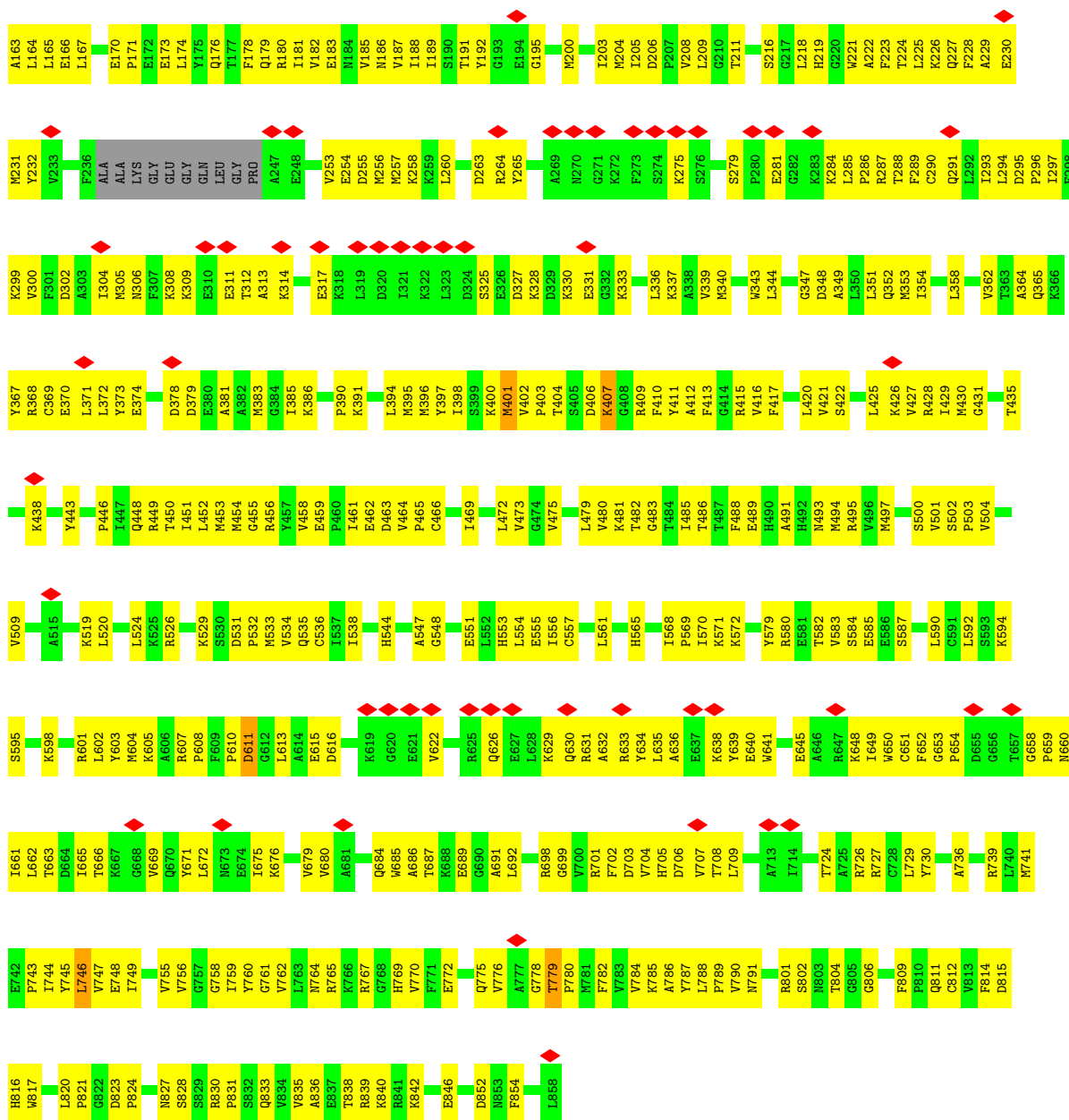




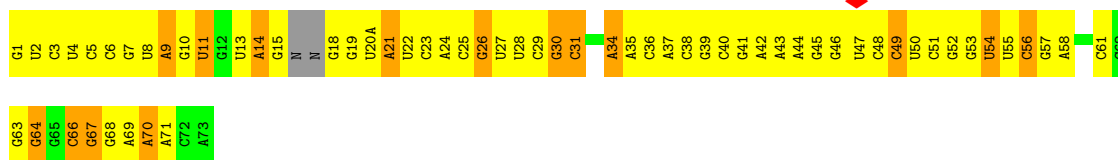
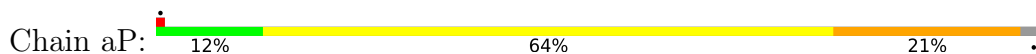
• Molecule 80: Elongation factor 2



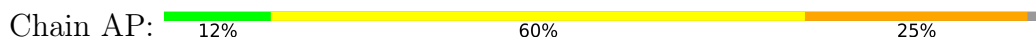


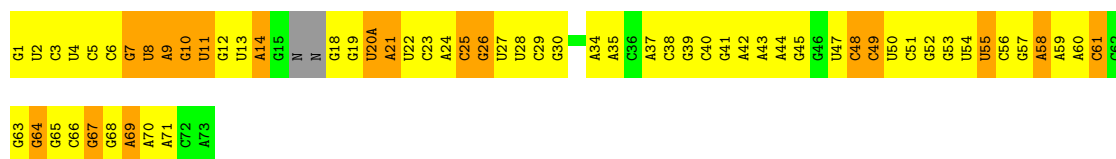


• Molecule 81: A/P site tRNA [Homo sapiens]

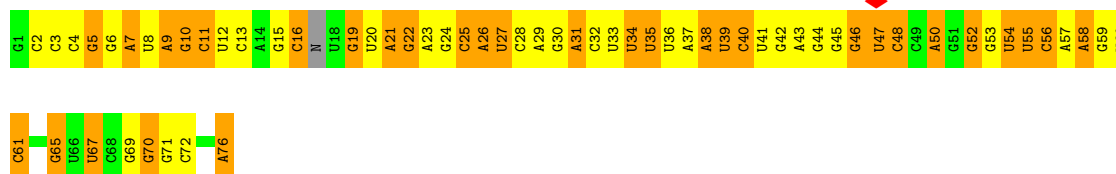
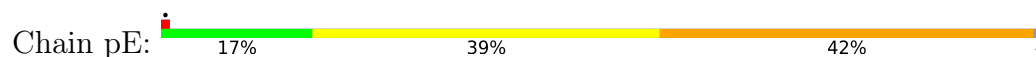


• Molecule 81: A/P site tRNA [Homo sapiens]

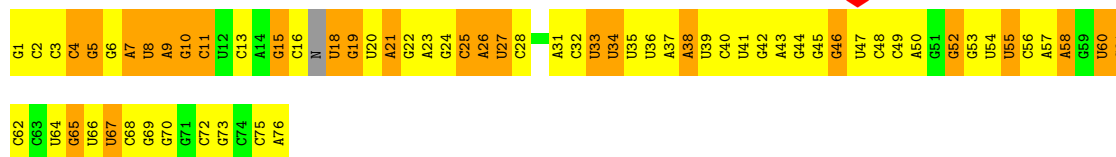
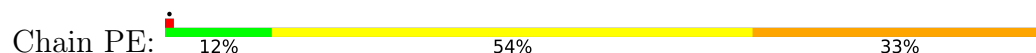




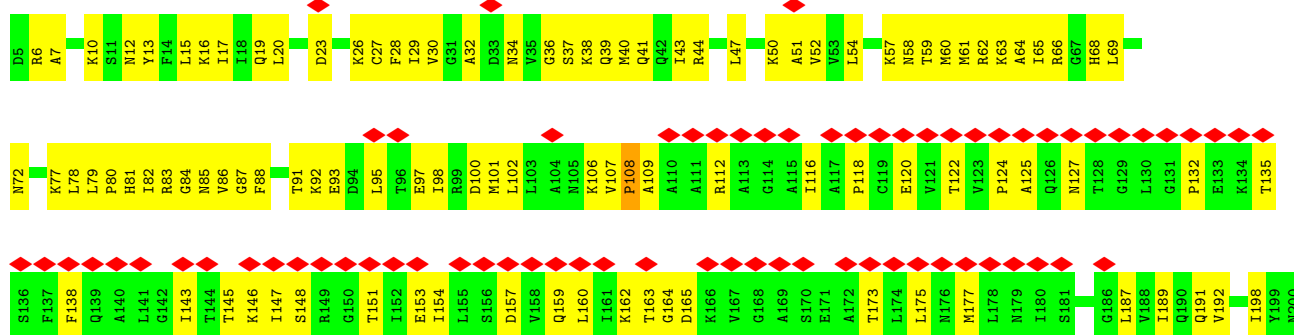
- Molecule 82: P/E site tRNA [Homo sapiens]



- Molecule 82: P/E site tRNA [Homo sapiens]

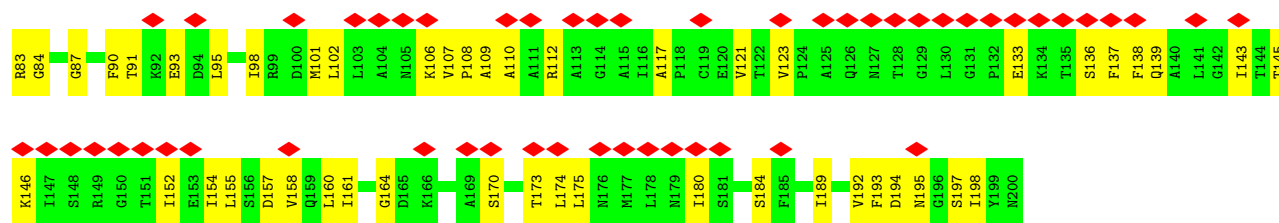


- Molecule 83: 60S acidic ribosomal protein P0

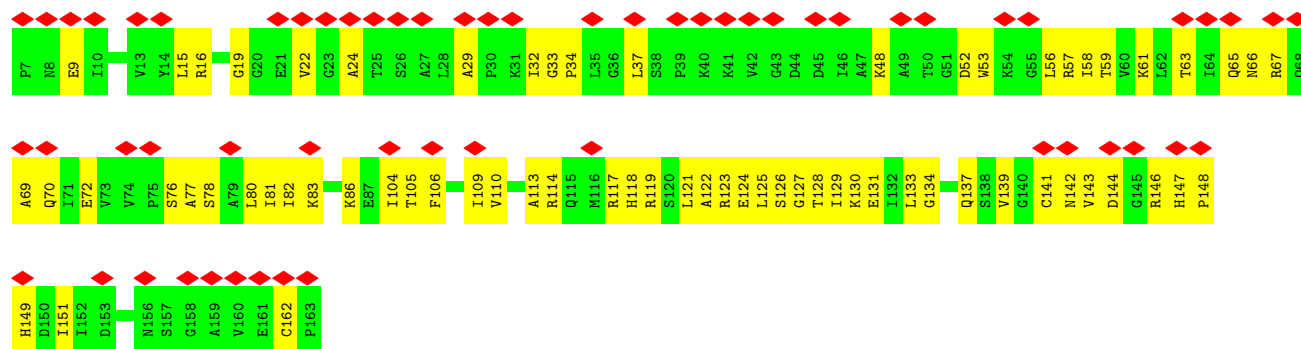
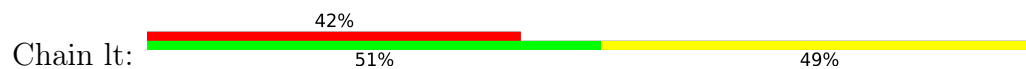


- Molecule 83: 60S acidic ribosomal protein P0

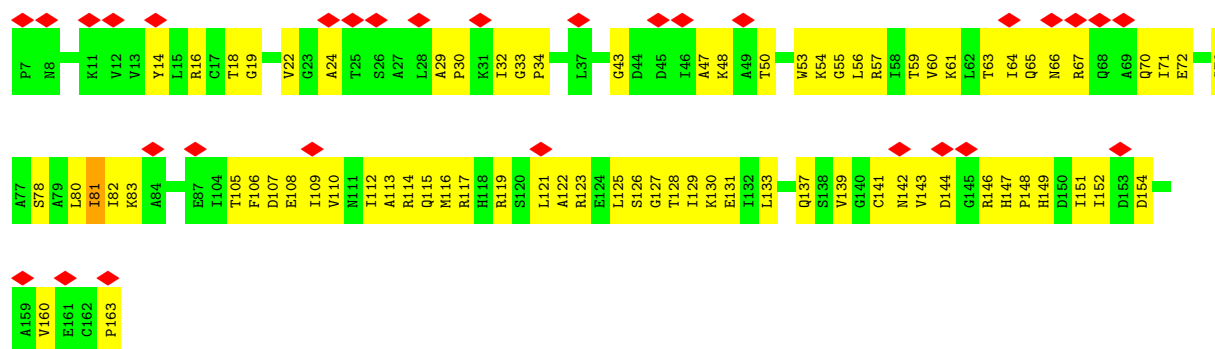




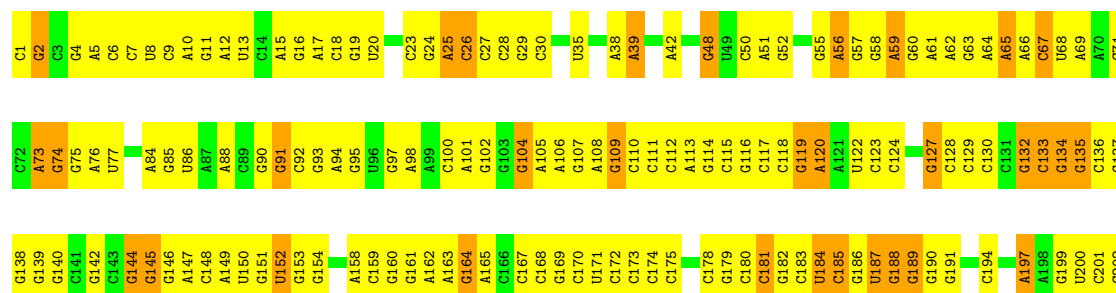
• Molecule 84: 60S ribosomal protein L12 [Homo sapiens]



• Molecule 84: 60S ribosomal protein L12 [Homo sapiens]



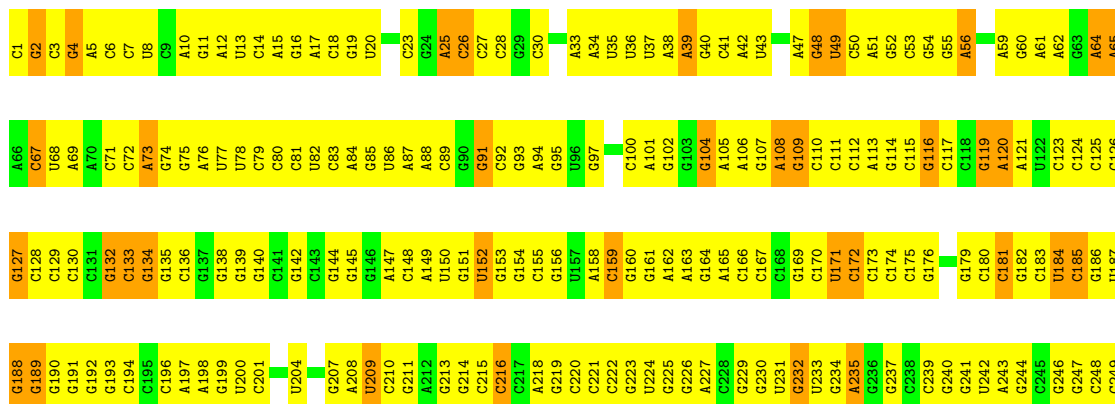
• Molecule 85: 28S rRNA [Homo sapiens]



|       |       |       |       |       |       |       |       |       |      |      |      |      |      |      |      |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|------|------|------|------|------|------|------|
| A1553 | A1554 | C1478 | U1410 | C1344 | A1279 | U1201 | G1075 | U945  | C736 | G669 | C485 | A419 | G341 | U272 | A208 |
| G1479 | G1480 | G1479 | C1411 | A1345 | C1280 | C1202 | C1076 | C946  | C737 | G670 | C486 | A420 | G342 | U273 | A428 |
| C1481 | C1412 | C1480 | C1413 | G1346 | G1281 | C1203 | A1077 | C947  | C738 | G671 | G487 | G423 | C343 | C274 | U209 |
| A1563 | G1482 | G1482 | G1414 | G1347 | G1282 | C1204 | C1078 | C948  | C739 | C672 | G488 | U424 | A344 | C275 | C210 |
| A1564 | A1563 | A1563 | G1415 | U1348 | G1283 | G1205 | C1079 | G949  | G740 | G673 | C489 | U425 | C345 | G276 | G211 |
| A1565 | G1484 | G1484 | G1416 | G1349 | G1284 | C1206 | C1080 | G950  | G741 | G674 | C490 | U426 | G346 | G277 | G212 |
| C1485 | G1485 | G1485 | G1417 | C1350 | U1285 | C1207 | C1081 | G951  | G742 | C675 | C491 | A427 | A347 | G278 | G213 |
| C1486 | C1486 | C1486 | C1418 | G1351 | C1286 | G1208 | C1082 | G952  | G743 | C676 | U492 | G428 | G348 | A427 | G216 |
| G1487 | A1420 | G1487 | G1419 | C1352 | U1209 | U1209 | U1083 | C953  | U750 | G677 | A349 | G431 | A349 | G280 | C217 |
| G1490 | G1426 | G1490 | G1426 | U1356 | G1211 | G1211 | C1084 | A956  | G751 | C678 | U494 | G432 | C350 | U281 | A218 |
| A1491 | A1427 | A1491 | G1430 | C1357 | G1212 | G1212 | C1085 | G957  | G752 | C679 | C351 | U433 | C351 | C282 | G219 |
| G1492 | G1437 | G1492 | U1438 | C1358 | G1213 | G1213 | C1086 | G958  | G753 | G680 | G352 | A434 | G353 | G283 | G220 |
| G1493 | U1439 | G1493 | G1440 | G1359 | C1215 | C1215 | C1087 | G959  | U754 | G681 | U495 | A435 | U286 | U287 | C221 |
| A1497 | C1430 | A1497 | C1431 | G1360 | C1216 | C1216 | G1089 | A960  | G758 | C685 | U496 | A436 | U288 | G288 | G222 |
| G1498 | G1432 | G1498 | G1432 | C1361 | G1217 | G1217 | C1090 | G961  | G759 | G686 | U497 | U437 | U289 | G289 | G223 |
| C1501 | G1437 | C1501 | C1437 | G1362 | G1218 | G1218 | C1091 | G962  | G760 | U688 | C501 | G438 | U290 | U290 | G224 |
| G1502 | U1440 | G1502 | U1440 | C1363 | G1219 | G1219 | C1092 | G963  | C903 | U689 | C502 | G439 | A360 | U291 | G225 |
| A1503 | C1438 | A1503 | C1438 | C1364 | G1220 | G1220 | C1093 | G964  | C904 | C690 | G503 | U440 | A361 | G226 | G226 |
| C1504 | U1441 | C1504 | U1441 | U1365 | G1221 | G1221 | C1094 | G965  | C905 | C691 | G504 | U441 | A362 | A227 | A227 |
| G1505 | C1442 | G1505 | C1442 | C1366 | G1222 | G1222 | C1095 | A966  | C906 | C692 | G505 | G442 | A296 | G229 | G229 |
| G1506 | U1443 | G1506 | U1443 | G1367 | G1223 | G1223 | C1096 | G967  | C907 | U687 | C506 | G443 | U297 | G230 | G230 |
| C1507 | G1444 | C1507 | G1444 | C1368 | G1234 | G1234 | C1097 | C968  | G908 | C693 | G507 | G444 | G298 | U297 | U297 |
| A1508 | C1445 | A1508 | C1445 | G1369 | G1235 | G1235 | C1098 | C969  | G909 | C694 | G508 | U445 | C369 | G298 | U298 |
| U1511 | G1446 | U1511 | G1446 | A1367 | A1238 | A1238 | C1099 | G970  | G910 | C695 | A509 | U446 | A371 | A300 | U233 |
| C1512 | C1447 | C1512 | C1447 | G1370 | G1239 | G1239 | C1100 | G971  | G911 | C696 | G510 | G447 | A372 | G301 | U234 |
| U1513 | G1448 | U1513 | G1448 | C1371 | G1240 | G1240 | C1101 | C972  | G912 | U700 | G511 | G448 | G373 | A302 | A235 |
| U1514 | C1449 | U1514 | C1449 | G1372 | G1241 | G1241 | C1102 | C973  | G913 | G701 | G512 | G449 | C303 | G303 | C239 |
| A1515 | G1450 | A1515 | G1450 | A1373 | G1242 | G1242 | C1103 | C974  | G914 | U702 | G513 | G450 | C304 | C304 | G240 |
| G1516 | C1451 | G1516 | C1451 | G1374 | G1243 | G1243 | C1104 | C975  | G915 | G703 | G514 | C451 | A305 | A305 | G241 |
| A1517 | U1452 | A1517 | U1452 | G1377 | G1244 | G1244 | C1105 | C976  | G916 | G704 | G515 | C452 | A306 | A306 | U242 |
| C1518 | G1455 | C1518 | G1455 | C1378 | G1253 | G1253 | C1106 | C977  | G917 | G705 | G516 | G453 | A307 | G308 | G246 |
| A1519 | C1456 | A1519 | C1456 | G1381 | G1254 | G1254 | C1107 | C978  | G918 | G706 | G517 | U454 | A308 | G309 | G247 |
| C1520 | G1457 | C1520 | G1457 | U1382 | A1255 | A1255 | C1108 | C979  | G919 | U707 | G518 | G455 | A385 | A385 | C248 |
| G1521 | C1458 | G1521 | C1458 | G1383 | G1256 | G1256 | C1109 | C980  | G920 | G708 | G519 | G456 | G387 | C249 | C249 |
| A1523 | G1459 | A1523 | G1459 | G1384 | G1257 | G1257 | C1110 | C981  | G921 | G709 | G642 | G457 | A386 | G310 | G250 |
| A1524 | C1460 | A1524 | C1460 | C1385 | G1258 | G1258 | C1111 | C982  | G922 | G710 | G643 | G458 | A387 | G311 | G251 |
| A1525 | C1461 | A1525 | C1461 | G1386 | G1259 | G1259 | C1112 | C983  | G923 | G711 | G644 | C459 | A388 | C252 | C252 |
| U1531 | G1462 | U1531 | G1462 | A1391 | G1260 | G1260 | C1113 | C984  | G924 | G712 | G645 | U460 | A389 | G312 | G253 |
| G1532 | C1463 | G1532 | C1463 | C1392 | G1261 | G1261 | C1114 | C985  | G925 | G713 | G646 | G461 | A390 | A317 | G254 |
| A1533 | G1464 | A1533 | G1464 | G1393 | G1262 | G1262 | C1115 | C986  | G926 | G714 | G647 | G462 | A391 | A318 | C255 |
| C1534 | G1465 | C1534 | G1465 | U1394 | G1263 | G1263 | C1116 | C987  | G927 | G715 | G648 | G463 | A392 | G323 | G256 |
| G1535 | C1466 | G1535 | C1466 | U1395 | G1264 | G1264 | C1117 | C988  | G928 | G716 | G649 | G464 | A393 | A324 | G257 |
| U1536 | G1467 | U1536 | G1467 | G1396 | G1265 | G1265 | C1118 | C989  | G929 | G717 | G650 | G465 | A394 | U325 | G258 |
| A1537 | C1468 | A1537 | C1468 | A1397 | G1266 | G1266 | C1119 | C990  | G930 | G718 | G651 | G466 | A395 | G326 | G259 |
| C1541 | G1469 | C1541 | G1469 | C1401 | G1267 | G1267 | C1120 | C991  | G931 | G719 | G652 | U467 | A396 | U327 | C260 |
| A1547 | C1470 | A1547 | C1470 | C1402 | G1268 | G1268 | C1121 | C992  | G932 | G720 | G653 | U468 | A397 | A328 | G261 |
| G1548 | G1471 | G1548 | G1471 | G1333 | G1269 | G1269 | C1122 | C993  | G933 | G721 | G654 | U469 | A398 | G329 | G262 |
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| A1621 | G1473 | A1621 | G1473 | G1335 | G1271 | G1271 | C1124 | C995  | G935 | G723 | G656 | G401 | A401 | C331 | C264 |
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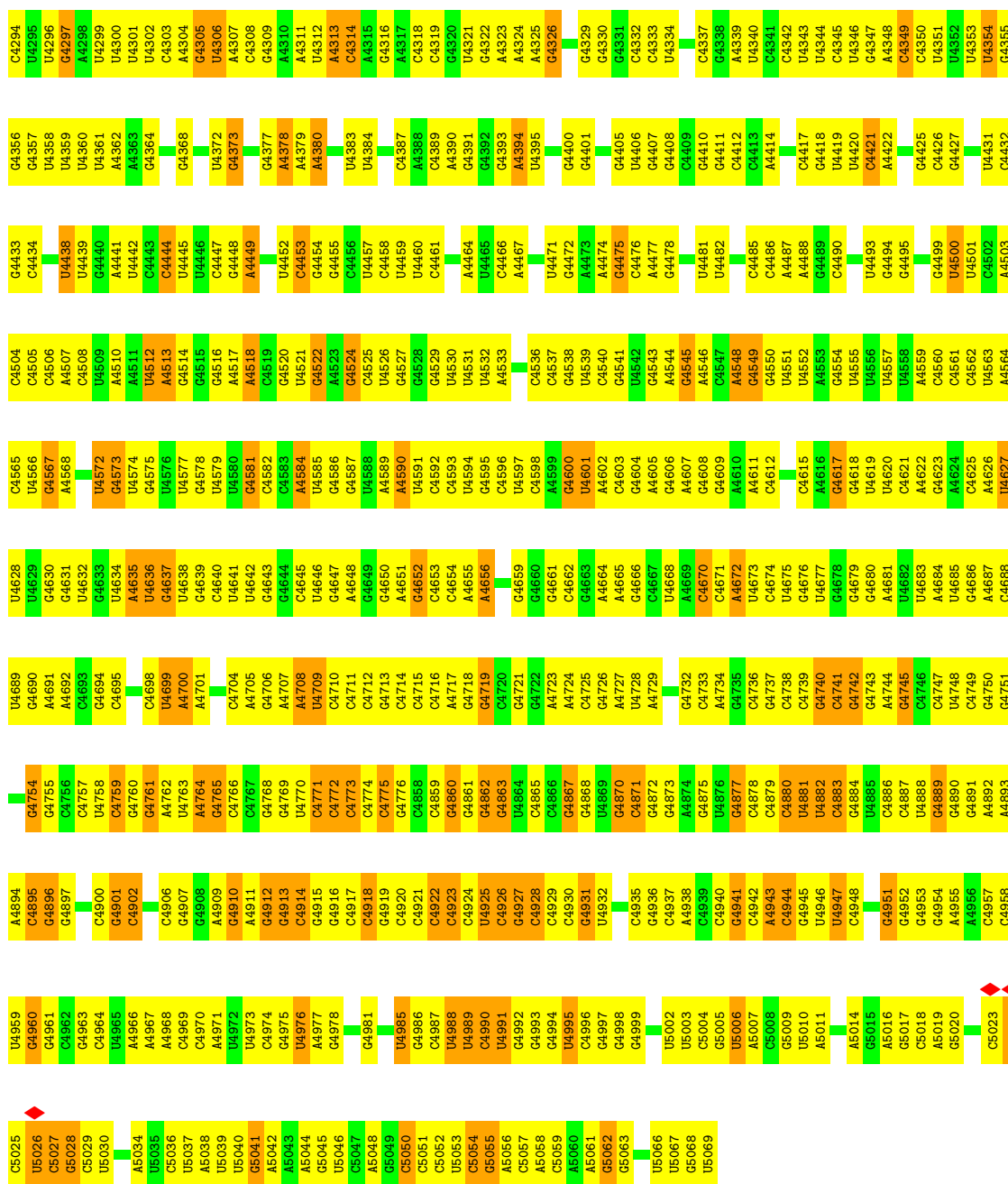


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| G1612 | G1613 | G1452 | G1388 | G1324 | G1261 | G1184 | G994  | C930 | G724 | C663 | G479 | G342 | G342 | G279 |
| A1614 | A1615 | G1453 | G1389 | C1325 | G1262 | G1185 | C995  | C931 | G725 | C664 | C480 | G343 | G343 | G280 |
| G1616 | G1617 | G1454 | G1390 | A1326 | G1263 | G1186 | C996  | C932 | G726 | C665 | C481 | G344 | G344 | G281 |
| A1618 | A1619 | G1455 | A1391 | C1327 | G1264 | G1187 | G997  | C933 | G727 | C666 | C482 | G345 | G345 | G282 |
| G1620 | G1621 | G1456 | G1392 | G1328 | G1265 | G1188 | G1048 | C934 | G728 | C667 | G483 | G346 | G346 | G283 |
| A1622 | A1623 | G1457 | G1393 | G1329 | G1266 | G1189 | C1049 | C935 | G729 | C668 | C484 | G347 | G347 | G284 |
| G1624 | G1625 | G1458 | G1394 | C1332 | G1267 | G1190 | C1050 | C936 | G730 | C669 | C485 | G348 | G348 | G285 |
| A1626 | A1627 | G1459 | G1395 | A1333 | G1268 | G1191 | C1051 | C937 | G731 | C670 | C486 | G349 | G349 | G286 |
| G1628 | G1629 | G1460 | G1396 | G1334 | G1269 | G1192 | G1052 | C938 | G732 | C671 | C487 | G350 | G350 | G287 |
| A1630 | A1631 | G1461 | G1397 | G1335 | G1270 | G1193 | G1053 | C939 | G733 | C672 | C488 | G351 | G351 | G288 |
| G1632 | G1633 | G1462 | A1398 | G1336 | G1271 | G1194 | G1054 | C940 | G734 | C673 | C489 | G352 | G352 | G289 |
| A1634 | A1635 | G1463 | G1399 | G1337 | G1272 | G1195 | G1055 | C941 | G735 | C674 | C490 | G353 | G353 | G290 |
| G1636 | G1637 | G1464 | G1401 | A1338 | G1273 | G1196 | G1056 | C942 | G736 | C675 | C491 | G354 | G354 | G291 |
| A1638 | A1639 | G1465 | G1402 | G1339 | G1274 | G1197 | G1057 | C943 | G737 | C676 | C492 | G355 | G355 | G292 |
| G1640 | G1641 | G1466 | G1403 | C1340 | G1275 | G1198 | G1058 | C944 | G738 | C677 | C493 | G356 | G356 | G293 |
| A1642 | A1643 | G1467 | G1404 | G1341 | G1276 | G1199 | G1059 | C945 | G739 | C678 | C494 | G357 | G357 | G294 |
| G1644 | G1645 | G1468 | G1405 | A1342 | G1277 | G1200 | G1060 | C946 | G740 | C679 | C495 | G358 | G358 | G295 |
| A1646 | A1647 | G1469 | G1406 | G1343 | G1278 | G1201 | G1061 | C947 | G741 | C680 | C496 | G359 | G359 | G296 |
| G1648 | G1649 | G1470 | G1407 | G1344 | G1279 | G1202 | G1062 | C948 | G742 | G681 | C497 | G360 | G360 | G297 |
| A1650 | A1651 | G1471 | G1408 | C1345 | G1280 | G1203 | G1063 | C949 | G743 | G682 | C498 | G361 | G361 | G298 |
| G1652 | G1653 | G1472 | G1409 | G1346 | G1281 | G1204 | G1064 | C950 | G744 | G683 | C499 | G362 | G362 | G299 |
| A1654 | A1655 | G1473 | G1410 | C1347 | G1282 | G1205 | G1065 | C951 | G745 | C684 | C500 | G363 | G363 | G300 |
| G1656 | G1657 | G1474 | G1411 | U1348 | G1283 | G1206 | G1066 | C952 | G746 | C685 | C501 | G364 | G364 | G301 |
| A1658 | A1659 | G1475 | G1412 | G1349 | G1284 | G1207 | G1067 | C953 | G747 | C686 | C502 | G365 | G365 | G302 |
| G1660 | G1661 | G1476 | G1413 | C1350 | G1285 | G1208 | G1068 | C954 | G748 | C687 | C503 | G366 | G366 | G303 |
| A1662 | A1663 | G1477 | G1414 | G1351 | G1286 | G1209 | G1069 | C955 | G749 | C688 | C504 | G367 | G367 | G304 |
| G1664 | G1665 | G1478 | G1415 | C1352 | G1287 | U1209 | C1081 | C956 | G750 | U688 | C505 | G368 | G368 | G305 |
| A1666 | A1667 | G1479 | G1416 | G1353 | G1288 | G1210 | C1082 | C957 | G751 | U689 | C506 | G369 | G369 | G306 |
| G1668 | G1669 | G1480 | G1417 | A1354 | G1289 | G1211 | C1083 | C958 | G752 | C690 | C507 | G370 | G370 | G307 |
| A1670 | A1671 | G1481 | G1418 | G1355 | G1290 | G1212 | C1084 | C959 | G753 | C691 | C508 | G371 | G371 | G308 |
| G1672 | G1673 | G1482 | G1419 | G1356 | G1291 | G1213 | C1085 | A960 | U754 | C692 | C509 | G372 | G372 | G309 |
| A1674 | A1675 | G1483 | G1420 | G1357 | G1292 | G1214 | C1086 |      |      | C693 | C510 | G373 | G373 | G310 |
| G1676 | G1677 | G1484 | G1421 | G1358 | G1293 | G1215 | C1087 |      |      | C694 | C511 | G374 | G374 | G311 |
| A1678 | A1679 | G1485 | G1422 | G1359 | G1294 | G1216 | C1088 |      |      | C695 | C512 | G375 | G375 | G312 |
| G1680 | G1681 | G1486 | G1423 | G1360 | G1295 | G1217 | C1089 |      |      | C696 | C513 | G376 | G376 | G313 |
| A1682 | A1683 | G1487 | G1424 | G1361 | G1296 | G1218 | C1090 |      |      | C697 | C514 | G377 | G377 | G314 |
| G1684 | G1685 | G1488 | G1425 | G1362 | G1297 | G1219 | C1091 |      |      | C698 | C515 | G378 | G378 | G315 |
| A1686 | A1687 | G1489 | G1426 | G1363 | G1298 | G1220 | C1092 |      |      | C699 | C516 | G379 | G379 | G316 |
| G1688 | G1689 | G1490 | G1427 | G1364 | G1299 | G1221 | C1093 |      |      | C700 | C517 | G380 | G380 | G317 |
| A1690 | A1691 | G1491 | G1428 | G1365 | G1300 | G1222 | C1094 |      |      | C701 | C518 | G381 | G381 | G318 |
| G1692 | G1693 | G1492 | G1429 | G1366 | G1301 | A1222 | C1095 |      |      | U702 | C519 | G382 | G382 | G319 |
| A1694 | A1695 | G1493 | G1430 | G1367 | G1302 | G1236 | C1096 |      |      | U703 | C520 | G383 | G383 | G320 |
| G1696 | G1697 | G1494 | G1431 | G1368 | G1303 | G1237 | C1097 |      |      | U704 | C521 | G384 | G384 | G321 |
| A1698 | A1699 | G1495 | G1432 | G1369 | G1304 | G1238 | C1098 |      |      | U705 | C522 | G385 | G385 | G322 |
| G1700 | G1701 | G1496 | G1433 | G1370 | G1305 | G1239 | C1099 |      |      | U706 | C523 | G386 | G386 | G323 |
| A1702 | A1703 | G1497 | G1434 | G1371 | G1306 | G1240 | C1100 |      |      | U707 | C524 | G387 | G387 | G324 |
| G1704 | G1705 | G1498 | G1435 | A1371 | A1307 | G1241 | C1167 |      |      | U708 | C525 | G388 | G388 | G325 |
| A1706 | A1707 | G1499 | G1436 | G1372 | C1308 | G1242 | G1168 |      |      | U709 | C526 | G389 | G389 | G326 |
| G1708 | G1709 | G1500 | G1437 | G1373 | G1309 | G1243 | G1169 |      |      | U710 | C527 | G390 | G390 | G327 |
| A1710 | A1711 | G1501 | U1438 | G1439 | G1433 | G1244 | G1170 |      |      | U711 | C528 | G391 | G391 | G328 |
| G1712 | G1713 | G1502 | U1439 | G1440 | G1434 | G1245 | G1171 |      |      | U712 | C529 | G392 | G392 | G329 |
| A1714 | A1715 | G1503 | U1440 | G1441 | G1435 | G1246 | G1172 |      |      | U713 | C530 | G393 | G393 | G330 |
| G1716 | G1717 | G1504 | U1441 | G1442 | G1436 | G1247 | G1173 |      |      | U714 | C531 | G394 | G394 | G331 |
| A1718 | A1719 | G1505 | U1442 | G1443 | G1437 | G1248 | G1174 |      |      | U715 | C532 | G395 | G395 | G332 |
| G1720 | G1721 | G1506 | U1443 | G1444 | G1438 | G1249 | G1175 |      |      | U716 | C533 | G396 | G396 | G333 |
| A1722 | A1723 | G1507 | U1444 | G1445 | U1439 | G1250 | G1176 |      |      | U717 | C534 | G397 | G397 | G334 |
| G1724 | G1725 | G1508 | U1445 | G1446 | U1440 | G1251 | G1177 |      |      | U718 | C535 | G398 | G398 | G335 |
| A1726 | A1727 | G1509 | U1446 | G1447 | U1441 | G1252 | G1178 |      |      | U719 | C536 | G399 | G399 | G336 |
| G1728 | G1729 | G1510 | U1447 | G1448 | U1442 | G1253 | G1179 |      |      | U720 | C537 | G400 | G400 | G337 |
| A1730 | A1731 | G1511 | U1448 | G1449 | U1443 | G1254 | U989  |      |      | U721 | C538 | G401 | G401 | G338 |
| G1732 | G1733 | G1512 | U1449 | G1450 | U1444 | G1255 | C990  |      |      | U722 | C539 | G402 | G402 | G339 |
| A1734 | A1735 | G1513 | U1450 | G1451 | U1445 | G1256 | C991  |      |      | U723 | C540 | G403 | G403 | G340 |
| G1736 | G1737 | G1514 | U1451 | G1452 | U1446 | G1257 | C992  |      |      | U724 | C541 | G404 | G404 | G341 |
| A1738 | A1739 | G1515 | U1452 | G1453 | U1447 | G1258 | C993  |      |      | U725 | C542 | G405 | G405 | G342 |
| G1740 | G1741 | G1516 | U1453 | G1454 | U1448 | G1259 | C994  |      |      | U726 | C543 | G406 | G406 | G343 |
| A1742 | A1743 | G1517 | U1454 | G1455 | U1449 |       |       |      |      |      |      |      |      |      |



|       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| G2609 | G2610 | A2611 | G2612 | G2613 | G2614 | G2615 | G2616 | G2617 | G2618 | G2619 | G2620 | A2621 | G2622 | A2623 | G2624 | G2625 | G2626 | G2627 | G2628 | G2629 | G2630 | G2631 | G2632 | G2633 | G2634 | G2635 | G2636 | G2637 | G2638 | G2639 | A2640 | A2641 | G2642 | G2643 | G2644 | G2645 | G2646 | G2647 | G2648 | G2649 | G2650 | G2651 | G2652 | G2653 | G2654 | G2655 | G2656 | G2657 | G2658 | G2659 | G2660 | G2661 | G2662 | G2663 | G2664 | G2665 | G2666 | G2667 | G2668 | G2669 | G2670 | G2671 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| G2541 | G2542 | G2543 | G2544 | G2545 | G2546 | G2547 | G2552 | G2553 | G2554 | G2555 | G2556 | G2557 | G2558 | G2559 | G2560 | G2561 | G2562 | G2563 | G2564 | G2565 | G2566 | G2567 | G2568 | G2569 | G2570 | G2571 | G2572 | G2573 | G2574 | G2575 | G2576 | G2577 | G2578 | G2579 | G2580 | G2581 | G2582 | G2583 | G2584 | G2585 | G2586 | G2587 | G2588 | G2589 | G2590 | G2591 | G2592 | G2593 | G2594 | G2595 | G2596 | G2597 | G2598 | G2599 | G2600 | G2601 | G2602 | G2603 | G2604 | G2605 | G2606 | G2607 | G2608 | G2609 | G2610 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| G2479 | G2480 | G2481 | G2482 | G2483 | G2484 | G2485 | G2486 | G2487 | G2488 | G2489 | G2490 | G2491 | G2492 | G2493 | G2494 | G2495 | G2496 | G2497 | G2498 | G2499 | G2500 | G2501 | G2502 | G2503 | G2504 | G2505 | G2506 | G2507 | G2508 | G2509 | G2510 | G2511 | G2512 | G2513 | G2514 | G2515 | G2516 | G2517 | G2518 | G2519 | G2520 | G2521 | G2522 | G2523 | G2524 | G2525 | G2526 | G2527 | G2528 | G2529 | G2530 | G2531 | G2532 | G2533 | G2534 | G2535 | G2536 | G2537 | G2538 | G2539 | G2540 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| A2341 | A2342 | A2343 | A2344 | G2345 | G2346 | G2347 | G2348 | A2349 | G2350 | G2351 | G2352 | G2353 | G2354 | G2355 | G2356 | G2357 | G2358 | G2359 | G2360 | G2361 | G2362 | G2363 | A2364 | A2365 | A2366 | A2367 | G2368 | A2369 | G2370 | G2371 | G2372 | G2373 | G2374 | G2375 | G2376 | G2377 | G2378 | G2379 | G2380 | G2381 | G2382 | G2383 | G2384 | G2385 | G2386 | G2387 | G2388 | A2389 | G2390 | G2391 | G2392 | G2393 | G2394 | G2395 | G2396 | G2397 | G2398 | G2399 | G2400 | A2401 | G2402 | A2403 | A2404 | G2405 | G2406 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| G2082 | G2083 | G2084 | G2085 | G2086 | G2087 | G2088 | G2089 | G2090 | G2091 | G2092 | G2093 | G2094 | G2095 | G2096 | G2097 | G2098 | G2099 | A2100 | G2101 | G2102 | G2103 | G2104 | A2105 | G2106 | G2107 | G2108 | G2109 | G2110 | G2111 | G2112 | G2113 | G2114 | G2115 | G2116 | G2117 | G2118 | G2119 | G2120 | G2121 | G2122 | G2123 | G2124 | G2125 | G2126 | G2127 | G2128 | G2129 | G2130 | G2131 | G2132 | G2133 | G2134 | G2135 | G2136 | G2137 | G2138 | G2139 | G2140 | G2141 | G2142 | G2143 | G2144 | G2145 | G2146 | G2147 | G2148 | G2149 | G2150 | G2151 | G2152 | G2153 | G2154 | G2155 | G2156 | G2157 | G2158 | G2159 | G2160 | G2161 | G2162 | G2163 | G2164 | G2165 | G2166 | G2167 | G2168 | G2169 | G2170 | G2171 | G2172 | G2173 | G2174 | G2175 | G2176 | G2177 | G2178 | G2179 | G2180 | G2181 | G2182 | G2183 | G2184 | G2185 | G2186 | G2187 | G2188 | G2189 | G2190 | G2191 | G2192 | G2193 | G2194 | G2195 | G2196 | G2197 | G2198 | G2199 | G2200 | G2201 | G2202 | G2203 | G2204 | G2205 | G2206 | G2207 | G2208 | G2209 | G2210 | G2211 | G2212 | G2213 | G2214 | G2215 | G2216 | G2217 | G2218 | G2219 | G2220 | G2221 | G2222 | G2223 | G2224 | G2225 | G2226 | G2227 | G2228 | G2229 | G2230 | G2231 | G2232 | G2233 | G2234 | G2235 | G2236 | G2237 | G2238 | G2239 | G2240 | G2241 | G2242 | G2243 | G2244 | G2245 | G2246 | G2247 | G2248 | G2249 | G2250 | G2251 | G2252 | G2253 | G2254 | G2255 | G2256 | G2257 | G2258 | G2259 | G2260 | G2261 | G2262 | G2263 | G2264 | G2265 | G2266 | G2267 | G2268 | G2269 | G2270 | G2271 | G2272 | G2273 | G2274 | G2275 | G2276 | G2277 | G2278 | G2279 | G2280 | G2281 | G2282 | G2283 | G2284 | G2285 | G2286 | G2287 | G2288 | G2289 | G2290 | G2291 | G2292 | G2293 | G2294 | G2295 | G2296 | G2297 | G2298 | G2299 | G2300 | G2301 | G2302 | G2303 | G2304 | G2305 | G2306 | G2307 | G2308 | G2309 | G2310 | G2311 | G2312 | G2313 | G2314 | G2315 | G2316 | G2317 | G2318 | G2319 | G2320 | G2321 | G2322 | G2323 | G2324 | G2325 | G2326 | G2327 | G2328 | G2329 | G2330 | G2331 | G2332 | G2333 | G2334 | G2335 | G2336 | G2337 | G2338 | G2339 | G2340 |
| U1954 | U1955 | U1956 | U1957 | U1958 | U1959 | U1960 | U1961 | U1962 | U1963 | U1967 | U1966 | U1965 | U1964 | U1965 | U1966 | U1967 | U1968 | U1969 | U1970 | U1971 | U1972 | U1973 | U1974 | U1975 | U1976 | U1977 | U1978 | U1979 | U1980 | U1981 | U1982 | U1983 | U1984 | U1985 | U1986 | U1987 | U1988 | U1989 | U1990 | U1991 | U1992 | U1993 | U1994 | U1995 | U1996 | U1997 | U1998 | U1999 | U2000 | G2001 | G2002 | G2003 | G2004 | G2005 | G2006 | G2007 | G2008 | G2009 | G2010 | G2011 | G2012 | G2013 | G2014 | G2015 | G2016 | G2017 | G2018 | G2019 | G2020 | G2021 | G2022 | G2023 | G2024 | G2025 | G2026 | G2027 | G2028 | G2029 | G2030 | G2031 | G2032 | G2033 | G2034 | G2035 | G2036 | G2037 | G2038 | G2039 | G2040 | G2041 | G2042 | G2043 | G2044 | G2045 | G2046 | G2047 | G2048 | G2049 | G2050 | G2051 | G2052 | G2053 | G2054 | G2055 | G2056 | G2057 | G2058 | G2059 | G2060 | G2061 | G2062 | G2063 | G2064 | G2065 | G2066 | G2067 | G2068 | G2069 | G2070 | G2071 | G2072 | G2073 | G2074 | G2075 | G2076 | G2077 | G2078 | G2079 | G2080 | G2081 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| G1818 | G1819 | G1820 | G1821 | G1822 | G1823 | G1824 | G1825 | G1826 | G1827 | G1831 | G1832 | G1833 | G1834 | U1835 | G1836 | G1837 | G1838 | G1839 | G1840 | G1841 | G1842 | G1843 | G1844 | G1845 | G1846 | G1847 | G1848 | G1849 | G1850 | G1852 | G1853 | G1854 | G1855 | G1856 | G1857 | G1858 | G1859 | G1860 | G1861 | G1862 | G1863 | G1864 | G1865 | G1866 | G1867 | G1868 | G1869 | G1870 | G1871 | G1872 | G1873 | G1874 | G1875 | G1876 | G1877 | G1878 | G1879 | G1880 | G1881 | G1882 | G1883 | G1884 | G1885 | G1886 | G1887 | G1888 | G1889 | G1890 | G1891 | G1892 | G1893 | G1894 | G1895 | G1896 | G1897 | G1898 | G1899 | G1900 | G1901 | G1902 | G1903 | G1904 | G1905 | G1906 | G1907 | G1908 | G1909 | G1910 | G1911 | G1912 | G1913 | G1914 | G1915 | G1916 | G1917 | G1918 | G1919 | G1920 | G1921 | G1922 | G1923 | G1924 | G1925 | G1926 | G1927 | G1928 | G1929 | G1930 | G1931 | G1932 | G1933 | G1934 | G1935 | G1936 | G1937 | G1938 | G1939 | G1940 | G1941 | G1942 | G1943 | G1944 | G1945 | G1946 | G1947 | G1948 | G1949 | G1950 | G1951 | G1952 | G1953 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| U1754 | U1755 | U1756 | U1757 | G1758 | G1759 | G1760 | G1761 | G1762 | G1763 | G1764 | A1765 | A1766 | A1767 | G1768 | G1769 | G1770 | G1771 | G1772 | U1773 | G1774 | A1775 | A1776 | G1777 | G1778 | U1779 | A1780 | G1781 | G1782 | G1783 | U1784 | G1785 | A1786 | G1787 | A1788 | G1789 | U1790 | U1791 | U1792 | U1793 | U1794 | U1795 | U1796 | U1797 | U1798 | U1799 | U1800 | A1801 | A1802 | G1803 | A1804 | A1805 | G1806 | G1807 | G1808 | G1809 | G1810 | G1811 | G1812 | U1813 | G1814 | G1815 | G1816 | G1817 | G1818 | G1819 | G1820 | G1821 | G1822 | G1823 | G1824 | G1825 | G1826 | G1827 | G1828 | G1829 | G1830 | G1831 | G1832 | G1833 | G1834 | G1835 | G1836 | G1837 | G1838 | G1839 | G1840 | G1841 | G1842 | G1843 | G1844 | G1845 | G1846 | G1847 | G1848 | G1849 | G1850 | G1851 | G1852 | G1853 | G1854 | G1855 | G1856 | G1857 | G1858 | G1859 | G1860 | G1861 | G1862 | G1863 | G1864 | G1865 | G1866 | G1867 | G1868 | G1869 | G1870 | G1871 | G1872 | G1873 | G1874 | G1875 | G1876 | G1877 | G1878 | G1879 | G1880 | G1881 | G1882 | G1883 | G1884 | G1885 | G1886 | G1887 | G1888 | G1889 | G1890 | G1891 | G1892 | G1893 | G1894 | G1895 | G1896 | G1897 | G1898 | G1899 | G1900 | G1901 | G1902 | G1903 | G1904 | G1905 | G1906 | G1907 | G1908 | G1909 | G1910 | G1911 | G1912 | G1913 | G1914 | G1915 | G1916 | G1917 | G1918 | G1919 | G1920 | G1921 | G1922 | G1923 | G1924 | G1925 | G1926 | G1927 | G1928 | G1929 | G1930 | G1931 | G1932 | G1933 | G1934 | G1935 | G1936 | G1937 | G1938 | G1939 | G1940 | G1941 | G1942 | G1943 | G1944 | G1945 | G1946 | G1947 | G1948 | G1949 | G1950 | G1951 | G1952 | G1953 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| A1682 | A1683 | A1684 | G1685 | G1686 | G1687 | G1688 | G1689 | G1690 | G1691 | G1692 | A1693 | A1694 | A1695 | A1696 | A1697 | A1698 | A1699 | A1700 | A1701 | G1702 | A1703 | A1704 | A1705 | A1706 | A1707 | A1708 | A1709 | A1710 | A1711 | A1712 | A1713 | A1714 | A1715 | A1716 | A1717 | A1718 | A1719 | A1720 | A1721 | A1722 | A1723 | A1724 | A1725 | A1726 | A1727 | A1728 | A1729 | A1730 | G1731 | G1732 | G1733 | G1734 | U1735 | G1736 | A1737 | A1738 | G1739 | G1740 | G1741 | G1742 | G1743 | G1744 | G1745 | A1746 | A1747 | A1748 | A1749 | G1750 | A1751 | A1752 | G1753 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| U1620 | A1621 | U1622 | G1623 | G1624 | G1625 | G1626 | G1627 | G1628 | G1629 | G1630 | A1631 | A1632 | A1633 | A1634 | U1635 | U1636 | A1637 | A1638 | U1639 | U1640 | G1641 | A1642 | A1643 | A1644 | A1645 | A1646 | U1647 | U1648 | U1649 | A1650 | A1651 | U1652 | U1653 | A1654 | G1655 | G1656 | G1657 | G1658 | G1659 | G1660 | G1661 | G1662 | G1663 | U1664 | G1665 | G1666 | G1667 | A1668 | A1669 | G1670 | U1671 | U1672 | U1673 | U1674 | G1675 | G1676 | G1677 | G1678 | G1679 | G1680 | G1681 | G1682 | G1683 | G1684 | G1685 | G1686 | G1687 | G1688 | G1689 | G1690 | G1691 | G1692 | A1693 | A1694 | A1695 | A1696 | A1697 | A1698 | A1699 | A1700 | A1701 | A1702 | A1703 | A1704 | A1705 | A1706 | A1707 | A1708 | A1709 | A1710 | A1711 | A1712 | A1713 | A1714 | A1715 | A1716 | A1717 | A1718 | A1719 | A1720 | A1721 | A1722 | A1723 | A1724 | A1725 | A1726 | A1727 | A1728 | A1729 | A1730 | A1731 | A1732 | A1733 | A1734 | A1735 | A1736 | A1737 | A1738 | A1739 | A1740 | A1741 | A1742 | A1743 | A1744 | A1745 | A1746 | A1747 | A1748 | A1749 | A1750 | A1751 | A1752 | G1753 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| U1620 | A1621 | U1622 | G1623 | G1624 | G1625 | G1626 | G1627 | G1628 | G1629 | G1630 | A1631 | A1632 | A1633 | A1634 | U1635 | U1636 | A1637 | A1638 | U1639 | U1640 | G1641 | A1642 | A1643 | A1644 | A1645 | A1646 | U1647 | U1648 | U1649 | A1650 | A1651 | U1652 | U1653 | A1654 | G1655 | G1656 | G1657 | G1658 | G1659 | G1660 | G1661 | G1662 | G1663 | U1664 | G1665 | G1666 | G1667 | A1668 | A1669 | G1670 | U1671 | U1672 | U1673 | U1674 | G1675 | G1676 | G1677 | G1678 | G1679 | G1680 | G1681 | G1682 | G1683 | G1684 | G1685 | G1686 | G1687 | G1688 | G1689 | G1690 | G1691 | G1692 | A1693 | A1694 | A1695 | A1696 | A1697 | A1698 | A1699 | A1700 | A1701 | A1702 | A1703 | A1704 | A1705 | A1706 | A1707 | A1708 | A1709 | A1710 | A1711 | A1712 | A1713 | A1714 | A1715 | A1716 | A1717 | A1718 | A1719 | A1720 | A1721 | A1722 | A1723 | A1724 | A1725 | A1726 | A1727 | A1728 | A1729 | A1730 | A1731 | A1732 | A1733 | A1734 | A1735 | A1736 | A1737 | A1738 | A1739 | A1740 | A1741 | A1742 | A1743 | A1744 | A1745 | A1746 | A1747 | A1748 | A1749 | A1750 | A1751 | A1752 | G1753 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| U1620 | A1621 | U1622 | G1623 | G1624 | G1625 | G1626 | G1627 | G1628 | G1629 | G1630 | A1631 | A1632 | A1633 | A1634 | U1635 | U1636 | A1637 | A1638 | U1639 | U1640 | G1641 | A1642 | A1643 | A1644 | A1645 | A1646 | U1647 | U1648 | U1649 | A1650 | A1651 | U1652 | U1653 | A1654 | G1655 | G1656 | G1657 | G1658 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |





- Molecule 86: Small ribosomal subunit protein eS30

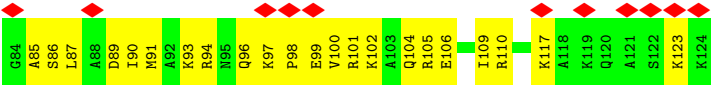


- Molecule 87: Ribosomal protein L24





• Molecule 87: Ribosomal protein L24



## 4 Experimental information

| Property                             | Value               | Source    |
|--------------------------------------|---------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE     | Depositor |
| Imposed symmetry                     | POINT, Not provided |           |
| Number of particles used             | 45867               | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF   | Depositor |
| CTF correction method                | NONE                | Depositor |
| Microscope                           | FEI TITAN KRIOS     | Depositor |
| Voltage (kV)                         | 300                 | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 50                  | Depositor |
| Minimum defocus (nm)                 | 1200                | Depositor |
| Maximum defocus (nm)                 | 2000                | Depositor |
| Magnification                        | Not provided        |           |
| Image detector                       | GATAN K3 (6k x 4k)  | Depositor |
| Maximum map value                    | 0.580               | Depositor |
| Minimum map value                    | -0.081              | Depositor |
| Average map value                    | 0.006               | Depositor |
| Map value standard deviation         | 0.032               | Depositor |
| Recommended contour level            | 0.096               | Depositor |
| Map size ( $\text{\AA}$ )            | 640.8, 640.8, 640.8 | wwPDB     |
| Map dimensions                       | 600, 600, 600       | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0    | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 1.068, 1.068, 1.068 | Depositor |

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths |               | Bond angles |               |
|-----|-------|--------------|---------------|-------------|---------------|
|     |       | RMSZ         | # Z  >5       | RMSZ        | # Z  >5       |
| 1   | CH    | 0.29         | 0/977         | 0.58        | 0/1306        |
| 1   | cH    | 0.29         | 0/977         | 0.67        | 0/1306        |
| 2   | SE    | 0.25         | 0/2118        | 0.46        | 2/2849 (0.1%) |
| 2   | sE    | 0.33         | 0/2118        | 0.58        | 3/2849 (0.1%) |
| 3   | SI    | 0.20         | 0/1715        | 0.43        | 0/2287        |
| 3   | sI    | 0.22         | 0/1715        | 0.42        | 0/2287        |
| 4   | SL    | 0.22         | 0/1268        | 0.44        | 0/1696        |
| 4   | sL    | 0.37         | 0/1268        | 0.59        | 1/1696 (0.1%) |
| 5   | SX    | 0.23         | 0/1116        | 0.43        | 0/1490        |
| 5   | sX    | 0.32         | 0/1116        | 0.54        | 1/1490 (0.1%) |
| 6   | SG    | 0.19         | 0/1946        | 0.42        | 0/2590        |
| 6   | sG    | 0.25         | 0/1946        | 0.50        | 2/2590 (0.1%) |
| 7   | SJ    | 0.20         | 0/1550        | 0.46        | 0/2069        |
| 7   | sJ    | 0.22         | 0/1550        | 0.45        | 0/2069        |
| 8   | SY    | 0.20         | 0/1083        | 0.42        | 0/1438        |
| 8   | sY    | 0.26         | 0/1083        | 0.49        | 0/1438        |
| 9   | se    | 0.23         | 0/465         | 0.54        | 0/612         |
| 10  | SA    | 0.25         | 0/1778        | 0.51        | 0/2416        |
| 10  | sA    | 0.48         | 1/1778 (0.1%) | 0.78        | 5/2416 (0.2%) |
| 11  | SB    | 0.22         | 0/1765        | 0.49        | 1/2362 (0.0%) |
| 11  | sB    | 0.39         | 0/1765        | 0.55        | 0/2362        |
| 12  | SH    | 0.22         | 0/1519        | 0.50        | 1/2033 (0.0%) |
| 12  | sH    | 0.23         | 0/1519        | 0.52        | 0/2033        |
| 13  | SV    | 0.23         | 0/643         | 0.50        | 0/860         |
| 13  | sV    | 0.43         | 0/643         | 0.70        | 1/860 (0.1%)  |
| 14  | Sa    | 0.35         | 1/836 (0.1%)  | 0.71        | 3/1121 (0.3%) |
| 14  | sa    | 0.34         | 0/836         | 0.56        | 1/1121 (0.1%) |
| 15  | SC    | 0.30         | 0/1762        | 0.55        | 0/2381        |
| 15  | sC    | 0.30         | 0/1762        | 0.57        | 0/2381        |
| 16  | SN    | 0.23         | 0/1232        | 0.45        | 0/1656        |
| 16  | sN    | 0.31         | 0/1232        | 0.52        | 0/1656        |
| 17  | SO    | 0.23         | 0/1062        | 0.59        | 2/1425 (0.1%) |

| Mol | Chain | Bond lengths |               | Bond angles |               |
|-----|-------|--------------|---------------|-------------|---------------|
|     |       | RMSZ         | # Z  >5       | RMSZ        | # Z  >5       |
| 17  | sO    | 0.27         | 0/1062        | 0.63        | 2/1425 (0.1%) |
| 18  | SW    | 0.28         | 0/1051        | 0.54        | 1/1406 (0.1%) |
| 18  | sW    | 0.31         | 0/1051        | 0.55        | 0/1406        |
| 19  | Sb    | 0.23         | 0/665         | 0.50        | 0/891         |
| 19  | sb    | 0.55         | 2/665 (0.3%)  | 0.88        | 3/891 (0.3%)  |
| 20  | L7    | 0.19         | 0/2861        | 0.26        | 0/4459        |
| 20  | l7    | 0.26         | 0/2861        | 0.30        | 0/4459        |
| 21  | L8    | 0.19         | 0/3701        | 0.29        | 0/5766        |
| 21  | l8    | 0.25         | 0/3701        | 0.30        | 0/5766        |
| 22  | LA    | 0.29         | 0/1936        | 0.56        | 2/2596 (0.1%) |
| 22  | lA    | 0.33         | 0/1936        | 0.50        | 0/2596        |
| 23  | LB    | 0.22         | 0/3306        | 0.43        | 0/4424        |
| 23  | lB    | 0.28         | 0/3306        | 0.50        | 1/4424 (0.0%) |
| 24  | LC    | 0.40         | 3/2981 (0.1%) | 0.59        | 4/4002 (0.1%) |
| 24  | lC    | 0.28         | 0/2981        | 0.50        | 2/4002 (0.0%) |
| 25  | LD    | 0.26         | 0/2428        | 0.52        | 2/3252 (0.1%) |
| 25  | lD    | 0.27         | 0/2428        | 0.48        | 0/3252        |
| 26  | LE    | 0.18         | 0/1942        | 0.42        | 0/2606        |
| 26  | lE    | 0.30         | 0/1942        | 0.50        | 1/2606 (0.0%) |
| 27  | LF    | 0.24         | 0/1905        | 0.43        | 0/2539        |
| 27  | lF    | 0.29         | 0/1905        | 0.50        | 0/2539        |
| 28  | LG    | 0.20         | 0/1960        | 0.44        | 0/2637        |
| 28  | lG    | 0.28         | 0/1960        | 0.48        | 1/2637 (0.0%) |
| 29  | LH    | 0.19         | 0/1537        | 0.43        | 0/2066        |
| 29  | lH    | 0.31         | 0/1537        | 0.52        | 0/2066        |
| 30  | LI    | 0.25         | 0/1673        | 0.48        | 0/2233        |
| 30  | lI    | 0.27         | 0/1673        | 0.48        | 0/2233        |
| 31  | LJ    | 0.23         | 0/1433        | 0.54        | 0/1915        |
| 31  | lJ    | 0.32         | 0/1433        | 0.59        | 0/1915        |
| 32  | LL    | 0.20         | 0/1732        | 0.42        | 0/2315        |
| 32  | lL    | 0.26         | 0/1732        | 0.46        | 0/2315        |
| 33  | LM    | 0.25         | 0/1161        | 0.51        | 0/1554        |
| 33  | lM    | 0.39         | 1/1161 (0.1%) | 0.66        | 1/1554 (0.1%) |
| 34  | LN    | 0.22         | 0/1746        | 0.42        | 0/2338        |
| 34  | lN    | 0.32         | 0/1746        | 0.48        | 0/2338        |
| 35  | LO    | 0.23         | 0/1682        | 0.46        | 0/2250        |
| 35  | lO    | 0.34         | 0/1682        | 0.54        | 0/2250        |
| 36  | LP    | 0.22         | 0/1268        | 0.41        | 0/1701        |
| 36  | lP    | 0.33         | 0/1268        | 0.50        | 0/1701        |
| 37  | LQ    | 0.25         | 0/1537        | 0.48        | 0/2052        |
| 37  | lQ    | 0.29         | 0/1537        | 0.45        | 0/2052        |
| 38  | LR    | 0.20         | 0/1582        | 0.41        | 0/2091        |
| 38  | lR    | 0.28         | 0/1582        | 0.47        | 0/2091        |

| Mol | Chain | Bond lengths |         | Bond angles |               |
|-----|-------|--------------|---------|-------------|---------------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5       |
| 39  | LS    | 0.21         | 0/1493  | 0.41        | 0/2003        |
| 39  | IS    | 0.30         | 0/1493  | 0.50        | 0/2003        |
| 40  | LT    | 0.26         | 0/1326  | 0.52        | 0/1770        |
| 40  | IT    | 0.30         | 0/1326  | 0.58        | 1/1770 (0.1%) |
| 41  | LU    | 0.23         | 0/839   | 0.55        | 0/1126        |
| 41  | IU    | 0.29         | 0/839   | 0.55        | 0/1126        |
| 42  | LV    | 0.20         | 0/993   | 0.37        | 0/1332        |
| 42  | IV    | 0.30         | 0/993   | 0.50        | 0/1332        |
| 43  | LX    | 0.24         | 0/1002  | 0.48        | 0/1345        |
| 43  | IX    | 0.29         | 0/1002  | 0.47        | 0/1345        |
| 44  | LY    | 0.20         | 0/1132  | 0.41        | 0/1504        |
| 44  | IY    | 0.24         | 0/1132  | 0.41        | 0/1504        |
| 45  | LZ    | 0.21         | 0/1130  | 0.44        | 0/1507        |
| 45  | IZ    | 0.35         | 0/1130  | 0.68        | 2/1507 (0.1%) |
| 46  | La    | 0.25         | 0/1191  | 0.47        | 0/1591        |
| 46  | la    | 0.30         | 0/1191  | 0.49        | 1/1591 (0.1%) |
| 47  | Lb    | 0.25         | 0/889   | 0.56        | 0/1175        |
| 47  | lb    | 0.31         | 0/889   | 0.55        | 0/1175        |
| 48  | Lc    | 0.24         | 0/774   | 0.58        | 0/1038        |
| 48  | lc    | 0.31         | 0/774   | 0.56        | 0/1038        |
| 49  | Ld    | 0.21         | 0/903   | 0.44        | 0/1216        |
| 49  | ld    | 0.28         | 0/903   | 0.46        | 0/1216        |
| 50  | Le    | 0.26         | 0/1071  | 0.51        | 1/1429 (0.1%) |
| 50  | le    | 0.31         | 0/1071  | 0.48        | 1/1429 (0.1%) |
| 51  | Lf    | 0.18         | 0/895   | 0.40        | 0/1198        |
| 51  | lf    | 0.29         | 0/895   | 0.52        | 0/1198        |
| 52  | Lg    | 0.20         | 0/916   | 0.38        | 0/1220        |
| 52  | lg    | 0.32         | 0/916   | 0.55        | 0/1220        |
| 53  | Lh    | 0.26         | 0/1023  | 0.50        | 0/1351        |
| 53  | lh    | 0.29         | 0/1023  | 0.47        | 0/1351        |
| 54  | Li    | 0.41         | 0/843   | 0.73        | 2/1115 (0.2%) |
| 54  | li    | 0.26         | 0/843   | 0.51        | 0/1115        |
| 55  | Lj    | 0.27         | 0/720   | 0.57        | 2/952 (0.2%)  |
| 55  | lj    | 0.34         | 0/720   | 0.60        | 2/952 (0.2%)  |
| 56  | Lk    | 0.23         | 0/575   | 0.49        | 0/761         |
| 56  | lk    | 0.27         | 0/575   | 0.51        | 0/761         |
| 57  | Ll    | 0.18         | 0/454   | 0.40        | 0/599         |
| 57  | ll    | 0.32         | 0/454   | 0.60        | 2/599 (0.3%)  |
| 58  | Lm    | 0.21         | 0/435   | 0.47        | 0/575         |
| 58  | lm    | 0.25         | 0/435   | 0.47        | 0/575         |
| 59  | Ln    | 0.23         | 0/231   | 0.55        | 0/294         |
| 59  | ln    | 0.28         | 0/231   | 0.58        | 0/294         |
| 60  | Lo    | 0.19         | 0/876   | 0.45        | 0/1156        |



| Mol | Chain | Bond lengths |               | Bond angles |                |
|-----|-------|--------------|---------------|-------------|----------------|
|     |       | RMSZ         | # Z  >5       | RMSZ        | # Z  >5        |
| 60  | lo    | 0.29         | 0/876         | 0.57        | 2/1156 (0.2%)  |
| 61  | Lp    | 0.23         | 0/718         | 0.47        | 0/953          |
| 61  | lp    | 0.33         | 0/718         | 0.52        | 1/953 (0.1%)   |
| 62  | Lr    | 0.26         | 0/1017        | 0.50        | 0/1364         |
| 62  | lr    | 0.41         | 0/1017        | 0.58        | 0/1364         |
| 63  | Lz    | 0.18         | 0/1769        | 0.49        | 0/2371         |
| 63  | lz    | 0.18         | 0/1769        | 0.49        | 0/2371         |
| 64  | SR    | 0.32         | 0/1105        | 0.65        | 2/1484 (0.1%)  |
| 64  | sR    | 0.71         | 2/1105 (0.2%) | 1.15        | 6/1484 (0.4%)  |
| 65  | SD    | 0.24         | 0/1793        | 0.46        | 0/2414         |
| 65  | sD    | 0.81         | 5/1793 (0.3%) | 0.96        | 6/2414 (0.2%)  |
| 66  | SF    | 0.25         | 0/1516        | 0.56        | 2/2037 (0.1%)  |
| 66  | sF    | 0.34         | 0/1516        | 0.59        | 3/2037 (0.1%)  |
| 67  | SK    | 0.29         | 0/851         | 0.66        | 0/1147         |
| 67  | sK    | 0.32         | 0/851         | 0.66        | 0/1147         |
| 68  | SP    | 0.23         | 0/1003        | 0.53        | 0/1342         |
| 68  | sP    | 0.28         | 0/1003        | 0.62        | 0/1342         |
| 69  | SQ    | 0.28         | 1/1160 (0.1%) | 0.64        | 2/1553 (0.1%)  |
| 69  | sQ    | 0.32         | 0/1160        | 0.63        | 1/1553 (0.1%)  |
| 70  | SS    | 0.24         | 0/1216        | 0.54        | 2/1628 (0.1%)  |
| 70  | sS    | 0.28         | 0/1216        | 0.58        | 1/1628 (0.1%)  |
| 71  | ST    | 0.26         | 0/1131        | 0.55        | 0/1515         |
| 71  | sT    | 0.32         | 0/1131        | 0.59        | 1/1515 (0.1%)  |
| 72  | SU    | 0.23         | 0/831         | 0.50        | 0/1115         |
| 72  | sU    | 0.32         | 0/831         | 0.55        | 1/1115 (0.1%)  |
| 73  | Sc    | 0.20         | 0/508         | 0.51        | 0/680          |
| 73  | sc    | 0.32         | 0/508         | 0.62        | 0/680          |
| 74  | Sd    | 0.21         | 0/470         | 0.51        | 0/623          |
| 74  | sd    | 0.27         | 0/470         | 0.46        | 0/623          |
| 75  | Sg    | 0.43         | 3/2493 (0.1%) | 0.81        | 5/3394 (0.1%)  |
| 75  | sg    | 0.26         | 0/2493        | 0.53        | 0/3394         |
| 76  | SM    | 0.25         | 0/950         | 0.53        | 0/1275         |
| 76  | sM    | 0.30         | 0/950         | 0.67        | 2/1275 (0.2%)  |
| 77  | SZ    | 0.30         | 0/604         | 0.73        | 1/810 (0.1%)   |
| 77  | sZ    | 0.34         | 0/604         | 0.69        | 1/810 (0.1%)   |
| 78  | Sf    | 0.17         | 0/560         | 0.46        | 0/745          |
| 78  | sf    | 0.21         | 0/560         | 0.52        | 0/745          |
| 79  | S2    | 0.19         | 0/41243       | 0.30        | 1/64259 (0.0%) |
| 79  | s2    | 0.24         | 0/41241       | 0.34        | 0/64251        |
| 80  | CB    | 0.25         | 0/6734        | 0.49        | 2/9094 (0.0%)  |
| 80  | cB    | 0.59         | 6/6734 (0.1%) | 0.74        | 13/9094 (0.1%) |
| 81  | AP    | 0.14         | 0/1692        | 0.26        | 0/2634         |
| 81  | aP    | 0.17         | 0/1692        | 0.29        | 0/2634         |

| Mol | Chain | Bond lengths |                  | Bond angles |                   |
|-----|-------|--------------|------------------|-------------|-------------------|
|     |       | RMSZ         | # Z  >5          | RMSZ        | # Z  >5           |
| 82  | PE    | 0.17         | 0/1778           | 0.36        | 0/2767            |
| 82  | pE    | 0.21         | 0/1778           | 0.38        | 0/2767            |
| 83  | Ls    | 0.19         | 0/1519           | 0.47        | 1/2052 (0.0%)     |
| 83  | ls    | 0.28         | 0/1519           | 0.63        | 3/2052 (0.1%)     |
| 84  | Lt    | 0.23         | 0/1058           | 0.57        | 0/1430            |
| 84  | lt    | 0.20         | 0/1058           | 0.53        | 0/1430            |
| 85  | L5    | 0.31         | 18/88929 (0.0%)  | 0.35        | 32/138727 (0.0%)  |
| 85  | l5    | 0.25         | 0/88929          | 0.33        | 0/138727          |
| 86  | Se    | 0.19         | 0/382            | 0.43        | 0/504             |
| 87  | LW    | 0.19         | 0/979            | 0.39        | 0/1295            |
| 87  | IW    | 0.27         | 0/979            | 0.46        | 0/1295            |
| All | All   | 0.28         | 43/492435 (0.0%) | 0.43        | 148/721182 (0.0%) |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | cH    | 0                   | 1                   |
| 5   | SX    | 0                   | 1                   |
| 5   | sX    | 0                   | 1                   |
| 12  | SH    | 0                   | 1                   |
| 12  | sH    | 0                   | 1                   |
| 22  | lA    | 0                   | 1                   |
| 23  | LB    | 0                   | 2                   |
| 23  | lB    | 0                   | 2                   |
| 31  | LJ    | 0                   | 1                   |
| 33  | LM    | 0                   | 2                   |
| 33  | lM    | 0                   | 2                   |
| 35  | LO    | 0                   | 1                   |
| 35  | lO    | 0                   | 1                   |
| 46  | la    | 0                   | 1                   |
| 51  | Lf    | 0                   | 1                   |
| 51  | lf    | 0                   | 1                   |
| 55  | Lj    | 0                   | 1                   |
| 55  | lj    | 0                   | 1                   |
| 64  | sR    | 0                   | 4                   |
| 66  | SF    | 0                   | 1                   |
| 68  | sP    | 0                   | 1                   |
| 69  | SQ    | 0                   | 1                   |
| 69  | sQ    | 0                   | 1                   |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 71  | ST    | 0                   | 1                   |
| 71  | sT    | 0                   | 1                   |
| All | All   | 0                   | 32                  |

All (43) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|--------|-------------|----------|
| 85  | L5    | 4105 | A    | C1'-N9  | 33.51  | 1.98        | 1.48     |
| 80  | cB    | 849  | PRO  | CG-CD   | -31.82 | 0.42        | 1.50     |
| 85  | L5    | 4102 | C    | N1-C2   | 23.76  | 1.87        | 1.40     |
| 85  | L5    | 4102 | C    | N3-C4   | 23.13  | 1.80        | 1.33     |
| 85  | L5    | 4102 | C    | C2-N3   | 23.11  | 1.81        | 1.35     |
| 80  | cB    | 831  | PRO  | CB-CG   | 21.02  | 2.54        | 1.49     |
| 85  | L5    | 4102 | C    | N1-C6   | 20.83  | 1.78        | 1.37     |
| 65  | sD    | 213  | PRO  | CG-CD   | -20.54 | 0.81        | 1.50     |
| 85  | L5    | 4102 | C    | C4-C5   | 20.37  | 1.83        | 1.43     |
| 85  | L5    | 4102 | C    | C5-C6   | 19.54  | 1.73        | 1.34     |
| 65  | sD    | 213  | PRO  | CB-CG   | 18.95  | 2.44        | 1.49     |
| 85  | L5    | 4105 | A    | N9-C4   | 17.93  | 1.73        | 1.37     |
| 64  | sR    | 134  | PRO  | CG-CD   | -16.95 | 0.93        | 1.50     |
| 80  | cB    | 831  | PRO  | CG-CD   | -14.19 | 1.02        | 1.50     |
| 75  | Sg    | 163  | PRO  | CG-CD   | -12.23 | 1.09        | 1.50     |
| 24  | LC    | 335  | MET  | CB-CG   | -11.61 | 1.17        | 1.52     |
| 80  | cB    | 849  | PRO  | CB-CG   | 11.35  | 2.06        | 1.49     |
| 10  | sA    | 207  | PRO  | CG-CD   | -9.81  | 1.17        | 1.50     |
| 85  | L5    | 4105 | A    | N9-C8   | 9.63   | 1.57        | 1.37     |
| 85  | L5    | 4104 | G    | O3'-P   | 7.51   | 1.72        | 1.61     |
| 85  | L5    | 4104 | G    | C3'-O3' | 6.99   | 1.53        | 1.43     |
| 85  | L5    | 4105 | A    | P-O5'   | 6.89   | 1.70        | 1.59     |
| 65  | sD    | 213  | PRO  | N-CD    | 6.70   | 1.57        | 1.47     |
| 85  | L5    | 4105 | A    | O5'-C5' | 6.43   | 1.52        | 1.42     |
| 85  | L5    | 4105 | A    | C5'-C4' | 6.24   | 1.60        | 1.51     |
| 65  | sD    | 212  | GLU  | C-N     | 6.18   | 1.48        | 1.33     |
| 85  | L5    | 4101 | C    | C1'-N1  | 6.15   | 1.57        | 1.48     |
| 80  | cB    | 831  | PRO  | N-CA    | -6.09  | 1.39        | 1.47     |
| 75  | Sg    | 163  | PRO  | CB-CG   | -5.86  | 1.20        | 1.49     |
| 65  | sD    | 213  | PRO  | N-CA    | -5.83  | 1.39        | 1.47     |
| 85  | L5    | 4101 | C    | O3'-P   | 5.79   | 1.69        | 1.61     |
| 33  | IM    | 118  | MET  | CB-CG   | -5.70  | 1.35        | 1.52     |
| 24  | LC    | 335  | MET  | CG-SD   | -5.55  | 1.66        | 1.80     |
| 80  | cB    | 849  | PRO  | CA-C    | 5.52   | 1.59        | 1.52     |
| 19  | sb    | 70   | LYS  | CG-CD   | -5.50  | 1.35        | 1.52     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 75  | Sg    | 163  | PRO  | N-CA    | -5.35 | 1.40        | 1.47     |
| 69  | SQ    | 41   | MET  | CB-CG   | -5.33 | 1.36        | 1.52     |
| 64  | sR    | 133  | GLY  | C-N     | 5.28  | 1.46        | 1.33     |
| 85  | L5    | 4102 | C    | C5'-C4' | 5.25  | 1.59        | 1.51     |
| 14  | Sa    | 13   | LYS  | CB-CG   | -5.19 | 1.36        | 1.52     |
| 24  | LC    | 335  | MET  | CA-C    | -5.14 | 1.46        | 1.52     |
| 85  | L5    | 4106 | G    | N9-C4   | 5.09  | 1.48        | 1.38     |
| 19  | sb    | 12   | PRO  | CG-CD   | -5.08 | 1.33        | 1.50     |

All (148) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 80  | cB    | 831  | PRO  | CB-CG-CD   | -33.15 | 0.03        | 106.10   |
| 85  | L5    | 4105 | A    | C8-N9-C4   | -22.64 | 37.87       | 105.80   |
| 75  | Sg    | 163  | PRO  | N-CD-CG    | -22.52 | 69.42       | 103.20   |
| 64  | sR    | 134  | PRO  | N-CD-CG    | -20.29 | 72.76       | 103.20   |
| 65  | sD    | 213  | PRO  | CB-CG-CD   | -19.43 | 43.92       | 106.10   |
| 75  | Sg    | 163  | PRO  | CB-CG-CD   | 18.64  | 165.74      | 106.10   |
| 65  | sD    | 213  | PRO  | N-CA-CB    | -18.01 | 84.34       | 103.25   |
| 65  | sD    | 213  | PRO  | CA-CB-CG   | -17.43 | 71.39       | 104.50   |
| 75  | Sg    | 163  | PRO  | CA-CB-CG   | -17.27 | 71.68       | 104.50   |
| 24  | LC    | 335  | MET  | CG-SD-CE   | -16.68 | 64.21       | 100.90   |
| 65  | sD    | 213  | PRO  | N-CD-CG    | -15.77 | 79.55       | 103.20   |
| 80  | cB    | 849  | PRO  | N-CD-CG    | -15.58 | 79.83       | 103.20   |
| 85  | L5    | 4105 | A    | C5-N7-C8   | -15.55 | 57.24       | 103.90   |
| 80  | cB    | 849  | PRO  | CA-CB-CG   | -15.11 | 75.80       | 104.50   |
| 64  | sR    | 134  | PRO  | CA-CB-CG   | -14.50 | 76.94       | 104.50   |
| 80  | cB    | 849  | PRO  | N-CA-CB    | -13.49 | 90.78       | 103.33   |
| 19  | sb    | 12   | PRO  | CA-N-CD    | -13.34 | 93.32       | 112.00   |
| 83  | ls    | 108  | PRO  | CA-N-CD    | -13.20 | 93.52       | 112.00   |
| 69  | SQ    | 41   | MET  | CG-SD-CE   | -12.41 | 73.59       | 100.90   |
| 80  | cB    | 831  | PRO  | CA-N-CD    | -12.18 | 94.94       | 112.00   |
| 85  | L5    | 4105 | A    | C8-N9-C1'  | 12.00  | 163.70      | 127.70   |
| 10  | sA    | 207  | PRO  | CA-N-CD    | -11.95 | 95.27       | 112.00   |
| 10  | sA    | 207  | PRO  | N-CD-CG    | -11.81 | 85.48       | 103.20   |
| 80  | cB    | 831  | PRO  | N-CA-CB    | -11.61 | 90.02       | 103.26   |
| 33  | lM    | 118  | MET  | CG-SD-CE   | -11.12 | 76.43       | 100.90   |
| 45  | lZ    | 90   | PRO  | CA-N-CD    | -11.08 | 96.48       | 112.00   |
| 85  | L5    | 4105 | A    | C4-N9-C1'  | 10.71  | 158.42      | 126.30   |
| 85  | L5    | 4106 | G    | N9-C1'-C2' | 10.27  | 127.40      | 112.00   |
| 80  | cB    | 849  | PRO  | CB-CG-CD   | -9.72  | 75.01       | 106.10   |
| 54  | Li    | 6    | PRO  | CA-N-CD    | -9.67  | 98.47       | 112.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 85  | L5    | 4105 | A    | N9-C1'-C2'  | 9.60  | 126.40      | 112.00   |
| 17  | sO    | 14   | VAL  | CA-C-N      | 9.29  | 138.41      | 121.70   |
| 17  | sO    | 14   | VAL  | C-N-CA      | 9.29  | 138.41      | 121.70   |
| 17  | SO    | 14   | VAL  | CA-C-N      | 9.23  | 138.32      | 121.70   |
| 17  | SO    | 14   | VAL  | C-N-CA      | 9.23  | 138.32      | 121.70   |
| 24  | LC    | 2    | ALA  | CA-C-N      | 9.21  | 138.28      | 121.70   |
| 24  | LC    | 2    | ALA  | C-N-CA      | 9.21  | 138.28      | 121.70   |
| 57  | ll    | 29   | MET  | CG-SD-CE    | -9.17 | 80.72       | 100.90   |
| 19  | sb    | 70   | LYS  | CD-CE-NZ    | -9.15 | 82.62       | 111.90   |
| 75  | Sg    | 25   | PRO  | CA-N-CD     | -9.11 | 99.25       | 112.00   |
| 69  | sQ    | 41   | MET  | CG-SD-CE    | -8.97 | 81.16       | 100.90   |
| 40  | lT    | 155  | PRO  | CA-N-CD     | -8.95 | 99.47       | 112.00   |
| 85  | L5    | 4105 | A    | O4'-C1'-N9  | 8.84  | 121.77      | 108.50   |
| 64  | SR    | 126  | MET  | CG-SD-CE    | -8.82 | 81.49       | 100.90   |
| 85  | L5    | 4105 | A    | N7-C8-N9    | 8.63  | 139.69      | 113.80   |
| 10  | sA    | 10   | MET  | CB-CG-SD    | 8.57  | 138.42      | 112.70   |
| 83  | ls    | 108  | PRO  | N-CD-CG     | -8.38 | 90.62       | 103.20   |
| 4   | sL    | 128  | VAL  | CB-CA-C     | 8.37  | 124.08      | 110.69   |
| 2   | sE    | 234  | PRO  | CA-N-CD     | -8.32 | 100.36      | 112.00   |
| 18  | SW    | 4    | MET  | CG-SD-CE    | -8.28 | 82.67       | 100.90   |
| 10  | sA    | 207  | PRO  | CA-CB-CG    | -8.21 | 88.90       | 104.50   |
| 66  | sF    | 77   | MET  | CG-SD-CE    | -8.16 | 82.95       | 100.90   |
| 83  | Ls    | 108  | PRO  | CA-N-CD     | -8.13 | 100.61      | 112.00   |
| 65  | sD    | 212  | GLU  | CA-CB-CG    | 8.12  | 130.34      | 114.10   |
| 64  | SR    | 1    | MET  | CB-CG-SD    | -8.04 | 88.58       | 112.70   |
| 85  | L5    | 4101 | C    | C6-N1-C2    | -7.96 | 96.30       | 120.20   |
| 80  | CB    | 46   | ILE  | N-CA-C      | -7.96 | 105.56      | 113.20   |
| 85  | L5    | 4106 | G    | C4-N9-C1'   | 7.91  | 150.22      | 126.50   |
| 85  | L5    | 4102 | C    | C4'-C3'-O3' | 7.75  | 121.03      | 109.40   |
| 50  | Le    | 7    | LEU  | CD1-CG-CD2  | -7.73 | 93.80       | 110.80   |
| 76  | sM    | 44   | LYS  | CA-CB-CG    | 7.69  | 129.48      | 114.10   |
| 64  | sR    | 134  | PRO  | N-CA-CB     | -7.69 | 95.18       | 103.25   |
| 55  | Lj    | 86   | PRO  | CA-N-CD     | -7.56 | 101.42      | 112.00   |
| 24  | lC    | 2    | ALA  | CA-C-N      | 7.41  | 135.03      | 121.70   |
| 24  | lC    | 2    | ALA  | C-N-CA      | 7.41  | 135.03      | 121.70   |
| 66  | sF    | 88   | MET  | CG-SD-CE    | -7.39 | 84.64       | 100.90   |
| 19  | sb    | 12   | PRO  | N-CD-CG     | -7.37 | 92.14       | 103.20   |
| 72  | sU    | 82   | MET  | CG-SD-CE    | -7.28 | 84.88       | 100.90   |
| 85  | L5    | 4101 | C    | C2'-C3'-O3' | 7.28  | 124.61      | 113.70   |
| 14  | Sa    | 13   | LYS  | CB-CG-CD    | -7.27 | 94.59       | 111.30   |
| 85  | L5    | 4106 | G    | O4'-C1'-N9  | 7.03  | 119.04      | 108.50   |
| 80  | cB    | 831  | PRO  | CA-CB-CG    | -6.96 | 91.28       | 104.50   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 2   | sE    | 19   | MET  | CG-SD-CE    | -6.93 | 85.64       | 100.90   |
| 85  | L5    | 4102 | C    | P-O5'-C5'   | 6.87  | 131.20      | 120.90   |
| 85  | L5    | 4105 | A    | C2'-C3'-O3' | -6.85 | 103.42      | 113.70   |
| 65  | sD    | 150  | MET  | CB-CA-C     | 6.85  | 121.47      | 109.89   |
| 2   | sE    | 15   | PRO  | CA-N-CD     | -6.69 | 102.64      | 112.00   |
| 22  | LA    | 106  | THR  | CA-C-N      | -6.69 | 107.84      | 121.48   |
| 22  | LA    | 106  | THR  | C-N-CA      | -6.69 | 107.84      | 121.48   |
| 85  | L5    | 4106 | G    | C1'-C2'-O2' | 6.65  | 118.38      | 108.40   |
| 75  | Sg    | 163  | PRO  | CA-N-CD     | -6.59 | 102.77      | 112.00   |
| 14  | Sa    | 13   | LYS  | CD-CE-NZ    | 6.56  | 132.91      | 111.90   |
| 85  | L5    | 4104 | G    | P-O3'-C3'   | 6.53  | 130.00      | 120.20   |
| 55  | lj    | 21   | ARG  | CA-C-N      | 6.52  | 133.99      | 121.54   |
| 55  | lj    | 21   | ARG  | C-N-CA      | 6.52  | 133.99      | 121.54   |
| 85  | L5    | 4105 | A    | C5'-C4'-O4' | 6.51  | 119.57      | 109.80   |
| 85  | L5    | 4105 | A    | O4'-C1'-C2' | -6.48 | 101.12      | 107.60   |
| 69  | SQ    | 41   | MET  | CA-CB-CG    | -6.46 | 101.18      | 114.10   |
| 55  | Lj    | 86   | PRO  | N-CD-CG     | -6.45 | 93.53       | 103.20   |
| 85  | L5    | 4101 | C    | C5-C6-N1    | 6.30  | 139.90      | 121.00   |
| 64  | sR    | 126  | MET  | CA-CB-CG    | 6.25  | 126.60      | 114.10   |
| 12  | SH    | 147  | LYS  | CA-CB-CG    | 6.23  | 126.56      | 114.10   |
| 6   | sG    | 169  | PRO  | CA-N-CD     | -6.14 | 103.40      | 112.00   |
| 25  | LD    | 231  | VAL  | CA-C-N      | 6.11  | 133.95      | 121.48   |
| 25  | LD    | 231  | VAL  | C-N-CA      | 6.11  | 133.95      | 121.48   |
| 77  | sZ    | 98   | LYS  | CD-CE-NZ    | -6.10 | 92.39       | 111.90   |
| 54  | Li    | 6    | PRO  | N-CA-CB     | -6.08 | 99.52       | 102.92   |
| 76  | sM    | 44   | LYS  | N-CA-C      | -6.01 | 99.40       | 108.96   |
| 85  | L5    | 4105 | A    | P-O5'-C5'   | 6.01  | 129.92      | 120.90   |
| 85  | L5    | 4116 | C    | N3-C4-N4    | -5.89 | 100.32      | 118.00   |
| 64  | sR    | 1    | MET  | CB-CA-C     | 5.86  | 121.23      | 110.10   |
| 85  | L5    | 4101 | C    | C2-N1-C1'   | 5.83  | 136.31      | 118.80   |
| 28  | lG    | 178  | GLY  | N-CA-C      | 5.83  | 122.72      | 114.85   |
| 85  | L5    | 4101 | C    | N1-C1'-C2'  | 5.81  | 120.72      | 112.00   |
| 46  | la    | 87   | ARG  | CG-CD-NE    | -5.80 | 99.24       | 112.00   |
| 6   | sG    | 217  | MET  | CA-CB-CG    | 5.77  | 125.64      | 114.10   |
| 85  | L5    | 4104 | G    | C5'-C4'-C3' | 5.75  | 123.82      | 115.20   |
| 85  | L5    | 4101 | C    | O4'-C1'-N1  | 5.68  | 117.01      | 108.50   |
| 23  | lB    | 148  | LYS  | CD-CE-NZ    | -5.66 | 93.80       | 111.90   |
| 2   | SE    | 19   | MET  | CG-SD-CE    | -5.64 | 88.50       | 100.90   |
| 60  | lo    | 104  | ILE  | CA-C-N      | 5.62  | 131.82      | 121.70   |
| 60  | lo    | 104  | ILE  | C-N-CA      | 5.62  | 131.82      | 121.70   |
| 64  | sR    | 1    | MET  | CB-CG-SD    | 5.61  | 129.52      | 112.70   |
| 66  | SF    | 134  | VAL  | N-CA-C      | -5.60 | 107.41      | 112.12   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 45  | lZ    | 35   | ASP  | N-CA-C      | -5.58 | 107.47      | 114.56   |
| 2   | SE    | 140  | VAL  | CA-CB-CG1   | -5.57 | 100.93      | 110.40   |
| 80  | cB    | 830  | ARG  | C-N-CD      | 5.56  | 147.81      | 125.00   |
| 70  | SS    | 57   | GLY  | CA-C-N      | -5.45 | 113.19      | 122.56   |
| 70  | SS    | 57   | GLY  | C-N-CA      | -5.45 | 113.19      | 122.56   |
| 80  | cB    | 497  | MET  | CG-SD-CE    | -5.44 | 88.94       | 100.90   |
| 26  | lE    | 203  | ILE  | N-CA-C      | -5.43 | 106.12      | 111.88   |
| 85  | L5    | 4107 | G    | C4'-C3'-O3' | 5.42  | 121.13      | 113.00   |
| 61  | lp    | 29   | ILE  | CB-CG1-CD1  | -5.42 | 102.42      | 113.80   |
| 77  | SZ    | 89   | GLN  | CA-CB-CG    | 5.40  | 124.91      | 114.10   |
| 66  | sF    | 134  | VAL  | N-CA-C      | -5.39 | 107.36      | 111.62   |
| 80  | cB    | 475  | VAL  | N-CA-C      | -5.31 | 107.30      | 112.29   |
| 83  | ls    | 108  | PRO  | N-CA-CB     | -5.31 | 98.85       | 102.73   |
| 66  | SF    | 78   | MET  | CA-CB-CG    | 5.25  | 124.60      | 114.10   |
| 14  | sa    | 41   | ILE  | N-CA-C      | -5.25 | 107.60      | 112.43   |
| 80  | CB    | 401  | MET  | CB-CG-SD    | 5.24  | 128.42      | 112.70   |
| 85  | L5    | 4105 | A    | O5'-C5'-C4' | 5.24  | 119.35      | 111.50   |
| 85  | L5    | 4100 | C    | O3'-P-O5'   | 5.20  | 111.80      | 104.00   |
| 10  | sA    | 207  | PRO  | N-CA-CB     | -5.20 | 97.79       | 103.25   |
| 80  | cB    | 848  | ILE  | CA-C-N      | -5.20 | 114.60      | 119.85   |
| 80  | cB    | 848  | ILE  | C-N-CA      | -5.20 | 114.60      | 119.85   |
| 85  | L5    | 4104 | G    | O3'-P-O5'   | 5.20  | 111.79      | 104.00   |
| 50  | le    | 90   | MET  | N-CA-C      | 5.19  | 119.19      | 111.87   |
| 24  | LC    | 335  | MET  | CB-CA-C     | -5.18 | 102.97      | 110.96   |
| 79  | S2    | 1133 | A    | C5'-C4'-C3' | 5.18  | 123.78      | 116.00   |
| 71  | sT    | 129  | ARG  | CG-CD-NE    | -5.18 | 100.61      | 112.00   |
| 5   | sX    | 86   | PRO  | CA-N-CD     | -5.12 | 104.83      | 112.00   |
| 14  | Sa    | 13   | LYS  | CG-CD-CE    | -5.12 | 99.53       | 111.30   |
| 11  | SB    | 222  | LYS  | N-CA-CB     | -5.09 | 108.36      | 114.17   |
| 70  | sS    | 71   | MET  | CG-SD-CE    | 5.08  | 112.09      | 100.90   |
| 85  | L5    | 4104 | G    | O4'-C1'-N9  | -5.08 | 100.58      | 108.20   |
| 85  | L5    | 4105 | A    | N3-C4-C5    | -5.04 | 111.69      | 126.80   |
| 13  | sV    | 32   | ILE  | CB-CG1-CD1  | -5.01 | 103.29      | 113.80   |
| 57  | ll    | 29   | MET  | CA-CB-CG    | 5.01  | 124.11      | 114.10   |

There are no chirality outliers.

All (32) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 23  | LB    | 17  | LEU  | Peptide |
| 23  | LB    | 258 | HIS  | Peptide |
| 31  | LJ    | 94  | LEU  | Peptide |

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| Mol | Chain | Res | Type | Group             |
|-----|-------|-----|------|-------------------|
| 33  | LM    | 87  | ALA  | Peptide           |
| 33  | LM    | 88  | ALA  | Peptide           |
| 35  | LO    | 110 | PRO  | Peptide           |
| 51  | Lf    | 106 | TYR  | Peptide           |
| 55  | Lj    | 39  | TYR  | Peptide           |
| 66  | SF    | 78  | MET  | Peptide           |
| 12  | SH    | 15  | LYS  | Peptide           |
| 69  | SQ    | 43  | GLU  | Peptide           |
| 71  | ST    | 46  | ALA  | Peptide           |
| 5   | SX    | 126 | ALA  | Peptide           |
| 1   | cH    | 51  | GLN  | Peptide           |
| 22  | lA    | 13  | GLY  | Peptide           |
| 23  | lB    | 17  | LEU  | Peptide           |
| 23  | lB    | 258 | HIS  | Peptide           |
| 33  | lM    | 87  | ALA  | Peptide           |
| 33  | lM    | 88  | ALA  | Peptide           |
| 35  | lO    | 110 | PRO  | Peptide           |
| 46  | la    | 87  | ARG  | Sidechain         |
| 51  | lf    | 106 | TYR  | Peptide           |
| 55  | lj    | 39  | TYR  | Peptide           |
| 12  | sH    | 15  | LYS  | Peptide           |
| 68  | sP    | 127 | LYS  | Peptide           |
| 69  | sQ    | 43  | GLU  | Peptide           |
| 64  | sR    | 133 | GLY  | Mainchain,Peptide |
| 64  | sR    | 26  | ASN  | Peptide           |
| 64  | sR    | 42  | PRO  | Peptide           |
| 71  | sT    | 129 | ARG  | Sidechain         |
| 5   | sX    | 126 | ALA  | Peptide           |

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | CH    | 968   | 0        | 1013     | 83      | 0            |
| 1   | cH    | 968   | 0        | 1013     | 109     | 0            |
| 2   | SE    | 2076  | 0        | 2177     | 162     | 0            |
| 2   | sE    | 2076  | 0        | 2177     | 149     | 0            |
| 3   | SI    | 1686  | 0        | 1772     | 116     | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 3   | sI    | 1686  | 0        | 1772     | 106     | 0            |
| 4   | SL    | 1247  | 0        | 1323     | 97      | 0            |
| 4   | sL    | 1247  | 0        | 1323     | 114     | 0            |
| 5   | SX    | 1098  | 0        | 1167     | 80      | 0            |
| 5   | sX    | 1098  | 0        | 1167     | 82      | 0            |
| 6   | SG    | 1923  | 0        | 2089     | 159     | 0            |
| 6   | sG    | 1923  | 0        | 2089     | 199     | 0            |
| 7   | SJ    | 1525  | 0        | 1640     | 120     | 0            |
| 7   | sJ    | 1525  | 0        | 1640     | 108     | 0            |
| 8   | SY    | 1065  | 0        | 1142     | 92      | 0            |
| 8   | sY    | 1065  | 0        | 1142     | 101     | 0            |
| 9   | se    | 459   | 0        | 503      | 64      | 0            |
| 10  | SA    | 1741  | 0        | 1746     | 161     | 0            |
| 10  | sA    | 1741  | 0        | 1746     | 190     | 0            |
| 11  | SB    | 1738  | 0        | 1809     | 149     | 0            |
| 11  | sB    | 1738  | 0        | 1809     | 157     | 0            |
| 12  | SH    | 1497  | 0        | 1590     | 132     | 0            |
| 12  | sH    | 1497  | 0        | 1590     | 114     | 0            |
| 13  | SV    | 636   | 0        | 637      | 60      | 0            |
| 13  | sV    | 636   | 0        | 637      | 85      | 0            |
| 14  | Sa    | 821   | 0        | 870      | 90      | 0            |
| 14  | sa    | 821   | 0        | 870      | 65      | 0            |
| 15  | SC    | 1725  | 0        | 1813     | 130     | 0            |
| 15  | sC    | 1725  | 0        | 1813     | 152     | 0            |
| 16  | SN    | 1208  | 0        | 1294     | 78      | 0            |
| 16  | sN    | 1208  | 0        | 1294     | 88      | 0            |
| 17  | SO    | 1049  | 0        | 1073     | 94      | 0            |
| 17  | sO    | 1049  | 0        | 1073     | 94      | 0            |
| 18  | SW    | 1034  | 0        | 1080     | 98      | 0            |
| 18  | sW    | 1034  | 0        | 1080     | 102     | 0            |
| 19  | Sb    | 651   | 0        | 672      | 40      | 0            |
| 19  | sb    | 651   | 0        | 672      | 67      | 0            |
| 20  | L7    | 2561  | 0        | 1295     | 89      | 0            |
| 20  | l7    | 2561  | 0        | 1294     | 99      | 0            |
| 21  | L8    | 3314  | 0        | 1683     | 149     | 0            |
| 21  | l8    | 3314  | 0        | 1682     | 144     | 0            |
| 22  | LA    | 1898  | 0        | 1993     | 133     | 0            |
| 22  | lA    | 1898  | 0        | 1993     | 134     | 0            |
| 23  | LB    | 3238  | 0        | 3376     | 169     | 0            |
| 23  | lB    | 3238  | 0        | 3376     | 160     | 0            |
| 24  | LC    | 2927  | 0        | 3104     | 201     | 0            |
| 24  | lC    | 2927  | 0        | 3104     | 156     | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 25  | LD    | 2382  | 0        | 2410     | 154     | 0            |
| 25  | ID    | 2382  | 0        | 2410     | 168     | 0            |
| 26  | LE    | 1904  | 0        | 2055     | 127     | 0            |
| 26  | IE    | 1904  | 0        | 2055     | 153     | 0            |
| 27  | LF    | 1870  | 0        | 1996     | 124     | 0            |
| 27  | IF    | 1870  | 0        | 1996     | 149     | 0            |
| 28  | LG    | 1927  | 0        | 2074     | 110     | 0            |
| 28  | IG    | 1927  | 0        | 2074     | 99      | 0            |
| 29  | LH    | 1518  | 0        | 1601     | 85      | 0            |
| 29  | IH    | 1518  | 0        | 1601     | 118     | 0            |
| 30  | LI    | 1634  | 0        | 1671     | 101     | 0            |
| 30  | II    | 1634  | 0        | 1671     | 79      | 0            |
| 31  | LJ    | 1410  | 0        | 1441     | 97      | 0            |
| 31  | IJ    | 1410  | 0        | 1441     | 96      | 0            |
| 32  | LL    | 1701  | 0        | 1818     | 104     | 0            |
| 32  | IL    | 1701  | 0        | 1818     | 111     | 0            |
| 33  | LM    | 1138  | 0        | 1204     | 95      | 0            |
| 33  | IM    | 1138  | 0        | 1204     | 106     | 0            |
| 34  | LN    | 1701  | 0        | 1749     | 125     | 0            |
| 34  | IN    | 1701  | 0        | 1749     | 143     | 0            |
| 35  | LO    | 1650  | 0        | 1794     | 108     | 0            |
| 35  | IO    | 1650  | 0        | 1794     | 116     | 0            |
| 36  | LP    | 1242  | 0        | 1269     | 74      | 0            |
| 36  | IP    | 1242  | 0        | 1269     | 80      | 0            |
| 37  | LQ    | 1513  | 0        | 1628     | 104     | 0            |
| 37  | IQ    | 1513  | 0        | 1628     | 99      | 0            |
| 38  | LR    | 1566  | 0        | 1729     | 109     | 0            |
| 38  | IR    | 1566  | 0        | 1729     | 86      | 0            |
| 39  | LS    | 1453  | 0        | 1490     | 90      | 0            |
| 39  | IS    | 1453  | 0        | 1490     | 94      | 0            |
| 40  | LT    | 1298  | 0        | 1366     | 98      | 0            |
| 40  | IT    | 1298  | 0        | 1366     | 106     | 0            |
| 41  | LU    | 825   | 0        | 850      | 63      | 0            |
| 41  | IU    | 825   | 0        | 850      | 83      | 0            |
| 42  | LV    | 979   | 0        | 1039     | 39      | 0            |
| 42  | IV    | 979   | 0        | 1039     | 86      | 0            |
| 43  | LX    | 985   | 0        | 1066     | 73      | 0            |
| 43  | IX    | 985   | 0        | 1066     | 77      | 0            |
| 44  | LY    | 1115  | 0        | 1205     | 73      | 0            |
| 44  | IY    | 1115  | 0        | 1205     | 66      | 0            |
| 45  | LZ    | 1107  | 0        | 1182     | 82      | 0            |
| 45  | IZ    | 1107  | 0        | 1182     | 79      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 46  | La    | 1162  | 0        | 1213     | 92      | 0            |
| 46  | la    | 1162  | 0        | 1213     | 61      | 0            |
| 47  | Lb    | 876   | 0        | 948      | 56      | 0            |
| 47  | lb    | 876   | 0        | 948      | 65      | 0            |
| 48  | Lc    | 764   | 0        | 804      | 58      | 0            |
| 48  | lc    | 764   | 0        | 804      | 62      | 0            |
| 49  | Ld    | 888   | 0        | 930      | 44      | 0            |
| 49  | ld    | 888   | 0        | 930      | 51      | 0            |
| 50  | Le    | 1053  | 0        | 1146     | 59      | 0            |
| 50  | le    | 1053  | 0        | 1147     | 55      | 0            |
| 51  | Lf    | 876   | 0        | 912      | 55      | 0            |
| 51  | lf    | 876   | 0        | 912      | 53      | 0            |
| 52  | Lg    | 906   | 0        | 998      | 47      | 0            |
| 52  | lg    | 906   | 0        | 998      | 67      | 0            |
| 53  | Lh    | 1015  | 0        | 1148     | 73      | 0            |
| 53  | lh    | 1015  | 0        | 1148     | 78      | 0            |
| 54  | Li    | 832   | 0        | 917      | 81      | 0            |
| 54  | li    | 832   | 0        | 917      | 46      | 0            |
| 55  | Lj    | 705   | 0        | 737      | 72      | 0            |
| 55  | lj    | 705   | 0        | 736      | 67      | 0            |
| 56  | Lk    | 569   | 0        | 637      | 39      | 0            |
| 56  | lk    | 569   | 0        | 637      | 50      | 0            |
| 57  | Ll    | 444   | 0        | 483      | 16      | 0            |
| 57  | ll    | 444   | 0        | 483      | 33      | 0            |
| 58  | Lm    | 429   | 0        | 465      | 25      | 0            |
| 58  | lm    | 429   | 0        | 465      | 31      | 0            |
| 59  | Ln    | 230   | 0        | 276      | 21      | 0            |
| 59  | ln    | 230   | 0        | 276      | 22      | 0            |
| 60  | Lo    | 862   | 0        | 929      | 53      | 0            |
| 60  | lo    | 862   | 0        | 930      | 57      | 0            |
| 61  | Lp    | 708   | 0        | 756      | 51      | 0            |
| 61  | lp    | 708   | 0        | 756      | 51      | 0            |
| 62  | Lr    | 1002  | 0        | 1068     | 84      | 0            |
| 62  | lr    | 1002  | 0        | 1068     | 83      | 0            |
| 63  | Lz    | 1741  | 0        | 1854     | 92      | 0            |
| 63  | lz    | 1741  | 0        | 1854     | 93      | 0            |
| 64  | SR    | 1090  | 0        | 1149     | 91      | 0            |
| 64  | sR    | 1090  | 0        | 1149     | 245     | 0            |
| 65  | SD    | 1765  | 0        | 1865     | 111     | 0            |
| 65  | sD    | 1765  | 0        | 1865     | 131     | 0            |
| 66  | SF    | 1495  | 0        | 1549     | 148     | 0            |
| 66  | sF    | 1495  | 0        | 1549     | 130     | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 67  | SK    | 827   | 0        | 854      | 78      | 0            |
| 67  | sK    | 827   | 0        | 854      | 97      | 0            |
| 68  | SP    | 985   | 0        | 1031     | 61      | 0            |
| 68  | sP    | 985   | 0        | 1031     | 79      | 0            |
| 69  | SQ    | 1142  | 0        | 1213     | 83      | 0            |
| 69  | sQ    | 1142  | 0        | 1213     | 122     | 0            |
| 70  | SS    | 1198  | 0        | 1261     | 109     | 0            |
| 70  | sS    | 1198  | 0        | 1261     | 120     | 0            |
| 71  | ST    | 1112  | 0        | 1146     | 116     | 0            |
| 71  | sT    | 1112  | 0        | 1146     | 121     | 0            |
| 72  | SU    | 821   | 0        | 883      | 77      | 0            |
| 72  | sU    | 821   | 0        | 883      | 57      | 0            |
| 73  | Sc    | 506   | 0        | 536      | 57      | 0            |
| 73  | sc    | 506   | 0        | 536      | 64      | 0            |
| 74  | Sd    | 459   | 0        | 452      | 52      | 0            |
| 74  | sd    | 459   | 0        | 452      | 51      | 0            |
| 75  | Sg    | 2436  | 0        | 2393     | 199     | 0            |
| 75  | sg    | 2436  | 0        | 2393     | 214     | 0            |
| 76  | SM    | 940   | 0        | 965      | 81      | 0            |
| 76  | sM    | 940   | 0        | 965      | 89      | 0            |
| 77  | SZ    | 598   | 0        | 656      | 73      | 0            |
| 77  | sZ    | 598   | 0        | 656      | 75      | 0            |
| 78  | Sf    | 548   | 0        | 555      | 36      | 0            |
| 78  | sf    | 548   | 0        | 555      | 32      | 0            |
| 79  | S2    | 36898 | 0        | 18603    | 1606    | 0            |
| 79  | s2    | 36898 | 0        | 18603    | 1960    | 0            |
| 80  | CB    | 6605  | 0        | 6679     | 456     | 0            |
| 80  | cB    | 6605  | 0        | 6679     | 504     | 0            |
| 81  | AP    | 1514  | 0        | 770      | 62      | 0            |
| 81  | aP    | 1514  | 0        | 770      | 66      | 0            |
| 82  | PE    | 1593  | 0        | 810      | 57      | 0            |
| 82  | pE    | 1593  | 0        | 810      | 69      | 0            |
| 83  | Ls    | 1496  | 0        | 1540     | 76      | 0            |
| 83  | ls    | 1496  | 0        | 1540     | 98      | 0            |
| 84  | Lt    | 1046  | 0        | 1076     | 94      | 0            |
| 84  | lt    | 1046  | 0        | 1076     | 66      | 0            |
| 85  | L5    | 79496 | 0        | 40159    | 3416    | 0            |
| 85  | l5    | 79496 | 0        | 40159    | 2938    | 0            |
| 86  | Se    | 378   | 0        | 420      | 27      | 0            |
| 87  | LW    | 965   | 0        | 1029     | 59      | 0            |
| 87  | lW    | 965   | 0        | 1029     | 81      | 0            |
| 88  | Lg    | 1     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 88  | Lj    | 1      | 0        | 0        | 0       | 0            |
| 88  | Lm    | 1      | 0        | 0        | 0       | 0            |
| 88  | Lo    | 1      | 0        | 0        | 0       | 0            |
| 88  | Lp    | 1      | 0        | 0        | 0       | 0            |
| 88  | Sa    | 1      | 0        | 0        | 0       | 0            |
| 88  | lg    | 1      | 0        | 0        | 0       | 0            |
| 88  | lj    | 1      | 0        | 0        | 0       | 0            |
| 88  | lm    | 1      | 0        | 0        | 0       | 0            |
| 88  | lo    | 1      | 0        | 0        | 0       | 0            |
| 88  | lp    | 1      | 0        | 0        | 0       | 0            |
| 88  | sa    | 1      | 0        | 0        | 0       | 0            |
| 89  | L5    | 213    | 0        | 0        | 0       | 0            |
| 89  | L7    | 3      | 0        | 0        | 0       | 0            |
| 89  | L8    | 5      | 0        | 0        | 0       | 0            |
| 89  | LA    | 1      | 0        | 0        | 0       | 0            |
| 89  | LP    | 1      | 0        | 0        | 0       | 0            |
| 89  | LV    | 1      | 0        | 0        | 0       | 0            |
| 89  | Le    | 1      | 0        | 0        | 0       | 0            |
| 89  | Lj    | 1      | 0        | 0        | 0       | 0            |
| 89  | S2    | 29     | 0        | 0        | 0       | 0            |
| 89  | l5    | 212    | 0        | 0        | 0       | 0            |
| 89  | l7    | 3      | 0        | 0        | 0       | 0            |
| 89  | l8    | 5      | 0        | 0        | 0       | 0            |
| 89  | lA    | 1      | 0        | 0        | 0       | 0            |
| 89  | lB    | 1      | 0        | 0        | 0       | 0            |
| 89  | le    | 2      | 0        | 0        | 0       | 0            |
| 89  | lg    | 1      | 0        | 0        | 0       | 0            |
| 89  | lj    | 1      | 0        | 0        | 0       | 0            |
| 89  | s2    | 29     | 0        | 0        | 0       | 0            |
| All | All   | 459641 | 0        | 345702   | 22392   | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 28.

All (22392) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 85:L5:4102:C:C4 | 85:L5:4102:C:C5 | 1.83                     | 1.59              |
| 85:L5:4102:C:C6 | 85:L5:4102:C:N1 | 1.78                     | 1.51              |
| 85:L5:4102:C:C2 | 85:L5:4105:A:N9 | 1.77                     | 1.50              |
| 85:L5:4102:C:C4 | 85:L5:4102:C:N3 | 1.80                     | 1.49              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 85:L5:4102:C:C2   | 85:L5:4102:C:N3    | 1.82                     | 1.47              |
| 85:L5:4102:C:C4   | 85:L5:4105:A:N9    | 1.88                     | 1.42              |
| 85:L5:4102:C:N1   | 85:L5:4102:C:C2    | 1.87                     | 1.42              |
| 85:L5:4102:C:C6   | 85:L5:4105:A:N9    | 1.89                     | 1.40              |
| 85:L5:4102:C:N3   | 85:L5:4105:A:N9    | 1.70                     | 1.40              |
| 85:L5:4102:C:N1   | 85:L5:4105:A:N9    | 1.79                     | 1.29              |
| 85:L5:4105:A:N9   | 85:L5:4105:A:C1'   | 1.98                     | 1.27              |
| 85:L5:4102:C:C5   | 85:L5:4105:A:N9    | 2.02                     | 1.25              |
| 85:L5:4102:C:C2   | 85:L5:4105:A:H1'   | 1.71                     | 1.25              |
| 33:IM:104:MET:HE1 | 33:IM:108:ASP:HB2  | 1.25                     | 1.19              |
| 85:l5:1176:C:H42  | 85:l5:1184:A:N6    | 1.41                     | 1.17              |
| 85:L5:4101:C:C2   | 85:L5:4104:G:H4'   | 1.80                     | 1.17              |
| 85:L5:1176:C:N4   | 85:L5:1184:A:H61   | 1.42                     | 1.15              |
| 85:L5:1176:C:H42  | 85:L5:1184:A:N6    | 1.41                     | 1.15              |
| 85:L5:1336:G:H1'  | 24:LC:95:MET:HE1   | 1.28                     | 1.15              |
| 85:l5:1176:C:N4   | 85:l5:1184:A:H61   | 1.42                     | 1.15              |
| 85:L5:2845:A:H61  | 85:L5:3843:C:N4    | 1.43                     | 1.15              |
| 85:L5:4102:C:C2   | 85:L5:4105:A:C4    | 2.33                     | 1.14              |
| 20:l7:61:G:H5''   | 25:ID:271:MET:HE3  | 1.27                     | 1.14              |
| 35:LO:175:MET:HE1 | 35:LO:178:ARG:HD2  | 1.27                     | 1.13              |
| 79:s2:878:G:H1    | 79:s2:908:A:N6     | 1.48                     | 1.12              |
| 8:sY:18:LEU:HG    | 8:sY:20:ARG:HD3    | 1.25                     | 1.11              |
| 85:L5:4102:C:C4   | 85:L5:4105:A:C8    | 2.39                     | 1.10              |
| 85:L5:1095:A:C2   | 85:L5:1200:G:N1    | 2.18                     | 1.09              |
| 22:lA:71:LYS:HE3  | 85:l5:2595:C:H5'   | 1.34                     | 1.09              |
| 82:pE:26:A:N6     | 82:pE:44:G:H1      | 1.49                     | 1.09              |
| 85:L5:2845:A:N6   | 85:L5:3843:C:H42   | 1.49                     | 1.09              |
| 85:L5:4102:C:H3'  | 85:L5:4106:G:H2'   | 1.24                     | 1.09              |
| 2:SE:128:LYS:HE2  | 2:SE:140:VAL:HG11  | 1.27                     | 1.08              |
| 85:L5:4102:C:C2   | 85:L5:4105:A:C1'   | 2.35                     | 1.08              |
| 80:CB:427:VAL:HB  | 80:CB:485:ILE:HD11 | 1.35                     | 1.07              |
| 14:Sa:13:LYS:HZ3  | 79:S2:1132:C:H2'   | 1.17                     | 1.07              |
| 34:IN:120:TRP:NE1 | 34:IN:123:GLU:OE2  | 1.87                     | 1.07              |
| 47:Lb:54:LEU:HA   | 47:Lb:57:MET:HG2   | 1.36                     | 1.06              |
| 53:Lh:105:LYS:HB2 | 53:Lh:108:GLN:HE21 | 1.17                     | 1.06              |
| 26:IE:118:THR:HB  | 50:le:90:MET:HE1   | 1.32                     | 1.06              |
| 85:L5:4102:C:H6   | 85:L5:4106:G:C4    | 1.74                     | 1.06              |
| 35:lO:93:LYS:HE3  | 85:l5:1308:C:H4'   | 1.32                     | 1.05              |
| 50:Le:82:VAL:HA   | 50:Le:85:LEU:HD23  | 1.36                     | 1.05              |
| 80:CB:43:ALA:HB2  | 80:CB:79:TYR:HE2   | 1.21                     | 1.05              |
| 25:LD:113:PHE:HB3 | 25:LD:115:MET:HE3  | 1.35                     | 1.05              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 85:l5:1762:C:N4    | 85:l5:1770:A:C2    | 2.25                     | 1.05              |
| 77:SZ:86:ALA:HA    | 77:SZ:89:GLN:HE22  | 1.22                     | 1.04              |
| 66:sF:139:VAL:HA   | 73:sc:63:ARG:HH22  | 1.21                     | 1.04              |
| 50:le:90:MET:HA    | 50:le:90:MET:HE3   | 1.33                     | 1.04              |
| 51:lf:2:SER:N      | 85:l5:4946:U:HO2'  | 1.55                     | 1.04              |
| 85:L5:1762:C:N4    | 85:L5:1770:A:C2    | 2.25                     | 1.04              |
| 85:L5:4102:C:C3'   | 85:L5:4106:G:H2'   | 1.86                     | 1.03              |
| 35:LO:118:MET:HE3  | 35:LO:119:VAL:H    | 1.21                     | 1.03              |
| 14:Sa:13:LYS:NZ    | 79:S2:1132:C:H2'   | 1.72                     | 1.03              |
| 55:Lj:19:CYS:SG    | 55:Lj:34:CYS:HB2   | 1.99                     | 1.03              |
| 85:L5:1095:A:H2    | 85:L5:1200:G:N1    | 1.54                     | 1.03              |
| 10:sA:85:ARG:HH22  | 10:sA:202:TYR:HA   | 1.25                     | 1.02              |
| 19:sb:70:LYS:HE3   | 79:s2:1106:C:H5''  | 1.37                     | 1.02              |
| 85:L5:4323:A:H2    | 25:LD:146:LEU:HD11 | 1.21                     | 1.02              |
| 85:L5:4102:C:C5    | 85:L5:4105:A:C8    | 2.46                     | 1.02              |
| 85:l5:1095:A:C2    | 85:l5:1200:G:N1    | 2.25                     | 1.02              |
| 80:CB:42:LYS:HE2   | 80:CB:347:GLY:H    | 1.25                     | 1.02              |
| 85:L5:1709:C:N4    | 85:L5:1716:G:H22   | 1.56                     | 1.02              |
| 85:L5:4102:C:C4    | 85:L5:4105:A:C1'   | 2.43                     | 1.02              |
| 2:SE:196:THR:HG21  | 2:SE:211:LYS:HG2   | 1.42                     | 1.01              |
| 85:L5:1709:C:H42   | 85:L5:1716:G:N2    | 1.57                     | 1.01              |
| 30:II:184:MET:HA   | 30:II:187:LYS:HE3  | 1.42                     | 1.01              |
| 85:l5:2845:A:H61   | 85:l5:3843:C:H42   | 1.02                     | 1.01              |
| 4:sL:128:VAL:C     | 4:sL:140:PHE:HE1   | 1.67                     | 1.00              |
| 27:IF:41:MET:HA    | 27:IF:44:LYS:HZ2   | 1.25                     | 1.00              |
| 14:Sa:74:CYS:SG    | 14:Sa:77:CYS:HB2   | 2.01                     | 1.00              |
| 13:sV:15:ARG:HH21  | 15:sC:84:PHE:HA    | 1.24                     | 1.00              |
| 6:SG:1:MET:HE2     | 6:SG:106:LEU:HB3   | 1.44                     | 1.00              |
| 3:sI:2:GLY:N       | 79:s2:1798:C:HO2'  | 1.60                     | 1.00              |
| 2:SE:72:ILE:HD11   | 2:SE:88:ASP:HB3    | 1.38                     | 1.00              |
| 85:l5:2845:A:H61   | 85:l5:3843:C:N4    | 1.60                     | 0.99              |
| 2:SE:128:LYS:NZ    | 79:S2:343:A:O3'    | 1.95                     | 0.99              |
| 80:CB:582:THR:HG21 | 80:CB:741:MET:HE3  | 1.41                     | 0.99              |
| 80:CB:77:LEU:HB3   | 80:CB:100:ILE:HB   | 1.44                     | 0.99              |
| 5:sX:101:LEU:HD23  | 5:sX:124:LYS:HB3   | 1.43                     | 0.99              |
| 64:sR:29:HIS:HA    | 64:sR:32:LYS:HD2   | 1.44                     | 0.99              |
| 85:L5:1094:G:H1    | 85:L5:1201:U:H3    | 1.06                     | 0.99              |
| 79:s2:1099:G:H1    | 79:s2:1133:A:N6    | 1.60                     | 0.98              |
| 60:Lo:12:CYS:HB3   | 60:Lo:15:CYS:SG    | 2.03                     | 0.98              |
| 1:CH:121:LEU:HD22  | 1:CH:133:ARG:HE    | 1.25                     | 0.98              |
| 60:lo:99:ARG:HH12  | 60:lo:102:GLN:HB2  | 1.26                     | 0.98              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 85:L5:679:C:H5''   | 62:Lr:82:ILE:HD12  | 1.46                     | 0.98              |
| 58:lm:99:CYS:HB2   | 58:lm:114:LYS:HE3  | 1.45                     | 0.98              |
| 31:lJ:94:LEU:HD21  | 31:lJ:98:ASN:HB3   | 1.43                     | 0.97              |
| 85:L5:1401:C:O2    | 85:L5:1416:G:N2    | 1.97                     | 0.97              |
| 27:lF:41:MET:HA    | 27:lF:44:LYS:NZ    | 1.78                     | 0.97              |
| 85:l5:493:G:H1     | 85:l5:660:A:H2     | 1.02                     | 0.97              |
| 59:Ln:17:ARG:HH12  | 79:S2:1173:A:H5''  | 1.28                     | 0.97              |
| 5:sX:140:ARG:HE    | 5:sX:141:PRO:HD2   | 1.27                     | 0.97              |
| 49:ld:90:ARG:HG2   | 49:ld:102:LEU:HD11 | 1.43                     | 0.97              |
| 85:L5:4102:C:N1    | 85:L5:4105:A:C4    | 2.33                     | 0.97              |
| 85:L5:3937:C:H1'   | 34:LN:125:SER:HB3  | 1.45                     | 0.96              |
| 67:SK:3:MET:SD     | 67:SK:7:ASN:ND2    | 2.39                     | 0.96              |
| 54:li:56:ARG:HA    | 54:li:59:GLU:OE1   | 1.64                     | 0.96              |
| 12:sH:46:THR:HG23  | 12:sH:65:PRO:HD3   | 1.46                     | 0.96              |
| 34:lN:120:TRP:CE3  | 85:l5:280:G:H5'    | 2.00                     | 0.96              |
| 28:LG:159:HIS:CD2  | 28:LG:185:LYS:HA   | 2.01                     | 0.96              |
| 85:L5:4101:C:H6    | 85:L5:4105:A:O5'   | 1.46                     | 0.96              |
| 15:sC:189:GLY:H    | 79:s2:1355:C:H42   | 1.02                     | 0.96              |
| 28:LG:159:HIS:HD2  | 28:LG:185:LYS:HA   | 1.26                     | 0.96              |
| 55:Lj:10:LYS:O     | 55:Lj:11:ARG:NH1   | 1.99                     | 0.96              |
| 85:L5:4103:C:C5'   | 85:L5:4106:G:H3'   | 1.94                     | 0.96              |
| 78:Sf:132:MET:HE3  | 78:Sf:139:HIS:HB3  | 1.47                     | 0.95              |
| 4:sL:84:ARG:HD3    | 79:s2:374:G:H4'    | 1.47                     | 0.95              |
| 80:CB:43:ALA:HB2   | 80:CB:79:TYR:CE2   | 2.01                     | 0.95              |
| 69:SQ:41:MET:HE1   | 71:ST:10:ASN:HA    | 1.45                     | 0.95              |
| 80:cB:333:LYS:HG3  | 80:cB:337:LYS:HZ2  | 1.30                     | 0.95              |
| 18:SW:4:MET:HE1    | 79:S2:683:G:H4'    | 1.44                     | 0.95              |
| 31:lJ:32:ARG:HH21  | 31:lJ:35:ARG:HD3   | 1.29                     | 0.95              |
| 24:LC:302:LEU:HD12 | 24:LC:303:ARG:H    | 1.31                     | 0.95              |
| 76:sM:124:ILE:HA   | 76:sM:127:TYR:HD2  | 1.32                     | 0.95              |
| 85:L5:4887:C:H42   | 85:L5:4932:U:H3    | 1.12                     | 0.95              |
| 34:lN:120:TRP:HE3  | 85:l5:280:G:H5'    | 1.29                     | 0.94              |
| 18:SW:4:MET:CE     | 79:S2:683:G:H4'    | 1.96                     | 0.94              |
| 79:s2:146:G:H1     | 79:s2:173:A:N6     | 1.63                     | 0.94              |
| 65:SD:214:LYS:HZ2  | 65:SD:215:ASP:H    | 1.14                     | 0.94              |
| 80:cB:337:LYS:HB3  | 80:cB:341:ARG:HH12 | 1.30                     | 0.94              |
| 79:S2:1652:G:H1    | 79:S2:1672:U:H3    | 1.04                     | 0.94              |
| 79:s2:1656:G:H1    | 79:s2:1668:U:H3    | 1.06                     | 0.94              |
| 80:CB:317:GLU:N    | 80:CB:317:GLU:OE1  | 2.01                     | 0.94              |
| 84:Lt:123:ARG:HB2  | 84:Lt:129:ILE:HD11 | 1.48                     | 0.94              |
| 75:Sg:128:THR:HG23 | 75:Sg:130:LYS:HZ2  | 1.33                     | 0.94              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 71:sT:129:ARG:HH22 | 79:s2:1416:C:H5'   | 1.31                     | 0.93              |
| 75:Sg:212:LYS:HA   | 75:Sg:235:ILE:HD13 | 1.50                     | 0.93              |
| 80:CB:18:ASN:HD21  | 80:CB:94:ASP:H     | 1.15                     | 0.93              |
| 14:Sa:28:ARG:NH2   | 14:Sa:74:CYS:HB2   | 1.84                     | 0.93              |
| 11:sB:217:MET:HE2  | 11:sB:220:LYS:HD3  | 1.47                     | 0.93              |
| 64:sR:53:TYR:H     | 79:s2:1466:G:H5''  | 1.33                     | 0.93              |
| 85:L5:1100:U:H3    | 85:L5:1194:G:H1    | 1.09                     | 0.93              |
| 77:sZ:104:ARG:NH2  | 79:s2:1594:A:N7    | 2.16                     | 0.93              |
| 56:Lk:5:ILE:HD11   | 56:Lk:43:TYR:HB3   | 1.51                     | 0.93              |
| 83:ls:47:LEU:HA    | 83:ls:50:LYS:HZ3   | 1.33                     | 0.92              |
| 85:L5:2486:G:N7    | 85:L5:2493:G:N1    | 2.17                     | 0.92              |
| 85:L5:1728:U:H5'   | 27:LF:127:LYS:NZ   | 1.83                     | 0.92              |
| 23:LB:213:GLN:HE22 | 23:LB:286:LYS:HA   | 1.34                     | 0.92              |
| 62:lr:58:LYS:HA    | 62:lr:121:GLN:HE21 | 1.33                     | 0.92              |
| 24:LC:298:ILE:HG22 | 37:LQ:131:PRO:HB3  | 1.47                     | 0.92              |
| 80:CB:745:TYR:HB2  | 80:CB:814:PHE:HA   | 1.51                     | 0.92              |
| 85:L5:4102:C:N3    | 85:L5:4105:A:C1'   | 2.33                     | 0.92              |
| 6:sG:142:ARG:HB2   | 6:sG:147:LEU:HB2   | 1.51                     | 0.92              |
| 62:lr:58:LYS:HA    | 62:lr:121:GLN:NE2  | 1.85                     | 0.92              |
| 76:sM:54:SER:HB3   | 76:sM:78:LYS:HD2   | 1.51                     | 0.92              |
| 10:sA:34:MET:HE1   | 10:sA:150:THR:HA   | 1.50                     | 0.92              |
| 23:IB:261:ARG:HE   | 35:lO:64:THR:HG21  | 1.33                     | 0.92              |
| 85:l5:1095:A:H2    | 85:l5:1200:G:H1    | 0.99                     | 0.92              |
| 71:ST:140:ALA:HA   | 71:ST:143:LYS:HE2  | 1.51                     | 0.92              |
| 71:sT:129:ARG:NH2  | 79:s2:1416:C:H5'   | 1.84                     | 0.92              |
| 10:SA:8:LEU:HD11   | 13:SV:79:VAL:HG21  | 1.52                     | 0.92              |
| 85:L5:4102:C:C6    | 85:L5:4105:A:C8    | 2.57                     | 0.92              |
| 85:L5:4102:C:C6    | 85:L5:4106:G:C4    | 2.58                     | 0.92              |
| 80:CB:429:ILE:HB   | 80:CB:443:TYR:HB2  | 1.52                     | 0.91              |
| 85:L5:4110:C:H3'   | 85:L5:4111:U:H2'   | 1.52                     | 0.91              |
| 41:lU:81:ARG:NH2   | 85:l5:2622:G:N7    | 2.17                     | 0.91              |
| 63:Lz:214:GLN:H    | 63:Lz:215:ARG:HH21 | 1.13                     | 0.91              |
| 79:s2:146:G:H1     | 79:s2:173:A:H61    | 0.92                     | 0.91              |
| 40:lT:159:MET:H    | 40:lT:159:MET:HE3  | 1.34                     | 0.91              |
| 4:SL:109:MET:HE3   | 4:SL:140:PHE:HD2   | 1.34                     | 0.91              |
| 85:L5:512:U:H3     | 85:L5:647:G:H1     | 1.18                     | 0.91              |
| 12:SH:133:LEU:HD21 | 12:SH:173:PHE:HB3  | 1.52                     | 0.91              |
| 67:sK:80:ARG:NH2   | 67:sK:89:ILE:O     | 2.03                     | 0.91              |
| 26:LE:150:LEU:HD11 | 26:LE:194:VAL:HB   | 1.51                     | 0.91              |
| 1:CH:37:ASP:OD1    | 86:Se:47:PRO:HD2   | 1.71                     | 0.91              |
| 64:sR:30:THR:H     | 79:s2:1455:A:H5'   | 1.33                     | 0.91              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 85:l5:1401:C:O2    | 85:l5:1416:G:N2    | 2.03                     | 0.91              |
| 85:L5:1072:C:O2    | 85:L5:1240:G:N2    | 2.03                     | 0.91              |
| 85:L5:4323:A:C2    | 25:LD:146:LEU:HD11 | 2.05                     | 0.91              |
| 63:Lz:159:MET:HE1  | 63:Lz:194:LEU:HD22 | 1.50                     | 0.91              |
| 10:sA:120:ARG:CZ   | 15:sC:266:TYR:HB3  | 2.00                     | 0.91              |
| 24:lC:284:MET:HE1  | 37:lQ:28:LEU:HB3   | 1.50                     | 0.91              |
| 85:L5:493:G:H1     | 85:L5:660:A:H2     | 0.93                     | 0.91              |
| 44:LY:30:MET:HE1   | 44:LY:78:TYR:HA    | 1.52                     | 0.91              |
| 51:Lf:25:THR:HG22  | 51:Lf:87:LYS:HE3   | 1.53                     | 0.91              |
| 79:s2:1099:G:H1    | 79:s2:1133:A:H61   | 1.02                     | 0.90              |
| 20:L7:2:U:H3       | 20:L7:117:G:H1     | 0.98                     | 0.90              |
| 34:lN:169:ARG:HH22 | 85:l5:63:G:P       | 1.93                     | 0.90              |
| 67:sK:65:ARG:HH22  | 74:sd:25:SER:HA    | 1.35                     | 0.90              |
| 23:LB:216:MET:HE1  | 23:LB:281:ASN:H    | 1.34                     | 0.90              |
| 17:sO:34:PHE:HB3   | 17:sO:41:PHE:HB2   | 1.53                     | 0.90              |
| 80:cB:558:LEU:HD13 | 80:cB:572:LYS:HZ2  | 1.35                     | 0.90              |
| 85:L5:4101:C:H3'   | 85:L5:4106:G:H1'   | 1.52                     | 0.90              |
| 73:sc:10:LYS:HD2   | 73:sc:11:LEU:H     | 1.37                     | 0.90              |
| 85:L5:1402:C:O2    | 85:L5:1415:G:N2    | 2.05                     | 0.90              |
| 25:LD:209:ARG:HA   | 25:LD:212:MET:HG2  | 1.54                     | 0.90              |
| 75:sg:100:ARG:HH12 | 79:s2:1399:C:H5''  | 1.36                     | 0.90              |
| 85:L5:1709:C:H42   | 85:L5:1716:G:H22   | 1.11                     | 0.90              |
| 85:L5:4102:C:C6    | 85:L5:4105:A:C1'   | 2.54                     | 0.90              |
| 85:l5:1094:G:H1    | 85:l5:1201:U:H3    | 1.19                     | 0.90              |
| 22:lA:71:LYS:CE    | 85:l5:2595:C:H5'   | 2.03                     | 0.89              |
| 66:sF:76:MET:HA    | 66:sF:155:CYS:SG   | 2.13                     | 0.89              |
| 53:Lh:105:LYS:HA   | 53:Lh:108:GLN:HG3  | 1.52                     | 0.89              |
| 71:sT:129:ARG:NH1  | 79:s2:1415:C:O3'   | 2.04                     | 0.89              |
| 79:S2:1729:U:H3    | 79:S2:1805:G:H1    | 0.93                     | 0.89              |
| 20:l7:39:C:O2'     | 31:lJ:46:GLN:NE2   | 2.05                     | 0.89              |
| 42:lV:60:MET:HE1   | 42:lV:78:PRO:HB3   | 1.53                     | 0.89              |
| 49:ld:64:ILE:HD11  | 85:l5:2373:C:H4'   | 1.52                     | 0.89              |
| 85:l5:1994:C:H2'   | 85:l5:1995:G:H8    | 1.33                     | 0.89              |
| 85:L5:4102:C:C5    | 85:L5:4105:A:C1'   | 2.56                     | 0.89              |
| 80:CB:254:GLU:HA   | 80:CB:257:MET:HG2  | 1.52                     | 0.89              |
| 12:sH:144:ILE:HD13 | 12:sH:154:ILE:HG13 | 1.55                     | 0.89              |
| 45:lZ:90:PRO:O     | 45:lZ:117:LYS:NZ   | 2.05                     | 0.89              |
| 52:lg:54:ARG:HE    | 85:l5:2683:C:H1'   | 1.37                     | 0.89              |
| 85:L5:173:C:H5''   | 32:LL:129:ARG:HH12 | 1.38                     | 0.89              |
| 85:l5:1072:C:O2    | 85:l5:1240:G:N2    | 2.05                     | 0.89              |
| 80:cB:632:ALA:HB1  | 80:cB:646:ALA:HB1  | 1.54                     | 0.89              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 63:Lz:68:LEU:HD12  | 63:Lz:85:MET:HE3   | 1.55                     | 0.88              |
| 35:IO:62:MET:HE3   | 35:IO:70:PRO:HD3   | 1.54                     | 0.88              |
| 80:CB:8:GLN:HB3    | 8:SY:130:LYS:HD2   | 1.56                     | 0.88              |
| 85:L5:1951:G:H1    | 85:L5:2032:U:H3    | 1.18                     | 0.88              |
| 66:sF:139:VAL:HA   | 73:sc:63:ARG:NH2   | 1.86                     | 0.88              |
| 12:sH:145:ARG:HH22 | 18:sW:52:ILE:HG13  | 1.37                     | 0.88              |
| 65:SD:42:THR:HG21  | 65:SD:45:ARG:HH21  | 1.39                     | 0.88              |
| 56:Lk:8:ILE:HD11   | 56:Lk:56:LEU:HD13  | 1.56                     | 0.88              |
| 63:Lz:62:LYS:HZ1   | 63:Lz:155:ILE:HD11 | 1.38                     | 0.88              |
| 22:IA:204:MET:HE3  | 22:IA:205:ASN:N    | 1.89                     | 0.88              |
| 75:sg:11:LEU:HB3   | 75:sg:43:TRP:CZ3   | 2.08                     | 0.88              |
| 85:l5:1095:A:H2    | 85:l5:1200:G:N1    | 1.64                     | 0.88              |
| 85:L5:493:G:N1     | 85:L5:660:A:C2     | 2.42                     | 0.88              |
| 1:CH:37:ASP:OD1    | 1:CH:38:VAL:N      | 2.07                     | 0.88              |
| 10:sA:81:ASN:HA    | 10:sA:84:GLN:HG3   | 1.54                     | 0.88              |
| 10:sA:85:ARG:HH21  | 10:sA:86:ALA:HA    | 1.36                     | 0.88              |
| 80:cB:89:ILE:HD13  | 80:cB:93:LYS:HB2   | 1.56                     | 0.88              |
| 10:sA:10:MET:HA    | 10:sA:55:TRP:CH2   | 2.09                     | 0.88              |
| 85:l5:2486:G:N7    | 85:l5:2493:G:N1    | 2.22                     | 0.88              |
| 14:Sa:13:LYS:HE2   | 79:S2:1133:A:H4'   | 1.55                     | 0.88              |
| 85:L5:4102:C:N1    | 85:L5:4105:A:H1'   | 1.88                     | 0.88              |
| 40:IT:127:GLN:NE2  | 40:IT:129:LYS:O    | 2.06                     | 0.87              |
| 85:l5:2557:G:H1    | 85:l5:2570:U:H3    | 0.87                     | 0.87              |
| 80:CB:38:SER:O     | 80:CB:42:LYS:NZ    | 2.07                     | 0.87              |
| 71:ST:62:ARG:HH12  | 79:S2:1542:C:H5''  | 1.38                     | 0.87              |
| 64:sR:56:HIS:HA    | 64:sR:59:LYS:HG3   | 1.54                     | 0.87              |
| 10:sA:208:GLU:O    | 10:sA:212:LYS:NZ   | 2.08                     | 0.87              |
| 80:cB:333:LYS:HG3  | 80:cB:337:LYS:NZ   | 1.90                     | 0.87              |
| 24:LC:331:TYR:CD1  | 24:LC:335:MET:HE1  | 2.09                     | 0.87              |
| 83:ls:15:LEU:O     | 83:ls:19:GLN:NE2   | 2.07                     | 0.87              |
| 10:SA:14:ASP:HA    | 10:SA:17:LYS:HD3   | 1.55                     | 0.87              |
| 6:sG:131:ARG:HH21  | 6:sG:132:ARG:HG2   | 1.37                     | 0.87              |
| 31:IJ:106:GLY:HA3  | 31:IJ:131:TYR:HA   | 1.54                     | 0.87              |
| 85:l5:1402:C:O2    | 85:l5:1415:G:N2    | 2.07                     | 0.87              |
| 32:LL:164:GLU:HB3  | 32:LL:167:ARG:HH12 | 1.37                     | 0.87              |
| 43:IX:80:PRO:HG2   | 43:IX:155:ILE:HG21 | 1.55                     | 0.87              |
| 80:CB:401:MET:HE2  | 80:CB:410:PHE:HB2  | 1.56                     | 0.87              |
| 66:SF:179:ASN:HA   | 66:SF:182:LYS:NZ   | 1.90                     | 0.87              |
| 27:IF:74:MET:HE1   | 85:l5:1089:G:H1'   | 1.57                     | 0.87              |
| 52:lg:54:ARG:NH2   | 85:l5:2682:G:N3    | 2.23                     | 0.87              |
| 69:sQ:51:LEU:HB2   | 69:sQ:81:ILE:HD11  | 1.55                     | 0.87              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 77:sZ:47:LEU:HD21  | 77:sZ:83:LEU:HB3   | 1.54                     | 0.87              |
| 32:LL:64:VAL:HA    | 32:LL:67:HIS:ND1   | 1.88                     | 0.87              |
| 77:SZ:86:ALA:HA    | 77:SZ:89:GLN:NE2   | 1.89                     | 0.87              |
| 49:ld:46:LEU:HD21  | 85:l5:2373:C:H5'   | 1.56                     | 0.87              |
| 79:s2:1324:G:H1    | 79:s2:1504:U:H3    | 1.19                     | 0.87              |
| 85:l5:2845:A:N6    | 85:l5:3843:C:H42   | 1.72                     | 0.87              |
| 61:Lp:56:HIS:HE1   | 61:Lp:61:MET:HE3   | 1.40                     | 0.87              |
| 64:SR:1:MET:N      | 79:S2:1454:A:N7    | 2.22                     | 0.87              |
| 65:SD:29:LEU:HB2   | 65:SD:34:TYR:HB2   | 1.53                     | 0.87              |
| 79:S2:1656:G:H1    | 79:S2:1668:U:H3    | 0.90                     | 0.87              |
| 29:lH:96:TYR:OH    | 29:lH:141:LYS:NZ   | 2.06                     | 0.86              |
| 34:lN:120:TRP:NE1  | 34:lN:122:GLY:H    | 1.73                     | 0.86              |
| 2:SE:128:LYS:CE    | 2:SE:140:VAL:HG11  | 2.04                     | 0.86              |
| 85:L5:1176:C:N3    | 85:L5:1184:A:N1    | 2.23                     | 0.86              |
| 85:L5:1414:C:H2'   | 85:L5:1415:G:H8    | 1.40                     | 0.86              |
| 75:Sg:79:LEU:HB3   | 75:Sg:89:LEU:HA    | 1.57                     | 0.86              |
| 7:sJ:31:LEU:O      | 7:sJ:35:TYR:HB2    | 1.75                     | 0.86              |
| 70:SS:50:ILE:HD11  | 70:SS:66:ARG:HH21  | 1.40                     | 0.86              |
| 23:IB:385:LYS:O    | 23:IB:389:MET:HB2  | 1.75                     | 0.86              |
| 24:lC:95:MET:SD    | 24:lC:95:MET:N     | 2.47                     | 0.86              |
| 58:Lm:94:MET:HA    | 58:Lm:94:MET:HE3   | 1.57                     | 0.86              |
| 79:S2:1418:C:H4'   | 79:S2:1420:G:H21   | 1.40                     | 0.86              |
| 85:l5:1072:C:N3    | 85:l5:1240:G:N1    | 2.23                     | 0.86              |
| 24:LC:95:MET:HA    | 24:LC:95:MET:HE3   | 1.55                     | 0.86              |
| 27:lF:132:MET:HA   | 27:lF:135:ILE:HD12 | 1.57                     | 0.86              |
| 17:SO:83:GLN:NE2   | 17:SO:87:GLU:OE2   | 2.08                     | 0.86              |
| 48:lc:77:ASN:OD1   | 48:lc:80:GLU:N     | 2.09                     | 0.86              |
| 75:sg:164:ILE:HD11 | 75:sg:176:VAL:HG13 | 1.58                     | 0.86              |
| 80:CB:284:LYS:HZ1  | 80:CB:286:PRO:HA   | 1.37                     | 0.86              |
| 79:S2:588:G:H4'    | 79:S2:589:G:H5'    | 1.56                     | 0.86              |
| 80:cB:822:GLY:H    | 80:cB:830:ARG:HH22 | 1.23                     | 0.86              |
| 40:LT:112:ASN:HA   | 40:LT:115:LYS:NZ   | 1.90                     | 0.86              |
| 75:Sg:125:ARG:HD2  | 75:Sg:150:TRP:CE2  | 2.08                     | 0.86              |
| 63:lz:59:PRO:HG2   | 63:lz:62:LYS:HD3   | 1.57                     | 0.86              |
| 55:Lj:11:ARG:HA    | 55:Lj:11:ARG:NE    | 1.89                     | 0.86              |
| 51:lF:33:VAL:HG23  | 51:lF:38:GLU:HB2   | 1.58                     | 0.85              |
| 85:L5:1951:G:N2    | 85:L5:2032:U:O2    | 2.09                     | 0.85              |
| 24:lC:325:MET:HE2  | 24:lC:325:MET:HA   | 1.56                     | 0.85              |
| 75:sg:159:ASN:HD21 | 75:sg:162:ASN:HD22 | 1.22                     | 0.85              |
| 82:pE:37:A:H3'     | 82:pE:38:A:H8      | 1.41                     | 0.85              |
| 65:sD:75:LYS:HZ3   | 67:sK:20:VAL:HG23  | 1.42                     | 0.85              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 6:SG:68:LEU:N      | 6:SG:100:CYS:SG    | 2.49                     | 0.85              |
| 32:LL:114:VAL:HA   | 32:LL:117:LEU:HD12 | 1.55                     | 0.85              |
| 1:CH:49:ASN:HD21   | 79:S2:638:C:H1'    | 1.40                     | 0.85              |
| 31:IJ:32:ARG:HE    | 31:IJ:35:ARG:NE    | 1.74                     | 0.85              |
| 43:IX:86:ALA:HB1   | 43:IX:97:VAL:HG21  | 1.58                     | 0.85              |
| 14:Sa:28:ARG:HH21  | 14:Sa:74:CYS:HB2   | 1.41                     | 0.85              |
| 70:SS:36:VAL:HB    | 70:SS:99:LEU:HD11  | 1.56                     | 0.85              |
| 85:L5:4773:C:O2    | 85:L5:4861:G:N2    | 2.09                     | 0.85              |
| 52:Lg:83:CYS:SG    | 52:Lg:86:CYS:HB2   | 2.16                     | 0.85              |
| 6:sG:136:LYS:HZ2   | 6:sG:174:PRO:HB2   | 1.41                     | 0.85              |
| 39:IS:83:ARG:HD2   | 39:IS:125:GLN:HE21 | 1.42                     | 0.85              |
| 80:cB:209:LEU:HA   | 80:cB:257:MET:HE1  | 1.57                     | 0.85              |
| 85:l5:493:G:N1     | 85:l5:660:A:C2     | 2.43                     | 0.85              |
| 17:SO:32:HIS:HD2   | 79:S2:975:G:H4'    | 1.42                     | 0.85              |
| 85:L5:493:G:O6     | 85:L5:660:A:N1     | 2.10                     | 0.85              |
| 79:S2:1461:G:H3'   | 79:S2:1463:U:H3    | 1.41                     | 0.85              |
| 64:sR:32:LYS:N     | 79:s2:1455:A:OP1   | 2.09                     | 0.84              |
| 25:LD:200:MET:HE2  | 25:LD:237:GLU:HA   | 1.59                     | 0.84              |
| 71:sT:129:ARG:HA   | 71:sT:129:ARG:NE   | 1.92                     | 0.84              |
| 85:l5:3946:G:H1    | 85:l5:4067:U:H3    | 1.24                     | 0.84              |
| 85:L5:2520:C:O2    | 85:L5:2640:G:N2    | 2.10                     | 0.84              |
| 38:LR:76:MET:HE1   | 38:LR:88:ARG:HH21  | 1.40                     | 0.84              |
| 1:cH:100:ASN:ND2   | 79:s2:608:C:O2     | 2.10                     | 0.84              |
| 26:lE:270:TYR:HE1  | 33:lM:110:PHE:HB3  | 1.43                     | 0.84              |
| 32:lL:41:ALA:HA    | 32:lL:44:ARG:HE    | 1.40                     | 0.84              |
| 47:lb:101:HIS:O    | 47:lb:109:ARG:NH2  | 2.10                     | 0.84              |
| 64:sR:49:LYS:NZ    | 79:s2:1368:U:O2'   | 2.09                     | 0.84              |
| 85:l5:2520:C:O2    | 85:l5:2640:G:N2    | 2.10                     | 0.84              |
| 85:L5:4101:C:C6    | 85:L5:4106:G:H4'   | 2.11                     | 0.84              |
| 22:LA:104:VAL:HA   | 22:LA:107:MET:HE3  | 1.59                     | 0.84              |
| 37:LQ:187:LYS:O    | 37:LQ:188:ASN:ND2  | 2.10                     | 0.84              |
| 69:SQ:41:MET:CE    | 71:ST:10:ASN:HA    | 2.08                     | 0.84              |
| 83:Ls:121:VAL:HG13 | 83:Ls:160:LEU:HD22 | 1.59                     | 0.84              |
| 13:sV:34:MET:HE1   | 13:sV:69:ILE:HG21  | 1.60                     | 0.84              |
| 14:sa:79:ILE:HD11  | 79:s2:1863:A:N3    | 1.92                     | 0.84              |
| 64:sR:49:LYS:HE2   | 79:s2:1370:A:H62   | 1.42                     | 0.84              |
| 83:ls:83:ARG:NH2   | 85:l5:2023:C:OP2   | 2.11                     | 0.84              |
| 75:Sg:87:LEU:HB3   | 75:Sg:101:PHE:HB2  | 1.60                     | 0.84              |
| 19:sb:31:TYR:HB2   | 19:sb:81:ARG:HE    | 1.42                     | 0.84              |
| 36:IP:112:LEU:HD13 | 36:IP:150:LEU:HD13 | 1.60                     | 0.84              |
| 41:IU:44:GLN:NE2   | 41:IU:45:GLU:OE1   | 2.10                     | 0.84              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 64:sR:9:VAL:HA     | 79:s2:1372:U:H3    | 1.39                     | 0.84              |
| 68:sP:37:TYR:O     | 70:sS:88:LYS:NZ    | 2.09                     | 0.84              |
| 71:sT:34:VAL:HG13  | 71:sT:52:TRP:HE1   | 1.41                     | 0.84              |
| 80:cB:454:MET:HE1  | 80:cB:459:GLU:HB2  | 1.59                     | 0.84              |
| 32:lL:71:ARG:NH1   | 85:l5:102:G:OP1    | 2.10                     | 0.84              |
| 36:lP:117:ILE:HG22 | 36:lP:148:MET:HB2  | 1.59                     | 0.84              |
| 62:lr:57:GLY:O     | 62:lr:121:GLN:NE2  | 2.11                     | 0.84              |
| 24:LC:10:VAL:HG23  | 24:LC:153:VAL:HG12 | 1.60                     | 0.84              |
| 8:sY:10:ARG:HA     | 79:s2:839:C:H41    | 1.43                     | 0.84              |
| 23:lB:2:SER:N      | 85:l5:4517:A:N7    | 2.25                     | 0.84              |
| 22:lA:205:ASN:OD1  | 22:lA:206:PRO:HD2  | 1.77                     | 0.84              |
| 34:lN:150:TRP:CZ3  | 85:l5:332:C:H5'    | 2.12                     | 0.84              |
| 63:lz:206:ILE:HG13 | 63:lz:215:ARG:HH12 | 1.40                     | 0.84              |
| 80:cB:724:THR:HA   | 80:cB:727:ARG:HE   | 1.43                     | 0.84              |
| 85:L5:4094:G:H21   | 85:L5:4109:G:H4'   | 1.43                     | 0.84              |
| 79:s2:289:G:N2     | 79:s2:293:C:O2     | 2.10                     | 0.84              |
| 85:L5:1768:C:N3    | 85:L5:1772:C:N4    | 2.26                     | 0.84              |
| 85:L5:4101:C:N1    | 85:L5:4104:G:H4'   | 1.92                     | 0.84              |
| 85:L5:4773:C:N3    | 85:L5:4861:G:N1    | 2.24                     | 0.84              |
| 22:LA:129:ALA:O    | 22:LA:169:VAL:HG21 | 1.78                     | 0.84              |
| 10:sA:84:GLN:OE1   | 10:sA:101:GLY:N    | 2.09                     | 0.83              |
| 80:cB:820:LEU:HG   | 80:cB:830:ARG:HH21 | 1.40                     | 0.83              |
| 85:L5:4101:C:C3'   | 85:L5:4106:G:H1'   | 2.08                     | 0.83              |
| 11:sB:60:ASP:HA    | 11:sB:63:LYS:HG2   | 1.59                     | 0.83              |
| 22:lA:207:VAL:HG23 | 22:lA:208:GLU:HG3  | 1.61                     | 0.83              |
| 54:li:4:ARG:NH1    | 85:l5:1482:G:O6    | 2.11                     | 0.83              |
| 31:lJ:35:ARG:NH1   | 31:lJ:122:SER:O    | 2.10                     | 0.83              |
| 85:L5:3967:G:H1    | 85:L5:4055:U:H3    | 0.85                     | 0.83              |
| 30:II:55:ASP:OD2   | 30:II:162:ARG:NH2  | 2.10                     | 0.83              |
| 48:lc:104:ILE:HG23 | 48:lc:106:ARG:HH12 | 1.42                     | 0.83              |
| 85:L5:1402:C:N3    | 85:L5:1415:G:N1    | 2.26                     | 0.83              |
| 85:L5:4103:C:H5'   | 85:L5:4106:G:H3'   | 1.59                     | 0.83              |
| 46:La:100:ILE:HD11 | 46:La:125:LYS:HG3  | 1.60                     | 0.83              |
| 79:S2:1536:G:H2'   | 79:S2:1537:A:H8    | 1.42                     | 0.83              |
| 2:sE:100:ARG:HB2   | 2:sE:114:ILE:HD13  | 1.61                     | 0.83              |
| 31:lJ:63:ARG:CZ    | 60:lo:105:GLN:H    | 1.91                     | 0.83              |
| 37:lQ:70:MET:HE1   | 37:lQ:137:VAL:HG21 | 1.59                     | 0.83              |
| 48:lc:77:ASN:OD1   | 48:lc:80:GLU:HG2   | 1.78                     | 0.83              |
| 82:pE:6:G:H1       | 82:pE:67:U:H3      | 1.25                     | 0.83              |
| 15:SC:75:ILE:HD11  | 15:SC:80:GLU:OE2   | 1.79                     | 0.83              |
| 23:lB:302:ASN:ND2  | 23:lB:314:ILE:H    | 1.76                     | 0.83              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 75:sg:87:LEU:HB2   | 75:sg:101:PHE:HB2  | 1.60                     | 0.83              |
| 83:ls:106:LYS:HZ2  | 83:ls:107:VAL:H    | 1.26                     | 0.83              |
| 85:l5:3615:G:N3    | 87:IW:44:ARG:NH1   | 2.25                     | 0.83              |
| 42:LV:112:MET:SD   | 42:LV:135:ASN:ND2  | 2.51                     | 0.83              |
| 80:cB:150:ARG:HH21 | 80:cB:200:MET:HB2  | 1.44                     | 0.83              |
| 85:L5:4049:U:O2    | 85:L5:4051:C:N4    | 2.12                     | 0.83              |
| 85:L5:4102:C:N1    | 85:L5:4105:A:C1'   | 2.42                     | 0.83              |
| 37:LQ:50:ARG:HB3   | 37:LQ:83:VAL:HG21  | 1.61                     | 0.83              |
| 85:l5:1346:C:H2'   | 85:l5:1347:G:H8    | 1.44                     | 0.83              |
| 12:SH:64:VAL:HG13  | 12:SH:68:GLN:HE21  | 1.44                     | 0.83              |
| 12:sH:144:ILE:HD11 | 12:sH:152:ARG:HB3  | 1.61                     | 0.83              |
| 75:sg:212:LYS:HA   | 75:sg:235:ILE:HD13 | 1.58                     | 0.83              |
| 78:sf:123:SER:HG   | 78:sf:126:CYS:HG   | 1.18                     | 0.83              |
| 80:cB:429:ILE:HB   | 80:cB:443:TYR:HB2  | 1.60                     | 0.83              |
| 85:l5:1176:C:N3    | 85:l5:1184:A:N1    | 2.26                     | 0.83              |
| 11:SB:82:ARG:HB3   | 11:SB:103:MET:HE1  | 1.60                     | 0.83              |
| 19:Sb:32:PHE:O     | 19:Sb:81:ARG:NH1   | 2.12                     | 0.83              |
| 41:lU:34:MET:SD    | 41:lU:38:ASN:ND2   | 2.51                     | 0.83              |
| 75:sg:32:LEU:H     | 75:sg:32:LEU:HD23  | 1.43                     | 0.83              |
| 73:Sc:29:GLN:HB3   | 73:Sc:43:ILE:HD11  | 1.61                     | 0.83              |
| 68:sP:88:GLU:N     | 68:sP:88:GLU:OE2   | 2.12                     | 0.82              |
| 85:L5:3705:G:H21   | 22:LA:224:THR:HG21 | 1.43                     | 0.82              |
| 29:LH:106:GLN:HB2  | 29:LH:111:LEU:HB3  | 1.61                     | 0.82              |
| 20:l7:114:U:H4'    | 25:ID:73:MET:HE1   | 1.61                     | 0.82              |
| 42:IV:40:ILE:HD11  | 85:l5:3799:A:C5    | 2.14                     | 0.82              |
| 75:sg:11:LEU:HB3   | 75:sg:43:TRP:HZ3   | 1.41                     | 0.82              |
| 12:SH:147:LYS:O    | 12:SH:147:LYS:HD2  | 1.77                     | 0.82              |
| 12:SH:182:GLY:HA3  | 79:S2:690:G:H8     | 1.42                     | 0.82              |
| 24:LC:287:THR:HG23 | 62:Lr:5:LEU:HD21   | 1.59                     | 0.82              |
| 59:Ln:17:ARG:HA    | 59:Ln:20:MET:HE3   | 1.60                     | 0.82              |
| 79:S2:1324:G:H1    | 79:S2:1504:U:H3    | 0.83                     | 0.82              |
| 43:lX:139:ARG:HH22 | 85:l5:2533:C:H5''  | 1.43                     | 0.82              |
| 50:le:90:MET:HE3   | 50:le:90:MET:CA    | 2.08                     | 0.82              |
| 74:sd:12:ARG:NH2   | 79:s2:1513:C:OP1   | 2.12                     | 0.82              |
| 11:SB:168:MET:HB2  | 11:SB:197:ILE:HD11 | 1.59                     | 0.82              |
| 85:l5:4907:G:N2    | 85:l5:4914:C:O2    | 2.11                     | 0.82              |
| 7:SJ:138:ARG:NH2   | 7:SJ:152:ASP:O     | 2.11                     | 0.82              |
| 85:L5:1995:G:H4'   | 84:Lt:128:THR:HB   | 1.60                     | 0.82              |
| 6:sG:151:ASP:HB3   | 87:IW:101:ARG:HH12 | 1.44                     | 0.82              |
| 21:l8:74:U:O4      | 44:lY:72:GLN:NE2   | 2.11                     | 0.82              |
| 85:l5:499:G:N2     | 85:l5:504:G:O6     | 2.13                     | 0.82              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 18:sW:24:GLN:HE21  | 19:sb:7:LEU:HD12   | 1.45                     | 0.82              |
| 21:l8:21:C:N3      | 85:l5:379:G:N1     | 2.27                     | 0.82              |
| 37:lQ:187:LYS:O    | 37:lQ:188:ASN:ND2  | 2.12                     | 0.82              |
| 85:l5:1994:C:H2'   | 85:l5:1995:G:C8    | 2.15                     | 0.82              |
| 85:L5:1709:C:N3    | 85:L5:1716:G:N1    | 2.27                     | 0.82              |
| 79:s2:1461:G:H21   | 79:s2:1465:A:H62   | 1.25                     | 0.82              |
| 67:SK:15:LEU:HD11  | 67:SK:21:MET:HE2   | 1.60                     | 0.82              |
| 77:SZ:50:PHE:HE1   | 77:SZ:55:TYR:HA    | 1.43                     | 0.82              |
| 4:sL:104:LYS:HD3   | 5:sX:8:ARG:HD3     | 1.60                     | 0.82              |
| 31:lJ:139:PHE:HE1  | 31:lJ:151:ILE:HD13 | 1.44                     | 0.82              |
| 46:la:77:LYS:NZ    | 85:l5:1502:G:N7    | 2.27                     | 0.82              |
| 85:L5:4094:G:O2'   | 85:L5:4109:G:N3    | 2.12                     | 0.82              |
| 32:LL:55:ILE:HA    | 32:LL:154:VAL:HG11 | 1.61                     | 0.82              |
| 77:SZ:104:ARG:NH2  | 79:S2:1594:A:N7    | 2.26                     | 0.82              |
| 37:lQ:104:ARG:NH2  | 85:l5:1353:G:N7    | 2.27                     | 0.82              |
| 52:lg:64:LEU:HA    | 52:lg:67:LEU:HD23  | 1.61                     | 0.82              |
| 85:l5:3615:G:H21   | 87:lW:44:ARG:HH22  | 1.27                     | 0.82              |
| 80:CB:180:ARG:NE   | 80:CB:183:GLU:OE2  | 2.12                     | 0.82              |
| 85:L5:679:C:H5''   | 62:Lr:82:ILE:CD1   | 2.09                     | 0.82              |
| 6:sG:55:GLY:O      | 6:sG:63:MET:HG2    | 1.80                     | 0.81              |
| 46:la:110:LYS:NZ   | 85:l5:1396:G:N7    | 2.28                     | 0.81              |
| 84:lt:57:ARG:HE    | 84:lt:83:LYS:HD2   | 1.45                     | 0.81              |
| 85:l5:1709:C:N4    | 85:l5:1716:G:H22   | 1.77                     | 0.81              |
| 85:L5:159:C:H5''   | 54:Li:25:ARG:HE    | 1.44                     | 0.81              |
| 85:L5:1095:A:H2    | 85:L5:1200:G:H1    | 0.93                     | 0.81              |
| 19:sb:33:MET:HE1   | 19:sb:79:PHE:HB2   | 1.61                     | 0.81              |
| 19:sb:70:LYS:NZ    | 79:s2:1107:G:P     | 2.53                     | 0.81              |
| 71:sT:43:LYS:NZ    | 79:s2:1540:G:OP2   | 2.13                     | 0.81              |
| 79:s2:1277:C:H2'   | 79:s2:1278:A:H8    | 1.45                     | 0.81              |
| 6:SG:137:ARG:NH2   | 79:S2:146:G:N7     | 2.27                     | 0.81              |
| 16:SN:70:LYS:HD2   | 16:SN:73:ARG:HH21  | 1.45                     | 0.81              |
| 22:LA:226:ARG:NH1  | 22:LA:228:ASP:OD2  | 2.12                     | 0.81              |
| 26:LE:164:PHE:HA   | 26:LE:175:VAL:HG12 | 1.61                     | 0.81              |
| 59:Ln:16:LYS:HG2   | 59:Ln:20:MET:HE2   | 1.59                     | 0.81              |
| 75:Sg:149:GLU:OE2  | 75:Sg:170:TRP:HB3  | 1.80                     | 0.81              |
| 79:S2:796:G:N2     | 79:S2:798:G:O6     | 2.13                     | 0.81              |
| 84:Lt:142:ASN:HD22 | 84:Lt:148:PRO:HB3  | 1.45                     | 0.81              |
| 4:sL:77:VAL:HG12   | 4:sL:124:ASP:H     | 1.45                     | 0.81              |
| 25:lD:287:PHE:O    | 25:lD:291:GLN:NE2  | 2.13                     | 0.81              |
| 60:lo:61:LYS:HA    | 60:lo:61:LYS:HE3   | 1.60                     | 0.81              |
| 66:sF:88:MET:SD    | 66:sF:91:ARG:NH2   | 2.53                     | 0.81              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 70:sS:59:LEU:HD21  | 70:sS:63:GLU:HB2   | 1.62                     | 0.81              |
| 80:cB:745:TYR:HB2  | 80:cB:814:PHE:HA   | 1.62                     | 0.81              |
| 85:L5:493:G:N1     | 85:L5:660:A:H2     | 1.77                     | 0.81              |
| 33:LM:52:PHE:HA    | 33:LM:55:MET:HE1   | 1.60                     | 0.81              |
| 79:S2:1550:G:H3'   | 79:S2:1579:A:H61   | 1.45                     | 0.81              |
| 80:cB:254:GLU:HA   | 80:cB:257:MET:HG2  | 1.62                     | 0.81              |
| 8:SY:21:LYS:HB3    | 8:SY:23:MET:HE1    | 1.60                     | 0.81              |
| 28:LG:173:LEU:HA   | 54:Li:43:MET:HE3   | 1.62                     | 0.81              |
| 79:s2:1372:U:OP1   | 79:s2:1385:G:N1    | 2.11                     | 0.81              |
| 85:L5:4101:C:C2'   | 85:L5:4106:G:H1'   | 2.11                     | 0.81              |
| 10:sA:85:ARG:NH1   | 10:sA:203:PHE:O    | 2.14                     | 0.81              |
| 22:1A:204:MET:HE3  | 22:1A:205:ASN:H    | 1.45                     | 0.81              |
| 80:CB:610:PRO:HG2  | 80:CB:613:LEU:HD11 | 1.61                     | 0.81              |
| 12:sH:133:LEU:HD21 | 12:sH:173:PHE:HB3  | 1.61                     | 0.81              |
| 64:sR:32:LYS:HG3   | 79:s2:1454:A:H4'   | 1.61                     | 0.81              |
| 85:L5:4907:G:N2    | 85:L5:4914:C:O2    | 2.12                     | 0.81              |
| 70:SS:17:ASN:OD1   | 70:SS:101:ASN:ND2  | 2.12                     | 0.81              |
| 27:1F:147:LEU:HD21 | 85:l5:943:A:N7     | 1.94                     | 0.81              |
| 45:lZ:88:ASP:OD2   | 45:lZ:121:ARG:NH2  | 2.13                     | 0.81              |
| 68:sP:28:MET:CE    | 68:sP:32:GLN:HG2   | 2.11                     | 0.81              |
| 79:s2:191:A:OP2    | 79:s2:208:G:N2     | 2.12                     | 0.81              |
| 80:CB:374:GLU:HG2  | 80:CB:495:ARG:HG3  | 1.62                     | 0.81              |
| 24:lC:109:ARG:NH2  | 85:l5:2343:G:OP2   | 2.14                     | 0.81              |
| 85:L5:1975:G:N2    | 85:L5:1983:A:OP1   | 2.13                     | 0.81              |
| 24:LC:331:TYR:CE1  | 24:LC:335:MET:HE1  | 2.16                     | 0.81              |
| 79:S2:928:G:H2'    | 79:S2:929:G:C8     | 2.16                     | 0.81              |
| 79:S2:1396:A:N7    | 79:S2:1449:G:O6    | 2.12                     | 0.81              |
| 16:sN:78:LYS:HG3   | 16:sN:80:LEU:HD23  | 1.63                     | 0.81              |
| 85:l5:4887:C:H42   | 85:l5:4932:U:H3    | 1.28                     | 0.81              |
| 16:SN:121:ARG:NH1  | 79:S2:925:G:OP1    | 2.14                     | 0.81              |
| 6:sG:144:LEU:O     | 87:1W:94:ARG:NH1   | 2.14                     | 0.80              |
| 73:sc:10:LYS:HE3   | 73:sc:34:PHE:HB3   | 1.62                     | 0.80              |
| 85:L5:4568:A:H2    | 36:LP:69:ARG:HH22  | 1.26                     | 0.80              |
| 85:L5:2601:A:N6    | 85:L5:2744:A:OP2   | 2.14                     | 0.80              |
| 79:S2:924:G:H1     | 79:S2:1018:U:H3    | 0.82                     | 0.80              |
| 7:sJ:134:HIS:NE2   | 79:s2:561:A:O2'    | 2.13                     | 0.80              |
| 11:sB:196:ASP:HA   | 11:sB:199:LYS:HG2  | 1.63                     | 0.80              |
| 23:lB:242:ARG:NH2  | 85:l5:2856:C:O2    | 2.14                     | 0.80              |
| 39:IS:29:ARG:HB2   | 40:lT:148:PRO:HB2  | 1.63                     | 0.80              |
| 85:l5:963:G:O6     | 85:l5:2095:A:N6    | 2.14                     | 0.80              |
| 85:l5:2318:G:N2    | 85:l5:2321:G:OP2   | 2.15                     | 0.80              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 85:l5:3971:G:N2    | 85:l5:3973:G:N3    | 2.29                     | 0.80              |
| 40:LT:14:MET:SD    | 40:LT:58:HIS:ND1   | 2.53                     | 0.80              |
| 79:S2:532:C:H42    | 79:S2:551:U:H3     | 1.28                     | 0.80              |
| 33:lM:118:MET:HE1  | 35:lO:192:TYR:CZ   | 2.17                     | 0.80              |
| 66:sF:127:ARG:HB3  | 66:sF:135:ARG:HH21 | 1.47                     | 0.80              |
| 79:s2:1406:G:N2    | 79:s2:1442:U:O4    | 2.14                     | 0.80              |
| 54:Li:60:LEU:HD22  | 54:Li:69:ALA:HB2   | 1.62                     | 0.80              |
| 15:sC:75:ILE:HB    | 15:sC:269:PHE:HE1  | 1.47                     | 0.80              |
| 26:lE:226:ARG:HH21 | 85:l5:695:G:H5''   | 1.46                     | 0.80              |
| 27:lF:175:ILE:HG21 | 27:lF:190:LEU:HD11 | 1.61                     | 0.80              |
| 56:lK:9:LYS:HE3    | 56:lK:13:LEU:HD23  | 1.64                     | 0.80              |
| 85:L5:1072:C:N3    | 85:L5:1240:G:N1    | 2.27                     | 0.80              |
| 24:lC:297:GLU:N    | 24:lC:297:GLU:OE1  | 2.13                     | 0.80              |
| 67:sK:65:ARG:NH2   | 74:sd:21:CYS:O     | 2.14                     | 0.80              |
| 6:SG:79:LYS:HB2    | 6:SG:86:PRO:HG3    | 1.64                     | 0.80              |
| 23:LB:14:LEU:HD23  | 23:LB:17:LEU:HD21  | 1.62                     | 0.80              |
| 63:Lz:206:ILE:H    | 63:Lz:215:ARG:HH12 | 1.28                     | 0.80              |
| 76:SM:28:HIS:HE1   | 76:SM:116:LYS:HZ3  | 1.27                     | 0.80              |
| 13:sV:15:ARG:NH2   | 15:sC:84:PHE:HA    | 1.96                     | 0.80              |
| 42:lV:123:LYS:HA   | 42:lV:139:ILE:HD11 | 1.64                     | 0.80              |
| 43:IX:93:ASN:ND2   | 85:l5:2532:C:O2'   | 2.15                     | 0.80              |
| 46:la:79:TRP:HB3   | 46:la:87:ARG:NH2   | 1.95                     | 0.80              |
| 66:sF:33:ILE:HA    | 66:sF:36:GLN:HG2   | 1.62                     | 0.80              |
| 77:sZ:46:ASN:HB2   | 77:sZ:78:LYS:HD2   | 1.64                     | 0.80              |
| 80:CB:4:PHE:N      | 80:CB:45:ILE:O     | 2.15                     | 0.80              |
| 14:Sa:7:ASN:HD21   | 14:Sa:11:ALA:HA    | 1.47                     | 0.80              |
| 51:Lf:70:ILE:HD11  | 51:Lf:90:SER:H     | 1.45                     | 0.80              |
| 69:SQ:86:GLN:NE2   | 69:SQ:118:THR:O    | 2.15                     | 0.80              |
| 71:ST:22:LEU:HB3   | 71:ST:28:LEU:HD21  | 1.63                     | 0.80              |
| 79:S2:508:A:H3'    | 79:S2:509:G:H8     | 1.45                     | 0.80              |
| 29:lH:106:GLN:HG3  | 29:lH:107:GLU:OE1  | 1.82                     | 0.80              |
| 75:sg:17:TRP:H     | 75:sg:36:ARG:HB2   | 1.45                     | 0.80              |
| 79:s2:1335:G:N2    | 79:s2:1495:G:O6    | 2.11                     | 0.80              |
| 81:AP:18:G:O6      | 81:AP:55:U:O2      | 2.00                     | 0.80              |
| 85:l5:1984:A:N7    | 85:l5:2010:A:O2'   | 2.15                     | 0.80              |
| 85:l5:4093:G:N7    | 85:l5:4095:G:N2    | 2.30                     | 0.80              |
| 21:L8:83:C:H42     | 44:LY:50:ARG:HH22  | 1.30                     | 0.80              |
| 22:LA:24:LYS:HD3   | 22:LA:49:ILE:HD12  | 1.64                     | 0.80              |
| 30:LI:188:LYS:HE3  | 30:LI:212:LEU:HD22 | 1.63                     | 0.80              |
| 4:sL:128:VAL:C     | 4:sL:140:PHE:CE1   | 2.57                     | 0.80              |
| 6:SG:131:ARG:HH12  | 87:LW:80:ARG:HD3   | 1.47                     | 0.80              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 12:SH:144:ILE:O   | 12:SH:145:ARG:NH1  | 2.15                     | 0.80              |
| 76:SM:58:GLU:HG3  | 76:SM:60:MET:SD    | 2.22                     | 0.80              |
| 11:sB:146:ARG:HG2 | 64:sR:135:VAL:HG22 | 1.65                     | 0.79              |
| 15:sC:113:GLN:C   | 15:sC:114:LYS:HD3  | 2.06                     | 0.79              |
| 31:lJ:16:ARG:HH12 | 31:lJ:18:ARG:HG3   | 1.46                     | 0.79              |
| 71:sT:105:GLN:NE2 | 79:s2:1564:C:OP1   | 2.14                     | 0.79              |
| 85:l5:1401:C:N3   | 85:l5:1416:G:N1    | 2.29                     | 0.79              |
| 85:l5:2557:G:N2   | 85:l5:2570:U:O2    | 2.15                     | 0.79              |
| 47:Lb:57:MET:SD   | 47:Lb:57:MET:N     | 2.54                     | 0.79              |
| 26:lE:281:ILE:HB  | 26:lE:286:LEU:HD21 | 1.65                     | 0.79              |
| 29:lH:173:ARG:HA  | 58:lm:90:ASN:HD21  | 1.47                     | 0.79              |
| 41:lU:45:GLU:HA   | 41:lU:54:GLY:HA2   | 1.62                     | 0.79              |
| 78:sf:138:ARG:NH1 | 79:s2:1292:C:O2    | 2.14                     | 0.79              |
| 80:cB:85:ASP:HA   | 80:cB:88:PHE:HB2   | 1.64                     | 0.79              |
| 80:cB:596:PRO:HB2 | 80:cB:720:GLN:HE22 | 1.47                     | 0.79              |
| 5:SX:63:ASN:OD1   | 79:S2:624:C:N4     | 2.15                     | 0.79              |
| 15:SC:94:ILE:HD11 | 15:SC:159:LYS:HB3  | 1.64                     | 0.79              |
| 77:SZ:98:LYS:NZ   | 77:SZ:111:ARG:O    | 2.16                     | 0.79              |
| 75:sg:29:ASP:OD2  | 75:sg:47:ARG:NH1   | 2.15                     | 0.79              |
| 85:l5:493:G:O6    | 85:l5:660:A:N1     | 2.16                     | 0.79              |
| 85:l5:3708:C:O2   | 85:l5:3742:G:N2    | 2.11                     | 0.79              |
| 85:L5:286:U:H3    | 85:L5:301:G:H1     | 1.29                     | 0.79              |
| 85:L5:1095:A:N1   | 85:L5:1200:G:O6    | 2.15                     | 0.79              |
| 69:SQ:43:GLU:O    | 69:SQ:45:ARG:N     | 2.15                     | 0.79              |
| 66:sF:172:CYS:O   | 66:sF:176:GLU:HG3  | 1.81                     | 0.79              |
| 85:L5:3708:C:N3   | 85:L5:3742:G:N1    | 2.31                     | 0.79              |
| 40:LT:112:ASN:HA  | 40:LT:115:LYS:HZ1  | 1.44                     | 0.79              |
| 4:sL:90:ARG:HH21  | 4:sL:109:MET:HE1   | 1.46                     | 0.79              |
| 34:lN:123:GLU:OE2 | 34:lN:123:GLU:N    | 2.14                     | 0.79              |
| 73:sc:49:PRO:O    | 73:sc:51:ARG:NH1   | 2.15                     | 0.79              |
| 79:s2:563:G:O6    | 79:s2:592:C:N4     | 2.16                     | 0.79              |
| 85:L5:1728:U:H5'  | 27:LF:127:LYS:HZ1  | 1.47                     | 0.79              |
| 85:L5:4334:U:H4'  | 40:LT:7:LYS:HB2    | 1.64                     | 0.79              |
| 1:cH:43:LYS:HG3   | 1:cH:45:ALA:H      | 1.48                     | 0.79              |
| 1:cH:121:LEU:HD11 | 1:cH:133:ARG:HD3   | 1.64                     | 0.79              |
| 20:l7:61:G:H5''   | 25:ID:271:MET:CE   | 2.11                     | 0.79              |
| 67:sK:28:HIS:CG   | 74:sd:8:TRP:HE1    | 2.01                     | 0.79              |
| 85:L5:74:G:H5''   | 32:LL:59:VAL:HB    | 1.62                     | 0.79              |
| 85:L5:308:G:OP2   | 85:L5:308:G:N2     | 2.14                     | 0.79              |
| 28:LG:29:ASN:HD21 | 28:LG:31:LEU:HB3   | 1.48                     | 0.79              |
| 45:LZ:68:ILE:HD11 | 45:LZ:118:PHE:HB3  | 1.65                     | 0.79              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 28:lG:110:LYS:NZ   | 85:l5:119:G:O2'    | 2.15                     | 0.79              |
| 36:lP:94:MET:HG3   | 36:lP:148:MET:HE1  | 1.63                     | 0.79              |
| 42:IV:90:ARG:HH22  | 42:IV:123:LYS:HG2  | 1.48                     | 0.79              |
| 50:le:102:ASN:HD22 | 85:l5:2307:A:H5''  | 1.47                     | 0.79              |
| 80:cB:228:PHE:HA   | 80:cB:231:MET:SD   | 2.23                     | 0.79              |
| 85:l5:4238:G:H2'   | 85:l5:4239:A:H8    | 1.47                     | 0.79              |
| 10:SA:30:LEU:HD11  | 10:SA:34:MET:HB2   | 1.63                     | 0.79              |
| 85:L5:4985:U:O2    | 23:LB:174:ARG:NH2  | 2.16                     | 0.79              |
| 71:ST:134:ILE:HA   | 71:ST:137:GLN:OE1  | 1.83                     | 0.79              |
| 1:CH:65:THR:HG23   | 65:SD:94:ARG:HH12  | 1.46                     | 0.79              |
| 24:lC:325:MET:HE1  | 27:lF:155:TYR:CE1  | 2.18                     | 0.79              |
| 27:lF:182:TYR:HB3  | 27:lF:200:ARG:HG3  | 1.64                     | 0.79              |
| 33:lM:118:MET:HE1  | 35:lO:192:TYR:CE2  | 2.18                     | 0.79              |
| 69:sQ:31:LEU:HD21  | 69:sQ:69:ARG:HE    | 1.46                     | 0.79              |
| 74:sd:10:HIS:NE2   | 79:s2:1261:C:O2    | 2.15                     | 0.79              |
| 80:cB:627:GLU:OE1  | 80:cB:629:LYS:HG2  | 1.82                     | 0.79              |
| 85:L5:2386:U:H2'   | 85:L5:2387:G:H8    | 1.45                     | 0.79              |
| 35:LO:42:ASN:HD21  | 35:LO:135:PHE:HD2  | 1.31                     | 0.79              |
| 22:lA:33:ASP:OD1   | 22:lA:34:PHE:N     | 2.15                     | 0.79              |
| 24:lC:80:ARG:NH2   | 85:l5:1646:A:OP2   | 2.16                     | 0.79              |
| 52:lg:24:ARG:HH22  | 85:l5:2639:U:H5'   | 1.48                     | 0.79              |
| 75:sg:7:LEU:HD11   | 75:sg:308:ARG:HB2  | 1.64                     | 0.79              |
| 82:pE:42:G:H2'     | 82:pE:43:A:C8      | 2.17                     | 0.79              |
| 84:lt:105:THR:HA   | 84:lt:143:VAL:HA   | 1.64                     | 0.79              |
| 85:l5:1402:C:N3    | 85:l5:1415:G:N1    | 2.29                     | 0.79              |
| 7:SJ:84:ILE:O      | 7:SJ:108:ARG:NH2   | 2.16                     | 0.79              |
| 16:SN:63:VAL:HG11  | 16:SN:71:ILE:HG23  | 1.63                     | 0.79              |
| 85:L5:369:G:N2     | 85:L5:372:A:OP2    | 2.16                     | 0.79              |
| 75:Sg:163:PRO:HB2  | 75:Sg:179:LEU:HG   | 1.62                     | 0.79              |
| 79:S2:1033:G:H1    | 79:S2:1080:A:HO2'  | 1.29                     | 0.79              |
| 5:sX:5:ARG:NH2     | 79:s2:1157:G:O4'   | 2.16                     | 0.79              |
| 8:sY:29:HIS:HB2    | 8:sY:32:LYS:HB2    | 1.65                     | 0.79              |
| 39:lS:154:LEU:HB3  | 39:lS:157:ARG:HD3  | 1.64                     | 0.79              |
| 42:IV:84:GLN:H     | 42:IV:98:PHE:HD2   | 1.31                     | 0.79              |
| 53:lh:97:LYS:H     | 53:lh:97:LYS:HZ3   | 1.29                     | 0.79              |
| 85:l5:1709:C:N4    | 85:l5:1716:G:N2    | 2.29                     | 0.79              |
| 85:L5:370:U:HO2'   | 55:Lj:16:HIS:HD1   | 1.26                     | 0.79              |
| 22:LA:229:ALA:HB3  | 22:LA:234:LYS:HB3  | 1.64                     | 0.79              |
| 39:LS:51:LEU:HD12  | 40:LT:151:LEU:HD12 | 1.64                     | 0.79              |
| 50:Le:90:MET:HA    | 50:Le:90:MET:HE3   | 1.65                     | 0.79              |
| 23:lB:224:LYS:HG2  | 23:lB:340:THR:HG22 | 1.65                     | 0.78              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 79:s2:1374:C:O2'  | 79:s2:1464:C:O2'   | 2.00                     | 0.78              |
| 80:cB:223:PHE:HB3 | 80:cB:344:LEU:HD13 | 1.65                     | 0.78              |
| 80:cB:254:GLU:O   | 80:cB:257:MET:HG3  | 1.83                     | 0.78              |
| 82:pE:26:A:H61    | 82:pE:44:G:H1      | 0.83                     | 0.78              |
| 85:l5:4129:G:O6   | 85:l5:4156:G:N2    | 2.16                     | 0.78              |
| 85:L5:4517:A:N7   | 23:LB:2:SER:N      | 2.30                     | 0.78              |
| 31:LJ:42:GLN:HE21 | 31:LJ:117:ILE:HD13 | 1.48                     | 0.78              |
| 16:sN:34:LYS:HZ3  | 16:sN:38:TYR:HE2   | 1.32                     | 0.78              |
| 16:sN:63:VAL:HG11 | 16:sN:71:ILE:HG23  | 1.65                     | 0.78              |
| 21:l8:21:C:O2     | 85:l5:379:G:N2     | 2.17                     | 0.78              |
| 29:lH:96:TYR:HE2  | 29:lH:142:ASP:OD2  | 1.65                     | 0.78              |
| 68:sP:28:MET:HE2  | 68:sP:32:GLN:HG2   | 1.65                     | 0.78              |
| 85:L5:513:U:H3'   | 85:L5:514:U:H4'    | 1.66                     | 0.78              |
| 47:Lb:43:MET:N    | 47:Lb:43:MET:SD    | 2.56                     | 0.78              |
| 79:S2:532:C:H2'   | 79:S2:533:A:H8     | 1.47                     | 0.78              |
| 66:sF:60:ARG:HD2  | 79:s2:1679:A:H2'   | 1.65                     | 0.78              |
| 66:sF:84:GLY:O    | 79:s2:1673:U:O2'   | 2.01                     | 0.78              |
| 79:s2:329:G:H2'   | 79:s2:330:G:H8     | 1.48                     | 0.78              |
| 85:l5:1709:C:H42  | 85:l5:1716:G:N2    | 1.79                     | 0.78              |
| 7:SJ:107:GLU:OE2  | 7:SJ:108:ARG:NH1   | 2.16                     | 0.78              |
| 11:SB:107:ARG:NH1 | 17:SO:133:THR:O    | 2.16                     | 0.78              |
| 76:SM:84:LYS:HG3  | 76:SM:88:TRP:CZ2   | 2.18                     | 0.78              |
| 26:lE:284:HIS:ND1 | 51:lF:42:TYR:OH    | 2.16                     | 0.78              |
| 76:sM:124:ILE:HA  | 76:sM:127:TYR:CD2  | 2.19                     | 0.78              |
| 85:l5:4992:G:H2'  | 85:l5:4993:G:C8    | 2.18                     | 0.78              |
| 18:SW:37:PHE:HE1  | 18:SW:41:MET:HE2   | 1.48                     | 0.78              |
| 85:L5:4101:C:H2'  | 85:L5:4106:G:C8    | 2.18                     | 0.78              |
| 85:L5:4686:G:OP2  | 58:Lm:112:LYS:NZ   | 2.15                     | 0.78              |
| 41:LU:19:LEU:HB2  | 41:LU:73:THR:HB    | 1.65                     | 0.78              |
| 44:LY:100:HIS:HD2 | 44:LY:102:SER:H    | 1.31                     | 0.78              |
| 36:lP:14:SER:HB3  | 36:lP:151:THR:HG22 | 1.63                     | 0.78              |
| 63:lz:33:GLU:HG3  | 63:lz:168:ALA:HA   | 1.65                     | 0.78              |
| 85:l5:3950:U:H2'  | 85:l5:3951:G:C8    | 2.19                     | 0.78              |
| 85:L5:102:G:OP1   | 32:LL:71:ARG:NH1   | 2.16                     | 0.78              |
| 65:SD:127:MET:SD  | 65:SD:127:MET:N    | 2.57                     | 0.78              |
| 69:SQ:43:GLU:OE1  | 69:SQ:80:GLN:NE2   | 2.16                     | 0.78              |
| 12:sH:148:LEU:HG  | 18:sW:49:GLU:OE1   | 1.83                     | 0.78              |
| 26:lE:270:TYR:CZ  | 33:lM:107:PHE:HA   | 2.18                     | 0.78              |
| 79:s2:835:C:H5'   | 79:s2:836:G:H5'    | 1.66                     | 0.78              |
| 8:SY:34:THR:O     | 79:S2:570:C:O2'    | 2.02                     | 0.78              |
| 85:L5:450:G:H1    | 85:L5:1297:U:H3    | 1.31                     | 0.78              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 85:L5:4101:C:H3'  | 85:L5:4106:G:O2'   | 1.82                     | 0.78              |
| 21:l8:145:C:O2    | 85:l5:11:G:N2      | 2.14                     | 0.78              |
| 24:lC:110:ARG:O   | 24:lC:113:ARG:NH1  | 2.17                     | 0.78              |
| 26:lE:94:LYS:HD3  | 26:lE:107:VAL:HG21 | 1.66                     | 0.78              |
| 26:lE:118:THR:CB  | 50:le:90:MET:HE1   | 2.12                     | 0.78              |
| 34:lN:191:ALA:O   | 34:lN:195:ARG:HG2  | 1.84                     | 0.78              |
| 66:sF:103:LEU:HA  | 77:sZ:66:LYS:HZ3   | 1.47                     | 0.78              |
| 85:l5:2906:G:H1'  | 85:l5:2908:U:H1'   | 1.65                     | 0.78              |
| 85:L5:1517:G:H1   | 24:LC:104:PRO:HD2  | 1.48                     | 0.78              |
| 66:SF:84:GLY:O    | 79:S2:1673:U:O2'   | 2.00                     | 0.78              |
| 2:sE:152:PRO:HG2  | 6:sG:216:ARG:HG2   | 1.63                     | 0.78              |
| 9:se:40:ARG:O     | 9:se:44:ASN:ND2    | 2.16                     | 0.78              |
| 35:lO:62:MET:HG2  | 35:lO:69:GLY:HA2   | 1.65                     | 0.78              |
| 40:lT:144:ASN:HB2 | 40:lT:146:LYS:HE2  | 1.65                     | 0.78              |
| 65:sD:127:MET:HA  | 65:sD:127:MET:HE3  | 1.66                     | 0.78              |
| 80:cB:350:LEU:O   | 80:cB:354:ILE:HG23 | 1.83                     | 0.78              |
| 85:l5:1974:U:H4'  | 85:l5:1975:G:H3'   | 1.65                     | 0.78              |
| 15:SC:187:ARG:NH2 | 15:SC:189:GLY:O    | 2.17                     | 0.78              |
| 85:L5:502:C:H3'   | 85:L5:503:C:H3'    | 1.66                     | 0.78              |
| 85:L5:909:A:C6    | 85:L5:910:G:O6     | 2.37                     | 0.78              |
| 71:ST:13:GLU:HA   | 71:ST:16:ARG:HE    | 1.49                     | 0.78              |
| 5:sX:22:TRP:HH2   | 79:s2:359:U:H5''   | 1.49                     | 0.78              |
| 20:l7:39:C:H1'    | 31:lJ:46:GLN:HE22  | 1.49                     | 0.78              |
| 42:IV:90:ARG:HH12 | 42:IV:123:LYS:HB3  | 1.49                     | 0.78              |
| 79:s2:804:U:H3    | 79:s2:859:G:H1     | 1.32                     | 0.78              |
| 80:CB:43:ALA:CB   | 80:CB:79:TYR:HE2   | 1.97                     | 0.78              |
| 85:L5:1534:A:H1'  | 55:Lj:11:ARG:HE    | 1.48                     | 0.78              |
| 33:LM:104:MET:SD  | 33:LM:105:THR:N    | 2.57                     | 0.78              |
| 59:ln:1:MET:HE1   | 79:s2:1852:C:OP2   | 1.84                     | 0.78              |
| 60:lo:99:ARG:NH1  | 60:lo:102:GLN:HB2  | 1.98                     | 0.78              |
| 69:sQ:14:GLY:HA3  | 69:sQ:86:GLN:HE22  | 1.49                     | 0.78              |
| 85:l5:909:A:C6    | 85:l5:910:G:O6     | 2.37                     | 0.78              |
| 29:LH:93:ARG:NH1  | 29:LH:143:GLU:OE1  | 2.16                     | 0.78              |
| 34:LN:124:ASP:HB3 | 34:LN:127:TYR:H    | 1.48                     | 0.78              |
| 4:sL:79:LYS:NZ    | 79:s2:396:U:OP2    | 2.15                     | 0.77              |
| 79:s2:1748:G:H1   | 79:s2:1786:U:H3    | 0.80                     | 0.77              |
| 85:L5:184:U:O2    | 85:L5:254:G:N1     | 2.17                     | 0.77              |
| 85:L5:3708:C:O2   | 85:L5:3742:G:N2    | 2.14                     | 0.77              |
| 85:L5:4102:C:N3   | 85:L5:4105:A:C8    | 2.53                     | 0.77              |
| 20:L7:114:U:H4'   | 25:LD:73:MET:HE1   | 1.65                     | 0.77              |
| 24:LC:25:PRO:HD2  | 24:LC:28:PHE:HE2   | 1.49                     | 0.77              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:LJ:108:GLY:HA2  | 31:LJ:129:ASP:HA   | 1.66                     | 0.77              |
| 75:Sg:125:ARG:HD2  | 75:Sg:150:TRP:CD2  | 2.19                     | 0.77              |
| 33:IM:136:LEU:HD12 | 33:IM:137:LYS:HZ2  | 1.49                     | 0.77              |
| 45:IZ:46:ILE:HD13  | 45:IZ:68:ILE:HD12  | 1.66                     | 0.77              |
| 54:Li:55:ARG:HA    | 54:Li:58:MET:HG3   | 1.65                     | 0.77              |
| 66:SF:126:THR:HA   | 66:SF:135:ARG:HG3  | 1.66                     | 0.77              |
| 12:sH:24:SER:HA    | 12:sH:27:LEU:HD12  | 1.64                     | 0.77              |
| 12:SH:143:ARG:HB2  | 12:SH:155:LYS:HG3  | 1.66                     | 0.77              |
| 85:L5:1336:G:H1'   | 24:LC:95:MET:CE    | 2.09                     | 0.77              |
| 85:L5:1511:U:H2'   | 85:L5:1512:G:H8    | 1.48                     | 0.77              |
| 30:LI:70:ILE:HG22  | 30:LI:74:LYS:HZ2   | 1.48                     | 0.77              |
| 57:Ll:9:ILE:HG23   | 57:Ll:51:LEU:HD21  | 1.66                     | 0.77              |
| 65:SD:42:THR:OG1   | 65:SD:45:ARG:O     | 2.01                     | 0.77              |
| 78:sf:95:ARG:NH2   | 79:s2:1306:U:O4    | 2.17                     | 0.77              |
| 79:s2:1488:C:O2'   | 79:s2:1490:G:OP2   | 2.02                     | 0.77              |
| 80:cB:153:PRO:HD2  | 80:cB:203:ILE:HD11 | 1.66                     | 0.77              |
| 85:l5:1100:U:H3    | 85:l5:1194:G:H1    | 1.33                     | 0.77              |
| 85:l5:3708:C:N3    | 85:l5:3742:G:N1    | 2.31                     | 0.77              |
| 12:SH:44:ASN:O     | 12:SH:68:GLN:NE2   | 2.16                     | 0.77              |
| 30:LI:52:MET:HE1   | 30:LI:165:ILE:HA   | 1.65                     | 0.77              |
| 68:sP:48:GLY:O     | 68:sP:50:ARG:NH1   | 2.16                     | 0.77              |
| 69:sQ:62:ARG:HH21  | 69:sQ:92:LEU:HD21  | 1.50                     | 0.77              |
| 69:sQ:146:ARG:NH2  | 82:pE:35:U:OP2     | 2.17                     | 0.77              |
| 85:l5:1269:G:H1    | 85:l5:2106:G:H1'   | 1.49                     | 0.77              |
| 80:CB:302:ASP:HA   | 80:CB:305:MET:HE3  | 1.65                     | 0.77              |
| 25:LD:89:LYS:HE2   | 25:LD:229:ASN:HB3  | 1.64                     | 0.77              |
| 14:sa:27:ALA:HA    | 17:sO:142:ARG:HH22 | 1.49                     | 0.77              |
| 15:sC:62:PRO:HG2   | 15:sC:68:ARG:HE    | 1.48                     | 0.77              |
| 79:s2:647:U:H2'    | 79:s2:648:A:H8     | 1.49                     | 0.77              |
| 80:cB:337:LYS:CB   | 80:cB:341:ARG:HH12 | 1.97                     | 0.77              |
| 85:l5:2601:A:N6    | 85:l5:2744:A:OP2   | 2.17                     | 0.77              |
| 85:L5:4102:C:H3'   | 85:L5:4106:G:C2'   | 2.10                     | 0.77              |
| 3:sI:190:LEU:HB3   | 3:sI:195:LEU:HD23  | 1.66                     | 0.77              |
| 4:sL:78:THR:HB     | 4:sL:87:VAL:HG23   | 1.65                     | 0.77              |
| 31:IJ:32:ARG:NH2   | 31:IJ:35:ARG:HD3   | 2.00                     | 0.77              |
| 32:IL:48:PRO:HB2   | 53:lh:120:ALA:HB2  | 1.67                     | 0.77              |
| 48:lc:51:ASN:OD1   | 48:lc:77:ASN:HB2   | 1.84                     | 0.77              |
| 54:li:4:ARG:NH2    | 85:l5:1482:G:N7    | 2.32                     | 0.77              |
| 66:sF:122:ARG:HG3  | 73:sc:59:LEU:HD11  | 1.66                     | 0.77              |
| 68:sP:33:LEU:HD12  | 68:sP:36:LEU:HB2   | 1.66                     | 0.77              |
| 70:sS:13:LEU:HB2   | 70:sS:20:ILE:HG23  | 1.67                     | 0.77              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 85:l5:1414:C:H2'   | 85:l5:1415:G:H8    | 1.47                     | 0.77              |
| 85:l5:4773:C:N3    | 85:l5:4861:G:N1    | 2.27                     | 0.77              |
| 10:SA:58:LEU:HD21  | 10:SA:181:GLU:HG3  | 1.65                     | 0.77              |
| 85:L5:1977:C:H5''  | 84:Lt:57:ARG:NH2   | 2.00                     | 0.77              |
| 85:L5:2461:G:H4'   | 34:LN:108:ARG:HH22 | 1.50                     | 0.77              |
| 84:Lt:141:CYS:SG   | 84:Lt:142:ASN:N    | 2.58                     | 0.77              |
| 6:sG:190:ARG:HH12  | 79:s2:333:G:H3'    | 1.49                     | 0.77              |
| 9:se:56:ASN:ND2    | 79:s2:637:U:O2'    | 2.18                     | 0.77              |
| 28:lG:73:ARG:NH1   | 85:l5:4076:G:OP1   | 2.17                     | 0.77              |
| 85:L5:1377:G:H4'   | 85:L5:1378:C:H3'   | 1.67                     | 0.77              |
| 85:L5:2906:G:H1'   | 85:L5:2908:U:H1'   | 1.67                     | 0.77              |
| 43:LX:108:GLN:HA   | 43:LX:111:GLN:NE2  | 2.00                     | 0.77              |
| 74:Sd:21:CYS:SG    | 74:Sd:38:MET:HG2   | 2.24                     | 0.77              |
| 27:lF:151:ASN:HD21 | 85:l5:943:A:H62    | 1.31                     | 0.77              |
| 79:s2:861:A:O2'    | 79:s2:862:A:N7     | 2.18                     | 0.77              |
| 85:L5:4103:C:H5''  | 85:L5:4106:G:H3'   | 1.64                     | 0.77              |
| 85:L5:4103:C:H5''  | 85:L5:4106:G:H5'   | 1.65                     | 0.77              |
| 3:sI:10:LYS:NZ     | 79:s2:370:G:O2'    | 2.17                     | 0.77              |
| 11:sB:150:ILE:HD12 | 64:sR:131:PRO:HD2  | 1.67                     | 0.77              |
| 15:sC:182:CYS:HB2  | 18:sW:95:PRO:HB2   | 1.67                     | 0.77              |
| 17:sO:99:ALA:H     | 17:sO:133:THR:HG22 | 1.49                     | 0.77              |
| 27:lF:243:LEU:O    | 27:lF:247:MET:HB2  | 1.85                     | 0.77              |
| 29:lH:14:GLU:N     | 29:lH:14:GLU:OE2   | 2.18                     | 0.77              |
| 52:lg:104:VAL:HA   | 52:lg:107:LEU:HD23 | 1.67                     | 0.77              |
| 64:sR:97:GLU:OE2   | 64:sR:118:GLN:NE2  | 2.18                     | 0.77              |
| 77:sZ:56:ASP:OD2   | 77:sZ:57:LYS:N     | 2.18                     | 0.77              |
| 10:SA:21:ALA:HB2   | 64:SR:91:LEU:HD21  | 1.67                     | 0.77              |
| 10:SA:126:ASP:HB2  | 10:SA:165:ASN:HD22 | 1.49                     | 0.77              |
| 85:L5:2557:G:N2    | 85:L5:2570:U:O2    | 2.17                     | 0.77              |
| 34:LN:143:ARG:HH21 | 53:Lh:95:LEU:HD23  | 1.49                     | 0.77              |
| 63:Lz:102:LYS:HE2  | 63:Lz:106:LYS:HD2  | 1.65                     | 0.77              |
| 70:SS:86:ARG:HH22  | 79:S2:1611:G:H4'   | 1.50                     | 0.77              |
| 11:sB:117:TRP:HB3  | 11:sB:153:THR:HA   | 1.67                     | 0.76              |
| 32:lL:121:ARG:O    | 32:lL:121:ARG:NH1  | 2.18                     | 0.76              |
| 79:s2:830:A:OP2    | 79:s2:846:G:N2     | 2.16                     | 0.76              |
| 80:cB:153:PRO:CD   | 80:cB:203:ILE:HD11 | 2.15                     | 0.76              |
| 85:l5:2386:U:H2'   | 85:l5:2387:G:H8    | 1.48                     | 0.76              |
| 80:CB:42:LYS:CE    | 80:CB:347:GLY:H    | 1.98                     | 0.76              |
| 80:CB:122:THR:O    | 80:CB:368:ARG:NH2  | 2.18                     | 0.76              |
| 79:S2:557:U:H5'    | 79:S2:558:G:C8     | 2.20                     | 0.76              |
| 8:sY:36:PRO:HG3    | 79:s2:570:C:H4'    | 1.66                     | 0.76              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 15:sC:230:THR:HG21 | 79:s2:4:C:H5'      | 1.68                     | 0.76              |
| 24:lC:155:GLU:HG3  | 24:lC:157:LYS:HE2  | 1.66                     | 0.76              |
| 28:lG:34:LYS:HE3   | 85:l5:4129:G:C1'   | 2.14                     | 0.76              |
| 36:lP:69:ARG:HH21  | 85:l5:3893:C:H1'   | 1.51                     | 0.76              |
| 85:l5:4629:U:O2'   | 87:lW:19:ARG:NH1   | 2.18                     | 0.76              |
| 15:SC:171:GLY:HA2  | 18:SW:98:GLN:HE22  | 1.49                     | 0.76              |
| 85:L5:49:U:OP2     | 34:LN:189:ARG:NH1  | 2.17                     | 0.76              |
| 85:L5:1401:C:N3    | 85:L5:1416:G:N1    | 2.28                     | 0.76              |
| 85:L5:2749:C:H2'   | 85:L5:2750:G:H8    | 1.49                     | 0.76              |
| 31:LJ:63:ARG:HH12  | 60:Lo:103:VAL:HG13 | 1.50                     | 0.76              |
| 26:lE:181:LEU:O    | 85:l5:4883:C:N4    | 2.14                     | 0.76              |
| 59:ln:1:MET:HE3    | 59:ln:2:ARG:N      | 2.00                     | 0.76              |
| 68:sP:89:MET:H     | 68:sP:89:MET:HE3   | 1.51                     | 0.76              |
| 80:CB:613:LEU:H    | 80:CB:613:LEU:HD12 | 1.50                     | 0.76              |
| 15:SC:271:ASP:O    | 15:SC:275:LYS:HG2  | 1.84                     | 0.76              |
| 85:L5:1406:G:H1    | 85:L5:1411:C:HO2'  | 1.31                     | 0.76              |
| 85:L5:4101:C:C6    | 85:L5:4105:A:P     | 2.77                     | 0.76              |
| 85:L5:4872:G:OP2   | 33:LM:94:LYS:NZ    | 2.18                     | 0.76              |
| 23:LB:216:MET:SD   | 23:LB:281:ASN:HA   | 2.24                     | 0.76              |
| 60:Lo:11:PHE:O     | 60:Lo:81:ARG:NH2   | 2.19                     | 0.76              |
| 62:Lr:8:MET:HA     | 62:Lr:11:ARG:HB2   | 1.67                     | 0.76              |
| 34:lN:150:TRP:CE3  | 85:l5:332:C:H5'    | 2.20                     | 0.76              |
| 45:lZ:36:ARG:NH1   | 45:lZ:38:TYR:OH    | 2.19                     | 0.76              |
| 64:sR:29:HIS:N     | 79:s2:1455:A:O5'   | 2.19                     | 0.76              |
| 85:l5:513:U:H3'    | 85:l5:514:U:H4'    | 1.66                     | 0.76              |
| 85:l5:1440:U:H3    | 85:l5:2105:A:H2    | 1.33                     | 0.76              |
| 85:l5:1916:G:N2    | 85:l5:2067:C:O2    | 2.18                     | 0.76              |
| 80:CB:43:ALA:HB3   | 80:CB:77:LEU:HD21  | 1.67                     | 0.76              |
| 59:Ln:1:MET:HE1    | 79:S2:1705:C:O3'   | 1.84                     | 0.76              |
| 79:S2:57:U:O2'     | 79:S2:499:G:N3     | 2.19                     | 0.76              |
| 45:lZ:94:THR:O     | 45:lZ:97:ASN:ND2   | 2.18                     | 0.76              |
| 55:lj:67:LEU:HG    | 55:lj:71:TYR:CE2   | 2.20                     | 0.76              |
| 80:cB:504:VAL:HG23 | 80:cB:812:CYS:HB2  | 1.65                     | 0.76              |
| 85:l5:4894:A:H3'   | 85:l5:4895:C:H5'   | 1.67                     | 0.76              |
| 85:L5:989:U:O2     | 85:L5:1064:G:O6    | 2.03                     | 0.76              |
| 85:L5:1364:U:OP2   | 32:LL:36:ARG:NH2   | 2.18                     | 0.76              |
| 85:L5:1994:C:H2'   | 85:L5:1995:G:H8    | 1.51                     | 0.76              |
| 85:L5:2300:A:N7    | 24:LC:143:ARG:NH1  | 2.32                     | 0.76              |
| 85:L5:4100:C:H3'   | 85:L5:4107:G:H5''  | 1.68                     | 0.76              |
| 85:L5:4101:C:C2    | 85:L5:4106:G:H4'   | 2.20                     | 0.76              |
| 20:L7:92:C:H2'     | 20:L7:93:G:H8      | 1.50                     | 0.76              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:sJ:164:PRO:HG2   | 79:s2:561:A:H5'    | 1.68                     | 0.76              |
| 16:sN:92:ILE:HG21  | 16:sN:149:LEU:HD11 | 1.68                     | 0.76              |
| 22:lA:133:TYR:HB3  | 22:lA:168:VAL:HG23 | 1.67                     | 0.76              |
| 35:lO:18:ARG:HH21  | 35:lO:128:ARG:HH21 | 1.32                     | 0.76              |
| 49:ld:114:PHE:HA   | 49:ld:117:LEU:HD22 | 1.66                     | 0.76              |
| 50:le:90:MET:HA    | 50:le:90:MET:CE    | 2.12                     | 0.76              |
| 64:sR:18:GLU:HG2   | 64:sR:68:GLY:HA2   | 1.66                     | 0.76              |
| 80:cB:290:CYS:HA   | 80:cB:294:LEU:HD13 | 1.68                     | 0.76              |
| 80:cB:670:GLN:O    | 80:cB:673:ASN:ND2  | 2.18                     | 0.76              |
| 12:SH:111:LYS:NZ   | 79:S2:747:U:O2     | 2.19                     | 0.76              |
| 20:L7:61:G:OP2     | 25:LD:270:LYS:NZ   | 2.17                     | 0.76              |
| 61:Lp:38:THR:HG22  | 61:Lp:45:THR:HG22  | 1.68                     | 0.76              |
| 76:SM:52:LEU:HD11  | 76:SM:65:VAL:HG21  | 1.68                     | 0.76              |
| 10:sA:52:LYS:NZ    | 13:sV:82:ASN:O     | 2.18                     | 0.76              |
| 24:lC:143:ARG:HH21 | 85:l5:2300:A:H62   | 1.34                     | 0.76              |
| 64:sR:30:THR:H     | 79:s2:1455:A:C5'   | 1.99                     | 0.76              |
| 85:L5:4676:G:OP1   | 23:LB:281:ASN:ND2  | 2.19                     | 0.76              |
| 26:LE:277:LEU:HB2  | 51:Lf:4:ARG:HB3    | 1.68                     | 0.76              |
| 41:lU:34:MET:HE2   | 41:lU:34:MET:HA    | 1.67                     | 0.76              |
| 56:lk:10:ASP:OD1   | 56:lk:11:PHE:N     | 2.18                     | 0.76              |
| 61:lp:29:ILE:HD11  | 61:lp:69:TRP:CB    | 2.15                     | 0.76              |
| 79:s2:1355:C:H2'   | 79:s2:1356:G:C4    | 2.21                     | 0.76              |
| 80:cB:755:VAL:HG21 | 80:cB:804:THR:HA   | 1.66                     | 0.76              |
| 85:L5:223:G:N3     | 24:LC:223:ASN:ND2  | 2.33                     | 0.76              |
| 85:L5:3848:U:H2'   | 85:L5:3849:A:H8    | 1.50                     | 0.76              |
| 85:L5:4101:C:O5'   | 85:L5:4106:G:O2'   | 2.04                     | 0.76              |
| 27:LF:247:MET:HE2  | 27:LF:247:MET:HA   | 1.68                     | 0.76              |
| 46:La:118:PRO:HG2  | 46:La:120:GLN:HE22 | 1.51                     | 0.76              |
| 53:Lh:105:LYS:HB2  | 53:Lh:108:GLN:NE2  | 1.99                     | 0.76              |
| 63:Lz:55:LEU:H     | 63:Lz:154:THR:HG21 | 1.49                     | 0.76              |
| 79:s2:981:A:H2'    | 79:s2:982:G:C8     | 2.21                     | 0.76              |
| 85:l5:3967:G:N1    | 85:l5:4055:U:N3    | 2.31                     | 0.76              |
| 85:L5:1269:G:H1    | 85:L5:2106:G:H1'   | 1.49                     | 0.76              |
| 26:LE:93:THR:HG22  | 26:LE:106:VAL:HG13 | 1.68                     | 0.76              |
| 60:Lo:21:HIS:CD2   | 60:Lo:70:LEU:HD13  | 2.20                     | 0.76              |
| 73:Sc:31:ARG:HA    | 73:Sc:43:ILE:HA    | 1.67                     | 0.76              |
| 79:S2:887:U:O2     | 79:S2:900:C:N4     | 2.18                     | 0.76              |
| 6:sG:5:ILE:HD11    | 6:sG:14:LYS:HG2    | 1.67                     | 0.76              |
| 7:sJ:93:LYS:HB2    | 7:sJ:96:TYR:CD1    | 2.21                     | 0.76              |
| 35:lO:121:PRO:HA   | 35:lO:124:LEU:HD12 | 1.68                     | 0.76              |
| 52:lg:24:ARG:HG3   | 52:lg:30:ILE:HD13  | 1.67                     | 0.76              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 80:CB:45:ILE:HD13  | 80:CB:78:PHE:HB2   | 1.66                     | 0.76              |
| 80:CB:121:VAL:HG13 | 80:CB:415:ARG:HB2  | 1.68                     | 0.76              |
| 85:L5:3619:G:H22   | 85:L5:3624:A:H1'   | 1.50                     | 0.76              |
| 85:L5:4751:G:N7    | 51:Lf:52:LYS:NZ    | 2.34                     | 0.76              |
| 85:L5:4907:G:N1    | 85:L5:4914:C:N3    | 2.29                     | 0.76              |
| 22:LA:7:GLY:HA2    | 22:LA:10:LYS:HD2   | 1.68                     | 0.76              |
| 32:LL:64:VAL:HA    | 32:LL:67:HIS:CE1   | 2.20                     | 0.76              |
| 79:S2:1652:G:N2    | 79:S2:1672:U:O2    | 2.18                     | 0.76              |
| 6:sG:139:SER:HA    | 6:sG:142:ARG:HE    | 1.50                     | 0.75              |
| 26:lE:223:ARG:NH2  | 26:lE:234:ASP:O    | 2.17                     | 0.75              |
| 33:lM:93:LYS:HA    | 33:lM:96:GLU:HG3   | 1.67                     | 0.75              |
| 38:lR:119:MET:N    | 38:lR:119:MET:SD   | 2.58                     | 0.75              |
| 85:l5:3697:U:H5''  | 85:l5:3698:G:H5'   | 1.69                     | 0.75              |
| 12:SH:191:GLU:O    | 12:SH:193:GLN:NE2  | 2.18                     | 0.75              |
| 14:Sa:6:ARG:NH2    | 79:S2:1148:A:OP2   | 2.17                     | 0.75              |
| 85:L5:364:G:H8     | 55:Lj:56:ARG:HH21  | 1.33                     | 0.75              |
| 85:L5:1969:G:H4'   | 83:Ls:36:GLY:HA2   | 1.67                     | 0.75              |
| 26:LE:224:LYS:NZ   | 26:LE:234:ASP:OD2  | 2.19                     | 0.75              |
| 53:Lh:79:LYS:O     | 53:Lh:84:ARG:NH2   | 2.18                     | 0.75              |
| 70:SS:40:TYR:CE1   | 70:SS:71:MET:HE2   | 2.21                     | 0.75              |
| 3:sI:151:GLU:HA    | 3:sI:154:LYS:HD3   | 1.68                     | 0.75              |
| 6:sG:191:ARG:NH2   | 79:s2:314:U:O4     | 2.19                     | 0.75              |
| 17:sO:13:GLN:HG3   | 17:sO:15:ILE:HA    | 1.68                     | 0.75              |
| 22:lA:217:GLN:NE2  | 85:l5:3819:G:OP2   | 2.20                     | 0.75              |
| 26:lE:241:GLU:N    | 26:lE:241:GLU:OE1  | 2.18                     | 0.75              |
| 31:lJ:121:PRO:HD3  | 70:sS:101:ASN:HB3  | 1.67                     | 0.75              |
| 51:lF:95:LYS:NZ    | 85:l5:1307:A:N3    | 2.35                     | 0.75              |
| 85:L5:4174:U:H2'   | 85:L5:4175:G:H8    | 1.50                     | 0.75              |
| 77:SZ:69:THR:HG22  | 77:SZ:72:VAL:HG12  | 1.67                     | 0.75              |
| 84:Lt:114:ARG:NE   | 84:Lt:130:LYS:HA   | 2.01                     | 0.75              |
| 11:sB:89:GLU:HG3   | 11:sB:228:LEU:HD22 | 1.69                     | 0.75              |
| 64:sR:56:HIS:HA    | 64:sR:59:LYS:CG    | 2.15                     | 0.75              |
| 68:sP:37:TYR:HD2   | 68:sP:41:GLN:HB2   | 1.51                     | 0.75              |
| 70:sS:2:SER:OG     | 70:sS:4:VAL:O      | 2.03                     | 0.75              |
| 77:sZ:41:ARG:NH2   | 79:s2:1600:G:OP1   | 2.19                     | 0.75              |
| 81:aP:50:U:H3      | 81:aP:64:G:H1      | 0.82                     | 0.75              |
| 85:l5:3967:G:H1    | 85:l5:4055:U:H3    | 1.29                     | 0.75              |
| 85:L5:4101:C:H3'   | 85:L5:4106:G:C1'   | 2.16                     | 0.75              |
| 66:SF:125:SER:HA   | 66:SF:138:ALA:HA   | 1.67                     | 0.75              |
| 7:sJ:122:SER:O     | 7:sJ:125:HIS:N     | 2.19                     | 0.75              |
| 10:sA:90:PHE:HA    | 10:sA:202:TYR:OH   | 1.87                     | 0.75              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:1B:95:THR:HG23  | 23:1B:97:ARG:H     | 1.49                     | 0.75              |
| 45:1Z:113:GLU:OE2  | 45:1Z:117:LYS:HE3  | 1.86                     | 0.75              |
| 85:L5:280:G:OP1    | 34:LN:47:LYS:NZ    | 2.19                     | 0.75              |
| 85:L5:4096:C:H1'   | 85:L5:4111:U:C2    | 2.21                     | 0.75              |
| 85:L5:4887:C:N4    | 85:L5:4932:U:H3    | 1.83                     | 0.75              |
| 20:L7:72:U:O2      | 20:L7:103:A:N6     | 2.19                     | 0.75              |
| 45:LZ:5:MET:HE1    | 45:LZ:82:PRO:HG3   | 1.68                     | 0.75              |
| 71:ST:11:GLN:HA    | 71:ST:14:PHE:HB3   | 1.68                     | 0.75              |
| 73:sc:10:LYS:HD2   | 73:sc:11:LEU:N     | 2.02                     | 0.75              |
| 80:cB:600:ASN:HD21 | 80:cB:716:ARG:HG2  | 1.51                     | 0.75              |
| 85:l5:2486:G:O6    | 85:l5:2493:G:O6    | 2.04                     | 0.75              |
| 85:L5:2667:C:H5''  | 38:LR:99:MET:HE1   | 1.67                     | 0.75              |
| 21:L8:47:C:H1'     | 21:L8:61:A:H2'     | 1.68                     | 0.75              |
| 24:LC:8:ILE:HD12   | 24:LC:24:LEU:HD13  | 1.67                     | 0.75              |
| 35:LO:34:VAL:HG23  | 35:LO:103:LYS:HB2  | 1.69                     | 0.75              |
| 36:LP:17:SER:OG    | 36:LP:94:MET:SD    | 2.43                     | 0.75              |
| 43:LX:91:GLU:HG3   | 43:LX:92:ASP:OD1   | 1.87                     | 0.75              |
| 52:Lg:41:ALA:O     | 52:Lg:52:ARG:NH1   | 2.19                     | 0.75              |
| 79:S2:958:G:N2     | 79:S2:965:U:O4     | 2.19                     | 0.75              |
| 6:sG:110:ASN:HD22  | 79:s2:165:G:C1'    | 1.99                     | 0.75              |
| 52:lg:24:ARG:NH2   | 85:l5:2638:G:O3'   | 2.19                     | 0.75              |
| 64:sR:60:ARG:HD2   | 79:s2:1464:C:H5'   | 1.69                     | 0.75              |
| 79:s2:1729:U:H3    | 79:s2:1805:G:H1    | 0.79                     | 0.75              |
| 85:L5:1346:C:H2'   | 85:L5:1347:G:H8    | 1.50                     | 0.75              |
| 66:SF:34:SER:HB3   | 73:Sc:11:LEU:HD21  | 1.66                     | 0.75              |
| 21:l8:125:C:H1'    | 21:l8:126:C:H2'    | 1.69                     | 0.75              |
| 25:1D:35:ARG:HH12  | 85:l5:4326:G:H1'   | 1.51                     | 0.75              |
| 36:1P:62:ARG:NH1   | 85:l5:423:G:OP1    | 2.19                     | 0.75              |
| 79:s2:928:G:H2'    | 79:s2:929:G:C8     | 2.22                     | 0.75              |
| 79:s2:1536:G:H2'   | 79:s2:1537:A:H8    | 1.52                     | 0.75              |
| 83:ls:62:ARG:HH22  | 83:ls:83:ARG:HH11  | 1.31                     | 0.75              |
| 12:SH:20:GLU:O     | 12:SH:24:SER:N     | 2.19                     | 0.75              |
| 85:L5:1705:G:H21   | 27:LF:46:ARG:HH21  | 1.34                     | 0.75              |
| 22:LA:114:CYS:HB2  | 22:LA:169:VAL:HG13 | 1.67                     | 0.75              |
| 27:LF:216:PRO:HG2  | 27:LF:220:MET:HE2  | 1.69                     | 0.75              |
| 81:aP:29:C:O2      | 81:aP:41:G:N1      | 2.19                     | 0.75              |
| 85:l5:1308:C:H2'   | 85:l5:1309:C:C6    | 2.22                     | 0.75              |
| 85:l5:2568:C:H2'   | 85:l5:2569:G:H8    | 1.50                     | 0.75              |
| 10:SA:139:TYR:OH   | 79:S2:1353:A:OP1   | 2.03                     | 0.75              |
| 85:L5:2296:G:O2'   | 24:LC:242:PRO:O    | 2.03                     | 0.75              |
| 22:LA:80:GLU:CD    | 22:LA:170:ALA:HA   | 2.12                     | 0.75              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:LO:175:MET:O    | 35:LO:175:MET:HE3  | 1.87                     | 0.75              |
| 6:sG:137:ARG:NH2   | 79:s2:146:G:N7     | 2.35                     | 0.75              |
| 62:lr:28:GLU:OE2   | 62:lr:28:GLU:N     | 2.20                     | 0.75              |
| 76:sM:117:GLU:O    | 76:sM:121:LYS:NZ   | 2.19                     | 0.75              |
| 79:s2:191:A:N6     | 79:s2:208:G:O2'    | 2.20                     | 0.75              |
| 82:pE:26:A:N1      | 82:pE:44:G:N2      | 2.33                     | 0.75              |
| 84:lt:141:CYS:SG   | 84:lt:142:ASN:N    | 2.59                     | 0.75              |
| 85:l5:184:U:O2     | 85:l5:254:G:N1     | 2.19                     | 0.75              |
| 85:L5:4101:C:H2'   | 85:L5:4106:G:H8    | 1.52                     | 0.75              |
| 85:L5:4670:C:O2'   | 85:L5:4672:A:OP2   | 2.05                     | 0.75              |
| 31:LJ:109:ILE:HD11 | 31:LJ:128:LEU:HG   | 1.68                     | 0.75              |
| 66:SF:33:ILE:HA    | 66:SF:36:GLN:HG2   | 1.67                     | 0.75              |
| 80:cB:305:MET:SD   | 80:cB:306:ASN:ND2  | 2.60                     | 0.74              |
| 83:ls:6:ARG:HG3    | 83:ls:10:LYS:HE2   | 1.69                     | 0.74              |
| 80:CB:396:MET:HB2  | 80:CB:485:ILE:HG23 | 1.68                     | 0.74              |
| 2:SE:69:PHE:HE1    | 8:SY:17:LEU:HD12   | 1.52                     | 0.74              |
| 3:SI:31:ARG:NH2    | 79:S2:381:C:OP2    | 2.20                     | 0.74              |
| 85:L5:1207:C:H2'   | 85:L5:1208:G:H8    | 1.52                     | 0.74              |
| 85:L5:1994:C:H2'   | 85:L5:1995:G:C8    | 2.22                     | 0.74              |
| 21:L8:19:C:H2'     | 21:L8:20:A:H8      | 1.51                     | 0.74              |
| 68:SP:86:LEU:HB2   | 68:SP:89:MET:HE1   | 1.69                     | 0.74              |
| 70:SS:105:ASN:HB2  | 70:SS:108:ARG:HH21 | 1.51                     | 0.74              |
| 72:SU:50:VAL:HA    | 72:SU:91:LEU:HD22  | 1.69                     | 0.74              |
| 28:lG:207:VAL:O    | 28:lG:212:LYS:NZ   | 2.15                     | 0.74              |
| 41:lU:21:PHE:HZ    | 41:lU:80:LYS:HG3   | 1.50                     | 0.74              |
| 79:s2:557:U:H5'    | 79:s2:558:G:H8     | 1.53                     | 0.74              |
| 79:s2:874:G:H2'    | 79:s2:875:A:H8     | 1.52                     | 0.74              |
| 79:s2:888:U:H4'    | 79:s2:889:U:H5'    | 1.70                     | 0.74              |
| 8:SY:105:LYS:NZ    | 79:S2:52:G:O2'     | 2.19                     | 0.74              |
| 20:L7:7:G:OP1      | 25:LD:33:ARG:NH1   | 2.20                     | 0.74              |
| 66:SF:88:MET:HE1   | 79:S2:1535:U:H1'   | 1.68                     | 0.74              |
| 81:AP:29:C:O2      | 81:AP:41:G:N1      | 2.18                     | 0.74              |
| 15:sC:117:ARG:O    | 15:sC:117:ARG:NH1  | 2.20                     | 0.74              |
| 30:II:177:ASN:ND2  | 30:II:180:GLU:OE2  | 2.18                     | 0.74              |
| 65:sD:94:ARG:O     | 65:sD:101:GLN:NE2  | 2.19                     | 0.74              |
| 79:s2:1341:C:N4    | 79:s2:1485:U:O4    | 2.20                     | 0.74              |
| 2:SE:151:ASP:HB3   | 2:SE:154:ILE:HG12  | 1.68                     | 0.74              |
| 5:SX:13:LEU:HD12   | 5:SX:14:ARG:N      | 2.02                     | 0.74              |
| 11:SB:214:LYS:NZ   | 11:SB:215:VAL:O    | 2.20                     | 0.74              |
| 85:L5:517:C:N4     | 85:L5:646:G:O2'    | 2.20                     | 0.74              |
| 85:L5:3950:U:H2'   | 85:L5:3951:G:C8    | 2.22                     | 0.74              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 38:LR:13:SER:OG   | 38:LR:38:ARG:NH2   | 2.20                     | 0.74              |
| 54:Li:43:MET:SD   | 54:Li:46:GLU:OE2   | 2.45                     | 0.74              |
| 6:sG:23:LYS:HD2   | 6:sG:41:LEU:HB2    | 1.68                     | 0.74              |
| 25:ID:38:ILE:HG21 | 40:IT:30:TYR:HE2   | 1.51                     | 0.74              |
| 40:IT:149:GLU:N   | 40:IT:149:GLU:OE1  | 2.20                     | 0.74              |
| 43:IX:64:SER:HB2  | 53:lh:69:LEU:HD23  | 1.69                     | 0.74              |
| 79:s2:1354:G:N2   | 79:s2:1357:A:OP2   | 2.18                     | 0.74              |
| 80:cB:9:ILE:O     | 80:cB:13:MET:HB2   | 1.86                     | 0.74              |
| 85:l5:4348:A:H61  | 85:l5:4364:G:H1    | 1.35                     | 0.74              |
| 2:SE:128:LYS:HG2  | 2:SE:140:VAL:CG1   | 2.17                     | 0.74              |
| 19:Sb:51:GLN:NE2  | 79:S2:927:C:O2     | 2.20                     | 0.74              |
| 11:sB:62:LEU:HA   | 11:sB:65:ARG:HD2   | 1.68                     | 0.74              |
| 23:lB:63:PRO:HA   | 23:lB:68:ASN:HD21  | 1.53                     | 0.74              |
| 23:lB:300:LYS:NZ  | 23:lB:309:LEU:O    | 2.20                     | 0.74              |
| 40:IT:43:LYS:O    | 40:IT:58:HIS:ND1   | 2.19                     | 0.74              |
| 79:s2:878:G:N2    | 79:s2:908:A:N1     | 2.34                     | 0.74              |
| 80:CB:396:MET:HB2 | 80:CB:485:ILE:CG2  | 2.18                     | 0.74              |
| 85:L5:1279:A:N3   | 24:LC:323:ARG:NH2  | 2.36                     | 0.74              |
| 65:SD:67:ARG:NH2  | 67:SK:97:SER:OG    | 2.20                     | 0.74              |
| 68:SP:81:ARG:NH2  | 68:SP:120:SER:O    | 2.19                     | 0.74              |
| 9:se:36:MET:H     | 9:se:36:MET:HE3    | 1.52                     | 0.74              |
| 64:sR:28:PHE:H    | 79:s2:1455:A:H3'   | 1.51                     | 0.74              |
| 69:sQ:134:GLY:HA3 | 69:sQ:140:ARG:HA   | 1.68                     | 0.74              |
| 80:cB:124:GLY:HA3 | 80:cB:358:LEU:HD12 | 1.70                     | 0.74              |
| 85:l5:369:G:N2    | 85:l5:372:A:OP2    | 2.19                     | 0.74              |
| 85:l5:1824:G:H2'  | 85:l5:1825:A:C8    | 2.22                     | 0.74              |
| 80:CB:223:PHE:HB3 | 80:CB:344:LEU:HD13 | 1.69                     | 0.74              |
| 85:L5:1563:A:N6   | 79:S2:1028:A:N1    | 2.35                     | 0.74              |
| 85:L5:4112:C:H41  | 85:L5:4116:C:H1'   | 1.51                     | 0.74              |
| 24:LC:142:HIS:CE1 | 24:LC:249:PHE:H    | 2.04                     | 0.74              |
| 70:SS:73:ASN:O    | 70:SS:76:GLN:NE2   | 2.19                     | 0.74              |
| 70:SS:84:LEU:HD12 | 70:SS:97:GLN:HB2   | 1.67                     | 0.74              |
| 75:Sg:171:ASP:O   | 75:Sg:172:LYS:HG2  | 1.87                     | 0.74              |
| 87:IW:1:MET:HE1   | 87:IW:3:VAL:HG23   | 1.67                     | 0.74              |
| 4:sL:81:LYS:NZ    | 79:s2:394:G:OP1    | 2.20                     | 0.74              |
| 14:sa:3:LYS:HZ2   | 14:sa:5:ARG:H      | 1.33                     | 0.74              |
| 15:sC:79:GLU:OE1  | 15:sC:79:GLU:N     | 2.19                     | 0.74              |
| 22:lA:116:LEU:HB2 | 22:lA:126:LEU:HB2  | 1.69                     | 0.74              |
| 25:ID:289:ARG:NH2 | 85:l5:1179:U:OP2   | 2.20                     | 0.74              |
| 61:lp:56:HIS:CD2  | 61:lp:63:THR:HG22  | 2.22                     | 0.74              |
| 64:sR:47:ARG:HH11 | 79:s2:1453:C:H4'   | 1.52                     | 0.74              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 64:sR:102:THR:HA   | 64:sR:105:MET:SD  | 2.28                     | 0.74              |
| 70:sS:26:ILE:HD11  | 70:sS:52:LEU:HA   | 1.67                     | 0.74              |
| 75:sg:49:GLU:HG3   | 75:sg:50:THR:HG23 | 1.70                     | 0.74              |
| 79:s2:1692:U:H2'   | 79:s2:1693:G:C8   | 2.22                     | 0.74              |
| 8:SY:114:MET:HE1   | 8:SY:127:ALA:HB3  | 1.68                     | 0.74              |
| 85:L5:119:G:C6     | 28:LG:132:ARG:HG3 | 2.23                     | 0.74              |
| 85:L5:4126:C:H5''  | 85:L5:4127:A:H5'' | 1.69                     | 0.74              |
| 24:LC:302:LEU:HD12 | 24:LC:303:ARG:N   | 2.01                     | 0.74              |
| 50:Le:7:LEU:HD23   | 50:Le:8:VAL:HG12  | 1.69                     | 0.74              |
| 79:S2:919:A:O2'    | 79:S2:1020:A:N1   | 2.19                     | 0.74              |
| 2:sE:181:CYS:HA    | 2:sE:227:VAL:HA   | 1.70                     | 0.74              |
| 3:sI:67:TRP:HZ3    | 3:sI:69:SER:HB2   | 1.51                     | 0.74              |
| 15:sC:60:TRP:HD1   | 15:sC:61:MET:N    | 1.86                     | 0.74              |
| 6:SG:25:ARG:O      | 6:SG:25:ARG:NH1   | 2.19                     | 0.74              |
| 85:L5:4102:C:C6    | 85:L5:4105:A:C4   | 2.76                     | 0.74              |
| 54:Li:86:LYS:O     | 54:Li:90:LEU:HD12 | 1.87                     | 0.74              |
| 62:Lr:21:ASN:OD1   | 62:Lr:23:GLN:NE2  | 2.21                     | 0.74              |
| 84:Lt:105:THR:HA   | 84:Lt:143:VAL:HA  | 1.69                     | 0.74              |
| 20:l7:110:G:P      | 25:ID:270:LYS:HZ1 | 2.11                     | 0.74              |
| 57:ll:20:ASN:ND2   | 57:ll:42:ARG:O    | 2.21                     | 0.74              |
| 79:s2:76:U:O2'     | 79:s2:78:C:OP1    | 2.06                     | 0.74              |
| 79:s2:639:C:H2'    | 79:s2:640:A:H8    | 1.53                     | 0.74              |
| 85:L5:4102:C:C2    | 85:L5:4105:A:N3   | 2.56                     | 0.74              |
| 85:L5:4713:G:OP1   | 35:LO:148:LYS:NZ  | 2.20                     | 0.74              |
| 71:ST:85:ASN:HB2   | 71:ST:88:MET:HB3  | 1.69                     | 0.74              |
| 10:sA:180:ARG:O    | 10:sA:184:ARG:HG3 | 1.86                     | 0.74              |
| 64:sR:11:LYS:NZ    | 79:s2:1371:U:O3'  | 2.21                     | 0.74              |
| 66:sF:29:GLN:NE2   | 66:sF:30:ILE:O    | 2.21                     | 0.74              |
| 85:l5:4524:G:OP1   | 85:l5:4559:A:N6   | 2.20                     | 0.74              |
| 80:CB:56:PHE:HB3   | 80:CB:455:GLY:HA3 | 1.70                     | 0.74              |
| 85:L5:138:G:H2'    | 85:L5:139:G:C8    | 2.23                     | 0.74              |
| 85:L5:1977:C:H5''  | 84:Lt:57:ARG:HH21 | 1.53                     | 0.74              |
| 85:L5:4096:C:H5''  | 85:L5:4108:G:C8   | 2.22                     | 0.74              |
| 85:L5:4102:C:O5'   | 85:L5:4106:G:O2'  | 2.05                     | 0.74              |
| 45:LZ:90:PRO:O     | 45:LZ:117:LYS:NZ  | 2.21                     | 0.74              |
| 78:Sf:96:LYS:HE2   | 78:Sf:97:LYS:H    | 1.52                     | 0.74              |
| 79:S2:531:A:H62    | 79:S2:554:A:H1'   | 1.53                     | 0.74              |
| 82:PE:8:U:N3       | 82:PE:15:G:O6     | 2.20                     | 0.74              |
| 5:sX:23:HIS:ND1    | 79:s2:1165:G:OP2  | 2.21                     | 0.73              |
| 15:sC:169:TYR:O    | 18:sW:98:GLN:NE2  | 2.21                     | 0.73              |
| 17:sO:62:VAL:HG12  | 17:sO:64:ALA:H    | 1.50                     | 0.73              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 24:1C:101:MET:HE1 | 85:l5:2343:G:C4    | 2.23                     | 0.73              |
| 29:lH:89:ARG:HH21 | 29:lH:187:VAL:HA   | 1.53                     | 0.73              |
| 30:lI:54:SER:HB2  | 30:lI:163:GLN:HG3  | 1.70                     | 0.73              |
| 39:lS:4:SER:HB2   | 85:l5:2062:C:H4'   | 1.68                     | 0.73              |
| 41:lU:21:PHE:CZ   | 41:lU:80:LYS:HG3   | 2.23                     | 0.73              |
| 17:SO:34:PHE:HB3  | 17:SO:41:PHE:HB2   | 1.69                     | 0.73              |
| 85:L5:1555:G:O6   | 61:Lp:4:ARG:NH1    | 2.20                     | 0.73              |
| 85:L5:4992:G:H2'  | 85:L5:4993:G:C8    | 2.23                     | 0.73              |
| 39:LS:154:LEU:HB3 | 39:LS:157:ARG:HD3  | 1.69                     | 0.73              |
| 56:Lk:16:ARG:HD2  | 56:Lk:61:PRO:HG3   | 1.69                     | 0.73              |
| 31:lJ:139:PHE:CE1 | 31:lJ:151:ILE:HD13 | 2.23                     | 0.73              |
| 66:sF:164:ARG:NH1 | 79:s2:1636:G:O2'   | 2.21                     | 0.73              |
| 79:s2:525:A:H2'   | 79:s2:526:A:H8     | 1.50                     | 0.73              |
| 85:l5:189:G:H2'   | 85:l5:190:G:H8     | 1.51                     | 0.73              |
| 85:l5:308:G:OP2   | 85:l5:308:G:N2     | 2.17                     | 0.73              |
| 85:l5:663:G:H2'   | 85:l5:664:G:C8     | 2.22                     | 0.73              |
| 26:LE:121:VAL:HB  | 50:Le:7:LEU:HD11   | 1.69                     | 0.73              |
| 56:Lk:16:ARG:CZ   | 56:Lk:61:PRO:HD3   | 2.18                     | 0.73              |
| 75:Sg:99:ARG:NH1  | 75:Sg:134:THR:O    | 2.22                     | 0.73              |
| 7:sJ:128:VAL:O    | 7:sJ:132:GLN:NE2   | 2.21                     | 0.73              |
| 60:lo:98:LYS:NZ   | 85:l5:4233:A:O5'   | 2.18                     | 0.73              |
| 67:sK:1:MET:HG3   | 67:sK:47:LYS:HD2   | 1.67                     | 0.73              |
| 79:s2:116:U:H3    | 79:s2:347:G:H1     | 1.35                     | 0.73              |
| 11:SB:114:VAL:O   | 79:S2:1869:A:N6    | 2.22                     | 0.73              |
| 85:L5:2544:G:N1   | 21:L8:124:U:OP1    | 2.21                     | 0.73              |
| 72:SU:18:HIS:HB3  | 72:SU:117:ALA:HB2  | 1.70                     | 0.73              |
| 76:SM:28:HIS:HE1  | 76:SM:116:LYS:NZ   | 1.85                     | 0.73              |
| 3:sI:165:GLN:NE2  | 3:sI:170:LYS:O     | 2.22                     | 0.73              |
| 6:sG:142:ARG:NH2  | 79:s2:144:U:OP1    | 2.22                     | 0.73              |
| 20:l7:92:C:H2'    | 20:l7:93:G:H8      | 1.52                     | 0.73              |
| 64:sR:28:PHE:N    | 79:s2:1455:A:O5'   | 2.21                     | 0.73              |
| 65:sD:62:LYS:NZ   | 67:sK:97:SER:OG    | 2.21                     | 0.73              |
| 67:sK:34:GLU:N    | 67:sK:34:GLU:OE1   | 2.21                     | 0.73              |
| 70:sS:36:VAL:HG13 | 70:sS:40:TYR:CD1   | 2.23                     | 0.73              |
| 80:cB:337:LYS:HB3 | 80:cB:341:ARG:NH1  | 2.02                     | 0.73              |
| 80:cB:689:GLU:O   | 80:cB:730:TYR:OH   | 2.06                     | 0.73              |
| 81:aP:23:C:H2'    | 81:aP:24:A:C8      | 2.24                     | 0.73              |
| 85:l5:512:U:H3    | 85:l5:647:G:H1     | 1.36                     | 0.73              |
| 85:l5:4954:G:H2'  | 85:l5:4955:A:H8    | 1.53                     | 0.73              |
| 80:CB:691:ALA:HA  | 80:CB:730:TYR:HE1  | 1.54                     | 0.73              |
| 12:SH:157:HIS:HB3 | 12:SH:190:PRO:HG3  | 1.70                     | 0.73              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 85:L5:2553:A:OP2   | 85:L5:2574:G:O2'   | 2.06                     | 0.73              |
| 85:L5:2656:U:OP1   | 45:LZ:78:ASN:ND2   | 2.21                     | 0.73              |
| 28:lG:29:ASN:HD21  | 28:lG:31:LEU:HB3   | 1.51                     | 0.73              |
| 32:lL:59:VAL:HG13  | 85:l5:74:G:H5'     | 1.70                     | 0.73              |
| 46:la:29:PRO:HB2   | 85:l5:1681:G:H5'   | 1.71                     | 0.73              |
| 80:cB:176:GLN:HB3  | 80:cB:180:ARG:HH22 | 1.52                     | 0.73              |
| 85:L5:1895:G:OP1   | 27:LF:96:ARG:NH2   | 2.21                     | 0.73              |
| 85:L5:4620:U:OP2   | 85:L5:4670:C:N4    | 2.18                     | 0.73              |
| 25:LD:193:GLU:OE1  | 25:LD:196:ARG:NH2  | 2.21                     | 0.73              |
| 29:LH:128:MET:SD   | 29:LH:132:VAL:HB   | 2.27                     | 0.73              |
| 79:S2:1581:C:H5'   | 79:S2:1582:C:H5    | 1.53                     | 0.73              |
| 20:l7:2:U:H3       | 20:l7:117:G:H1     | 1.34                     | 0.73              |
| 22:lA:215:ASN:ND2  | 85:l5:4546:A:N7    | 2.37                     | 0.73              |
| 47:lb:62:ALA:O     | 47:lb:65:MET:SD    | 2.46                     | 0.73              |
| 64:sR:29:HIS:NE2   | 79:s2:1476:A:N1    | 2.37                     | 0.73              |
| 70:sS:142:ARG:NH2  | 79:s2:1228:A:OP1   | 2.22                     | 0.73              |
| 79:s2:1513:C:H2'   | 79:s2:1514:G:H8    | 1.53                     | 0.73              |
| 80:cB:176:GLN:HB3  | 80:cB:180:ARG:HH12 | 1.53                     | 0.73              |
| 83:ls:173:THR:O    | 83:ls:177:MET:HG2  | 1.88                     | 0.73              |
| 80:CB:50:ARG:HH22  | 79:S2:463:C:H4'    | 1.52                     | 0.73              |
| 4:SL:103:GLU:OE2   | 5:SX:11:ARG:NH1    | 2.21                     | 0.73              |
| 85:L5:3697:U:H5''  | 85:L5:3698:G:H5'   | 1.69                     | 0.73              |
| 25:LD:51:MET:SD    | 25:LD:53:VAL:HG23  | 2.28                     | 0.73              |
| 59:Ln:9:ARG:NH2    | 79:S2:1851:A:OP1   | 2.22                     | 0.73              |
| 69:SQ:132:PHE:HE2  | 72:SU:76:THR:HA    | 1.54                     | 0.73              |
| 83:Ls:62:ARG:NH2   | 83:Ls:82:ILE:O     | 2.21                     | 0.73              |
| 10:sA:10:MET:HA    | 10:sA:55:TRP:CZ3   | 2.24                     | 0.73              |
| 24:lC:323:ARG:NH1  | 85:l5:975:C:O2     | 2.20                     | 0.73              |
| 32:IL:129:ARG:HH22 | 85:l5:173:C:H3'    | 1.54                     | 0.73              |
| 72:sU:27:ARG:HD2   | 72:sU:82:MET:SD    | 2.29                     | 0.73              |
| 75:sg:14:HIS:HE1   | 75:sg:18:VAL:HG22  | 1.54                     | 0.73              |
| 85:l5:493:G:N1     | 85:l5:660:A:H2     | 1.84                     | 0.73              |
| 18:SW:69:LEU:HD11  | 18:SW:129:PHE:HB2  | 1.70                     | 0.73              |
| 85:L5:4087:G:N7    | 22:LA:67:TYR:OH    | 2.22                     | 0.73              |
| 85:L5:4472:G:H5''  | 58:Lm:102:ARG:HH21 | 1.53                     | 0.73              |
| 27:LF:220:MET:SD   | 27:LF:220:MET:N    | 2.62                     | 0.73              |
| 39:LS:95:ARG:NH2   | 39:LS:112:ASP:OD2  | 2.22                     | 0.73              |
| 15:sC:60:TRP:CE3   | 15:sC:96:PHE:HE2   | 2.06                     | 0.73              |
| 18:sW:115:GLU:N    | 18:sW:115:GLU:OE1  | 2.22                     | 0.73              |
| 34:lN:65:ARG:NH2   | 85:l5:2457:G:OP1   | 2.21                     | 0.73              |
| 35:lO:169:ARG:NH2  | 85:l5:4860:G:OP1   | 2.22                     | 0.73              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 42:IV:88:TYR:CZ   | 42:IV:96:LEU:HD21  | 2.24                     | 0.73              |
| 80:cB:334:PRO:HA  | 80:cB:337:LYS:HD2  | 1.69                     | 0.73              |
| 85:l5:1802:A:H5'' | 85:l5:1803:G:H5'   | 1.68                     | 0.73              |
| 85:l5:4260:U:H2'  | 85:l5:4261:C:H6    | 1.54                     | 0.73              |
| 80:CB:162:ARG:O   | 80:CB:166:GLU:HB3  | 1.87                     | 0.73              |
| 85:L5:1857:C:H2'  | 85:L5:1858:A:H8    | 1.54                     | 0.73              |
| 85:L5:1961:G:N2   | 85:L5:2024:G:O2'   | 2.20                     | 0.73              |
| 85:L5:2759:G:O2'  | 85:L5:2762:G:N2    | 2.21                     | 0.73              |
| 85:L5:4101:C:C6   | 85:L5:4105:A:O5'   | 2.38                     | 0.73              |
| 32:LL:48:PRO:HB2  | 53:Lh:120:ALA:HB2  | 1.71                     | 0.73              |
| 45:LZ:12:LEU:HB2  | 45:LZ:81:MET:HB3   | 1.71                     | 0.73              |
| 53:Lh:70:ARG:HG2  | 53:Lh:83:LEU:HD11  | 1.70                     | 0.73              |
| 67:SK:27:VAL:HG13 | 67:SK:43:LEU:HD21  | 1.69                     | 0.73              |
| 79:S2:1403:C:N4   | 79:S2:1433:C:OP1   | 2.22                     | 0.73              |
| 38:lR:60:ARG:NH1  | 85:l5:2808:G:O3'   | 2.21                     | 0.73              |
| 62:lr:108:MET:HE1 | 85:l5:2263:A:H5''  | 1.70                     | 0.73              |
| 73:sc:12:ALA:HB1  | 73:sc:32:VAL:HB    | 1.71                     | 0.73              |
| 80:cB:741:MET:HG3 | 80:cB:817:TRP:HB3  | 1.70                     | 0.73              |
| 85:l5:4174:U:H2'  | 85:l5:4175:G:H8    | 1.54                     | 0.73              |
| 5:SX:23:HIS:ND1   | 79:S2:1165:G:OP2   | 2.19                     | 0.73              |
| 85:L5:1866:U:OP1  | 30:LI:4:ARG:NH1    | 2.22                     | 0.73              |
| 25:LD:67:ALA:HA   | 25:LD:72:ASP:HA    | 1.71                     | 0.73              |
| 39:LS:91:HIS:HB2  | 39:LS:93:MET:HE1   | 1.71                     | 0.73              |
| 52:Lg:98:GLU:OE1  | 52:Lg:101:LYS:NZ   | 2.22                     | 0.73              |
| 63:Lz:47:LYS:O    | 63:Lz:48:ARG:NH1   | 2.22                     | 0.73              |
| 2:sE:19:MET:HE1   | 79:s2:846:G:C4     | 2.23                     | 0.73              |
| 9:se:34:ARG:HA    | 9:se:37:GLN:HE22   | 1.53                     | 0.73              |
| 26:lE:108:LYS:NZ  | 85:l5:2260:C:OP1   | 2.20                     | 0.73              |
| 37:lQ:173:LYS:NZ  | 85:l5:88:A:N7      | 2.36                     | 0.73              |
| 59:ln:1:MET:HE2   | 59:ln:5:TRP:HB2    | 1.69                     | 0.73              |
| 66:sF:124:ASP:O   | 66:sF:139:VAL:N    | 2.19                     | 0.73              |
| 75:sg:80:SER:OG   | 75:sg:90:TRP:NE1   | 2.22                     | 0.73              |
| 80:cB:395:MET:HG2 | 80:cB:418:SER:HB3  | 1.70                     | 0.73              |
| 80:cB:641:TRP:HE1 | 80:cB:646:ALA:HA   | 1.54                     | 0.73              |
| 80:CB:171:PRO:HA  | 80:CB:174:LEU:HD13 | 1.71                     | 0.73              |
| 85:L5:2403:A:OP1  | 52:Lg:10:ARG:NH1   | 2.22                     | 0.73              |
| 31:LJ:18:ARG:HB2  | 31:LJ:133:VAL:HG23 | 1.70                     | 0.73              |
| 76:SM:69:CYS:SG   | 76:SM:70:ALA:N     | 2.62                     | 0.73              |
| 26:lE:118:THR:HB  | 50:le:90:MET:CE    | 2.15                     | 0.72              |
| 42:IV:98:PHE:HD1  | 87:IW:22:ALA:HB3   | 1.53                     | 0.72              |
| 70:sS:8:LYS:O     | 70:sS:8:LYS:HD2    | 1.89                     | 0.72              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 74:sd:16:GLN:NE2   | 79:s2:1262:C:N3    | 2.37                     | 0.72              |
| 79:s2:375:U:H2'    | 79:s2:376:A:C8     | 2.23                     | 0.72              |
| 79:s2:1144:A:H2'   | 79:s2:1145:A:C8    | 2.23                     | 0.72              |
| 85:l5:517:C:N4     | 85:l5:646:G:O2'    | 2.22                     | 0.72              |
| 85:l5:1095:A:N1    | 85:l5:1200:G:O6    | 2.21                     | 0.72              |
| 85:L5:1095:A:N1    | 85:L5:1200:G:C6    | 2.57                     | 0.72              |
| 85:L5:2772:C:O2'   | 56:Lk:17:ARG:NH1   | 2.22                     | 0.72              |
| 85:L5:2822:G:OP2   | 38:LR:21:LYS:NZ    | 2.21                     | 0.72              |
| 51:Lf:46:ARG:HD2   | 51:Lf:106:TYR:HD2  | 1.54                     | 0.72              |
| 62:Lr:5:LEU:H      | 62:Lr:5:LEU:HD22   | 1.53                     | 0.72              |
| 79:S2:925:G:H1     | 79:S2:1017:U:H3    | 0.76                     | 0.72              |
| 1:cH:61:LEU:O      | 65:sD:108:LYS:NZ   | 2.22                     | 0.72              |
| 2:sE:87:MET:HE1    | 2:sE:122:LYS:HE2   | 1.70                     | 0.72              |
| 4:sL:7:GLU:OE1     | 4:sL:11:GLN:NE2    | 2.22                     | 0.72              |
| 21:l8:154:G:H5'    | 28:lG:189:ARG:HH21 | 1.54                     | 0.72              |
| 41:lU:19:LEU:HB2   | 41:lU:73:THR:HB    | 1.69                     | 0.72              |
| 75:sg:217:MET:HA   | 75:sg:229:THR:HA   | 1.69                     | 0.72              |
| 85:l5:1824:G:H2'   | 85:l5:1825:A:H8    | 1.54                     | 0.72              |
| 85:L5:1478:C:H2'   | 85:L5:1479:G:H8    | 1.54                     | 0.72              |
| 72:SU:56:MET:HE2   | 79:S2:1580:A:H5'   | 1.71                     | 0.72              |
| 75:Sg:126:ASP:OD2  | 75:Sg:130:LYS:NZ   | 2.22                     | 0.72              |
| 76:SM:23:LYS:NZ    | 76:SM:88:TRP:O     | 2.21                     | 0.72              |
| 76:SM:28:HIS:CE1   | 76:SM:116:LYS:HZ3  | 2.07                     | 0.72              |
| 79:S2:981:A:H2'    | 79:S2:982:G:C8     | 2.23                     | 0.72              |
| 84:Lt:114:ARG:HG2  | 84:Lt:119:ARG:NH2  | 2.03                     | 0.72              |
| 12:sH:7:LYS:HE2    | 12:sH:25:GLN:HE21  | 1.53                     | 0.72              |
| 17:sO:103:ASN:HD22 | 17:sO:142:ARG:HG3  | 1.52                     | 0.72              |
| 25:lD:38:ILE:HG21  | 40:lT:30:TYR:CE2   | 2.23                     | 0.72              |
| 34:lN:120:TRP:CD1  | 34:lN:122:GLY:H    | 2.07                     | 0.72              |
| 45:lZ:76:ASN:HB3   | 45:lZ:79:HIS:CE1   | 2.24                     | 0.72              |
| 50:le:91:CYS:SG    | 50:le:95:TYR:N     | 2.61                     | 0.72              |
| 53:lh:8:ASP:O      | 53:lh:12:LYS:NZ    | 2.21                     | 0.72              |
| 79:s2:835:C:H4'    | 79:s2:836:G:H8     | 1.54                     | 0.72              |
| 85:L5:2658:G:N2    | 85:L5:2676:A:OP2   | 2.21                     | 0.72              |
| 75:Sg:145:GLU:O    | 75:Sg:175:LYS:NZ   | 2.22                     | 0.72              |
| 75:Sg:257:LYS:HD3  | 75:Sg:259:TRP:HZ3  | 1.53                     | 0.72              |
| 79:S2:366:U:H3     | 79:S2:394:G:H1     | 1.37                     | 0.72              |
| 79:S2:1536:G:H2'   | 79:S2:1537:A:C8    | 2.25                     | 0.72              |
| 1:cH:133:ARG:NH1   | 79:s2:534:G:O3'    | 2.21                     | 0.72              |
| 18:sW:28:ARG:HD3   | 79:s2:921:G:C6     | 2.24                     | 0.72              |
| 22:lA:57:PRO:HG2   | 22:lA:170:ALA:HB3  | 1.72                     | 0.72              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 26:IE:270:TYR:CE1  | 33:IM:110:PHE:HB3  | 2.24                     | 0.72              |
| 27:IF:247:MET:HA   | 27:IF:247:MET:HE3  | 1.70                     | 0.72              |
| 32:IL:177:LYS:HB3  | 32:IL:180:ALA:HB3  | 1.72                     | 0.72              |
| 43:IX:77:ILE:HD11  | 43:IX:98:PHE:CD2   | 2.24                     | 0.72              |
| 45:IZ:97:ASN:O     | 45:IZ:100:VAL:HG23 | 1.88                     | 0.72              |
| 67:sK:95:ARG:O     | 67:sK:97:SER:N     | 2.22                     | 0.72              |
| 79:s2:454:U:H2'    | 79:s2:455:A:H8     | 1.55                     | 0.72              |
| 85:l5:1709:C:N3    | 85:l5:1716:G:N1    | 2.37                     | 0.72              |
| 85:L5:1984:A:N7    | 85:L5:2010:A:O2'   | 2.23                     | 0.72              |
| 85:L5:4097:G:H3'   | 85:L5:4111:U:N3    | 2.05                     | 0.72              |
| 85:L5:4101:C:H2'   | 85:L5:4106:G:H1'   | 1.70                     | 0.72              |
| 32:LL:104:ASN:HD22 | 32:LL:110:LEU:HD13 | 1.55                     | 0.72              |
| 54:Li:66:ASP:HB2   | 54:Li:87:ARG:HH22  | 1.52                     | 0.72              |
| 63:Lz:62:LYS:NZ    | 63:Lz:155:ILE:HD11 | 2.03                     | 0.72              |
| 36:IP:126:ARG:HA   | 36:IP:140:MET:HE1  | 1.70                     | 0.72              |
| 45:IZ:5:MET:O      | 45:IZ:28:ASN:ND2   | 2.23                     | 0.72              |
| 58:lm:99:CYS:HB2   | 58:lm:114:LYS:CE   | 2.19                     | 0.72              |
| 73:sc:21:THR:OG1   | 73:sc:66:ARG:NH2   | 2.22                     | 0.72              |
| 76:sM:45:ARG:HH22  | 76:sM:74:ILE:HG12  | 1.52                     | 0.72              |
| 80:CB:815:ASP:OD1  | 80:CB:816:HIS:ND1  | 2.22                     | 0.72              |
| 2:SE:64:ILE:HG23   | 8:SY:17:LEU:HD11   | 1.72                     | 0.72              |
| 14:Sa:5:ARG:HH21   | 79:S2:1864:U:H3'   | 1.53                     | 0.72              |
| 85:L5:280:G:OP2    | 34:LN:44:ARG:NH1   | 2.21                     | 0.72              |
| 85:L5:2373:C:H5'   | 49:Ld:46:LEU:HD11  | 1.71                     | 0.72              |
| 23:LB:140:GLU:HA   | 23:LB:143:LYS:HD2  | 1.72                     | 0.72              |
| 79:S2:28:U:H2'     | 79:S2:29:G:H8      | 1.55                     | 0.72              |
| 83:Ls:123:VAL:HG12 | 83:Ls:180:ILE:HD12 | 1.70                     | 0.72              |
| 6:sG:110:ASN:HD22  | 79:s2:165:G:H1'    | 1.54                     | 0.72              |
| 25:ID:284:LYS:HZ3  | 30:II:209:TRP:CD1  | 2.07                     | 0.72              |
| 26:IE:127:SER:O    | 26:IE:128:HIS:ND1  | 2.22                     | 0.72              |
| 29:IH:140:GLN:NE2  | 29:IH:142:ASP:OD1  | 2.22                     | 0.72              |
| 72:sU:32:LEU:HD12  | 72:sU:87:ARG:HD2   | 1.70                     | 0.72              |
| 75:sg:5:MET:HE1    | 75:sg:298:LEU:HD13 | 1.71                     | 0.72              |
| 80:CB:420:LEU:HA   | 80:CB:465:PRO:HA   | 1.71                     | 0.72              |
| 5:SX:25:LYS:NZ     | 79:S2:1166:G:N7    | 2.37                     | 0.72              |
| 22:LA:19:HIS:CD2   | 22:LA:193:ARG:HA   | 2.25                     | 0.72              |
| 28:LG:182:CYS:HB3  | 28:LG:222:ILE:HD11 | 1.71                     | 0.72              |
| 33:LM:37:LEU:HD21  | 33:LM:47:ARG:HD3   | 1.71                     | 0.72              |
| 40:LT:51:GLY:HA3   | 40:LT:92:ARG:HG3   | 1.71                     | 0.72              |
| 46:La:73:VAL:HB    | 46:La:108:TYR:CD1  | 2.23                     | 0.72              |
| 72:SU:19:ARG:NH2   | 79:S2:1433:C:O2    | 2.22                     | 0.72              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 74:Sd:19:ARG:HD3   | 74:Sd:32:ARG:HD3   | 1.70                     | 0.72              |
| 75:Sg:152:SER:H    | 75:Sg:169:GLY:HA2  | 1.54                     | 0.72              |
| 76:SM:84:LYS:HD2   | 76:SM:88:TRP:HE1   | 1.53                     | 0.72              |
| 79:S2:532:C:H2'    | 79:S2:533:A:C8     | 2.24                     | 0.72              |
| 79:S2:553:U:H3'    | 79:S2:554:A:H4'    | 1.71                     | 0.72              |
| 10:sA:113:GLN:HE22 | 10:sA:115:ALA:HB3  | 1.55                     | 0.72              |
| 25:ID:68:ARG:HG2   | 25:ID:73:MET:HG2   | 1.70                     | 0.72              |
| 33:IM:76:ALA:HA    | 33:IM:79:LYS:HE2   | 1.70                     | 0.72              |
| 34:IN:127:TYR:HB3  | 34:IN:129:PHE:HE2  | 1.55                     | 0.72              |
| 38:IR:176:ARG:HH22 | 38:IR:180:LYS:HE3  | 1.52                     | 0.72              |
| 79:s2:526:A:H2'    | 79:s2:527:C:C6     | 2.24                     | 0.72              |
| 80:cB:221:TRP:HE3  | 80:cB:344:LEU:HD11 | 1.55                     | 0.72              |
| 84:It:15:LEU:HD23  | 84:It:15:LEU:H     | 1.55                     | 0.72              |
| 85:l5:2870:A:OP2   | 85:l5:2879:A:N6    | 2.22                     | 0.72              |
| 85:L5:382:G:N1     | 85:L5:385:A:OP2    | 2.23                     | 0.72              |
| 85:L5:2019:C:OP1   | 83:Ls:6:ARG:NH2    | 2.22                     | 0.72              |
| 85:L5:2044:U:O3'   | 35:LO:63:ASN:ND2   | 2.23                     | 0.72              |
| 31:LJ:141:ILE:HA   | 31:LJ:144:LYS:HD2  | 1.72                     | 0.72              |
| 35:LO:175:MET:HE1  | 35:LO:178:ARG:CD   | 2.13                     | 0.72              |
| 46:La:75:LEU:HB3   | 46:La:117:LEU:HD21 | 1.70                     | 0.72              |
| 4:sL:36:TYR:OH     | 79:s2:294:U:OP1    | 2.08                     | 0.72              |
| 27:IF:171:ASP:OD2  | 27:IF:173:ALA:N    | 2.23                     | 0.72              |
| 33:IM:96:GLU:HA    | 33:IM:99:GLU:OE2   | 1.90                     | 0.72              |
| 43:IX:102:VAL:HA   | 43:IX:134:LYS:HG3  | 1.70                     | 0.72              |
| 63:lz:55:LEU:H     | 63:lz:154:THR:HG21 | 1.55                     | 0.72              |
| 79:s2:1244:U:H2'   | 79:s2:1245:G:H8    | 1.53                     | 0.72              |
| 79:s2:1384:C:H2'   | 79:s2:1385:G:H8    | 1.54                     | 0.72              |
| 85:L5:1482:G:O6    | 54:Li:4:ARG:NH1    | 2.20                     | 0.72              |
| 85:L5:4452:U:OP2   | 85:L5:4522:G:N1    | 2.22                     | 0.72              |
| 33:LM:104:MET:SD   | 33:LM:108:ASP:HB2  | 2.29                     | 0.72              |
| 60:Lo:21:HIS:HD2   | 60:Lo:70:LEU:HD13  | 1.55                     | 0.72              |
| 79:S2:866:U:H2'    | 79:S2:867:G:C8     | 2.25                     | 0.72              |
| 25:ID:211:LEU:HD21 | 25:ID:219:TYR:HA   | 1.71                     | 0.72              |
| 55:lj:64:MET:HB3   | 55:lj:68:LYS:HB3   | 1.70                     | 0.72              |
| 79:s2:974:C:H2'    | 79:s2:975:G:H8     | 1.55                     | 0.72              |
| 80:cB:19:ILE:HD12  | 80:cB:21:ASN:HD21  | 1.54                     | 0.72              |
| 85:l5:4773:C:O2    | 85:l5:4861:G:N2    | 2.17                     | 0.72              |
| 85:L5:2557:G:H1    | 85:L5:2570:U:H3    | 0.78                     | 0.72              |
| 24:LC:284:MET:HE1  | 37:LQ:124:ASP:HB3  | 1.71                     | 0.72              |
| 43:LX:76:ILE:HD12  | 43:LX:76:ILE:H     | 1.55                     | 0.72              |
| 71:ST:9:VAL:HG11   | 71:ST:138:VAL:HG23 | 1.72                     | 0.72              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:ID:40:ASP:OD1  | 25:ID:42:ASN:N    | 2.21                     | 0.72              |
| 34:IN:160:GLU:OE1 | 34:IN:160:GLU:N   | 2.20                     | 0.72              |
| 42:IV:56:GLY:N    | 42:IV:59:ASP:OD2  | 2.21                     | 0.72              |
| 64:sR:8:THR:HB    | 79:s2:1371:U:H4'  | 1.72                     | 0.72              |
| 79:s2:822:U:H3    | 79:s2:826:A:H62   | 1.36                     | 0.72              |
| 12:SH:37:LYS:HB3  | 12:SH:41:ARG:HE   | 1.53                     | 0.72              |
| 15:SC:272:HIS:HA  | 15:SC:275:LYS:HZ2 | 1.53                     | 0.72              |
| 85:L5:1974:U:H4'  | 85:L5:1975:G:H3'  | 1.71                     | 0.72              |
| 85:L5:3877:A:N3   | 85:L5:4401:G:O2'  | 2.22                     | 0.72              |
| 60:Lo:12:CYS:SG   | 60:Lo:79:SER:OG   | 2.47                     | 0.72              |
| 72:SU:28:ASN:ND2  | 72:SU:31:SER:OG   | 2.21                     | 0.72              |
| 79:S2:1488:C:O2'  | 79:S2:1490:G:OP2  | 2.07                     | 0.72              |
| 9:se:11:LYS:HE2   | 9:se:15:GLN:HE22  | 1.52                     | 0.71              |
| 19:sb:81:ARG:NH1  | 19:sb:82:LYS:O    | 2.22                     | 0.71              |
| 21:l8:11:C:O3'    | 36:lP:3:ARG:NH2   | 2.23                     | 0.71              |
| 23:lB:133:TYR:HA  | 23:lB:136:LYS:HE3 | 1.71                     | 0.71              |
| 73:sc:22:GLY:O    | 73:sc:26:GLN:NE2  | 2.21                     | 0.71              |
| 84:lt:128:THR:HB  | 85:l5:1995:G:H4'  | 1.71                     | 0.71              |
| 85:l5:1174:G:N2   | 85:l5:1187:G:N7   | 2.38                     | 0.71              |
| 6:SG:56:ASN:HD22  | 79:S2:156:G:H1'   | 1.54                     | 0.71              |
| 11:SB:182:LYS:NZ  | 11:SB:183:GLU:OE2 | 2.23                     | 0.71              |
| 85:L5:278:G:OP2   | 54:Li:30:ARG:NH2  | 2.23                     | 0.71              |
| 85:L5:364:G:N7    | 55:Lj:55:ARG:NH1  | 2.37                     | 0.71              |
| 27:LF:187:MET:N   | 27:LF:187:MET:SD  | 2.61                     | 0.71              |
| 37:LQ:122:THR:H   | 37:LQ:125:GLN:NE2 | 1.88                     | 0.71              |
| 59:Ln:2:ARG:NE    | 79:S2:1842:C:OP2  | 2.23                     | 0.71              |
| 59:Ln:9:ARG:HA    | 59:Ln:12:ARG:HG3  | 1.72                     | 0.71              |
| 74:Sd:13:LYS:NZ   | 79:S2:1556:A:O2'  | 2.22                     | 0.71              |
| 2:sE:45:ILE:HG13  | 2:sE:61:VAL:HG11  | 1.72                     | 0.71              |
| 2:sE:134:LYS:NZ   | 79:s2:127:C:O2    | 2.21                     | 0.71              |
| 3:sI:37:LYS:NZ    | 3:sI:93:THR:O     | 2.22                     | 0.71              |
| 13:sV:33:GLN:NE2  | 13:sV:53:TYR:O    | 2.23                     | 0.71              |
| 13:sV:57:GLY:O    | 13:sV:61:ARG:HB2  | 1.91                     | 0.71              |
| 22:lA:205:ASN:ND2 | 85:l5:1633:G:C8   | 2.59                     | 0.71              |
| 24:lC:281:MET:SD  | 37:lQ:110:ARG:NH2 | 2.63                     | 0.71              |
| 59:ln:11:ARG:HH11 | 79:s2:1183:A:H5'  | 1.54                     | 0.71              |
| 61:lp:29:ILE:HD11 | 61:lp:69:TRP:CG   | 2.24                     | 0.71              |
| 64:sR:41:ILE:HB   | 79:s2:1388:A:O4'  | 1.89                     | 0.71              |
| 79:s2:1536:G:H2'  | 79:s2:1537:A:C8   | 2.24                     | 0.71              |
| 81:aP:50:U:O4     | 81:aP:64:G:O6     | 2.08                     | 0.71              |
| 85:l5:1202:C:N3   | 85:l5:1203:G:O2'  | 2.23                     | 0.71              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 19:Sb:70:LYS:HZ2   | 79:S2:1106:C:H5''  | 1.56                     | 0.71              |
| 24:LC:208:CYS:SG   | 24:LC:248:ARG:NE   | 2.64                     | 0.71              |
| 55:Lj:11:ARG:HA    | 55:Lj:11:ARG:CZ    | 2.20                     | 0.71              |
| 1:CH:128:ILE:HG22  | 1:CH:130:LEU:H     | 1.53                     | 0.71              |
| 2:sE:15:PRO:HD3    | 2:sE:18:TRP:HZ3    | 1.54                     | 0.71              |
| 15:sC:60:TRP:CZ3   | 15:sC:96:PHE:HE2   | 2.09                     | 0.71              |
| 29:IH:44:GLU:HB3   | 29:IH:58:ASP:HB2   | 1.71                     | 0.71              |
| 34:IN:135:ILE:HG21 | 34:IN:151:ILE:HG21 | 1.71                     | 0.71              |
| 45:IZ:57:MET:N     | 45:IZ:57:MET:SD    | 2.63                     | 0.71              |
| 85:l5:1705:G:H2'   | 85:l5:1706:A:O4'   | 1.91                     | 0.71              |
| 8:SY:10:ARG:HA     | 79:S2:839:C:H41    | 1.54                     | 0.71              |
| 12:SH:55:GLY:O     | 12:SH:58:LYS:NZ    | 2.23                     | 0.71              |
| 15:SC:88:ILE:HD11  | 15:SC:93:ILE:HD11  | 1.72                     | 0.71              |
| 15:SC:267:GLN:HA   | 15:SC:270:THR:HB   | 1.72                     | 0.71              |
| 28:LG:219:VAL:HA   | 28:LG:222:ILE:HG22 | 1.71                     | 0.71              |
| 64:SR:9:VAL:HG23   | 64:SR:50:ILE:HD13  | 1.69                     | 0.71              |
| 67:SK:85:LEU:HD13  | 67:SK:89:ILE:HG21  | 1.71                     | 0.71              |
| 68:SP:107:ILE:HA   | 68:SP:111:MET:SD   | 2.30                     | 0.71              |
| 7:sJ:67:ASP:HB3    | 7:sJ:70:ARG:HB3    | 1.72                     | 0.71              |
| 19:sb:70:LYS:HE3   | 79:s2:1106:C:C5'   | 2.19                     | 0.71              |
| 23:IB:97:ARG:NH2   | 85:l5:4911:A:OP1   | 2.23                     | 0.71              |
| 37:IQ:11:ARG:NH2   | 85:l5:1690:C:OP2   | 2.23                     | 0.71              |
| 71:sT:42:HIS:HB3   | 71:sT:93:SER:HB3   | 1.70                     | 0.71              |
| 78:sf:133:ALA:O    | 78:sf:139:HIS:ND1  | 2.23                     | 0.71              |
| 80:cB:430:MET:SD   | 80:cB:484:THR:HG23 | 2.31                     | 0.71              |
| 85:l5:1367:C:O2'   | 85:l5:1369:C:OP2   | 2.07                     | 0.71              |
| 85:l5:1857:C:H2'   | 85:l5:1858:A:H8    | 1.55                     | 0.71              |
| 85:l5:4740:G:O6    | 85:l5:4959:U:O2    | 2.07                     | 0.71              |
| 85:L5:2333:G:H5''  | 24:LC:195:LYS:HE3  | 1.71                     | 0.71              |
| 85:L5:3946:G:H1    | 85:L5:4067:U:H3    | 1.36                     | 0.71              |
| 65:SD:18:LYS:NZ    | 74:Sd:49:ASP:O     | 2.23                     | 0.71              |
| 4:sL:128:VAL:HG13  | 4:sL:140:PHE:CE1   | 2.24                     | 0.71              |
| 24:IC:28:PHE:HD2   | 24:IC:132:ALA:HB2  | 1.56                     | 0.71              |
| 48:lc:36:LYS:NZ    | 48:lc:40:GLN:HE21  | 1.88                     | 0.71              |
| 64:sR:60:ARG:NH2   | 79:s2:1463:U:OP1   | 2.23                     | 0.71              |
| 65:sD:29:LEU:HB2   | 65:sD:34:TYR:HB2   | 1.73                     | 0.71              |
| 79:s2:557:U:H2'    | 79:s2:558:G:C8     | 2.26                     | 0.71              |
| 2:SE:133:THR:HG22  | 2:SE:134:LYS:HG2   | 1.73                     | 0.71              |
| 85:L5:1933:G:H2'   | 85:L5:1934:A:C8    | 2.25                     | 0.71              |
| 23:LB:216:MET:HG2  | 23:LB:354:GLN:OE1  | 1.89                     | 0.71              |
| 34:LN:138:PHE:HA   | 34:LN:143:ARG:HD3  | 1.71                     | 0.71              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 40:LT:45:MET:HE3   | 40:LT:94:GLU:HB2   | 1.72                     | 0.71              |
| 8:sY:17:LEU:HD23   | 8:sY:17:LEU:N      | 2.03                     | 0.71              |
| 10:sA:37:TYR:OH    | 13:sV:66:ASP:OD1   | 2.07                     | 0.71              |
| 33:IM:29:ASP:OD1   | 33:IM:30:VAL:N     | 2.23                     | 0.71              |
| 44:IY:1:MET:HA     | 44:IY:1:MET:HE3    | 1.72                     | 0.71              |
| 69:sQ:43:GLU:O     | 69:sQ:45:ARG:N     | 2.23                     | 0.71              |
| 81:aP:40:C:H2'     | 81:aP:41:G:H8      | 1.55                     | 0.71              |
| 85:l5:1269:G:O2'   | 85:l5:1440:U:O2'   | 2.06                     | 0.71              |
| 85:l5:3970:G:O2'   | 85:l5:4052:C:N4    | 2.20                     | 0.71              |
| 80:CB:305:MET:SD   | 80:CB:306:ASN:ND2  | 2.64                     | 0.71              |
| 80:CB:396:MET:SD   | 80:CB:416:VAL:HA   | 2.31                     | 0.71              |
| 2:SE:136:ILE:HB    | 2:SE:149:TYR:HE2   | 1.55                     | 0.71              |
| 6:SG:189:ARG:NH2   | 79:S2:332:G:O6     | 2.23                     | 0.71              |
| 7:SJ:31:LEU:O      | 7:SJ:35:TYR:HB2    | 1.91                     | 0.71              |
| 85:L5:1424:G:H1'   | 47:Lb:29:TYR:HE2   | 1.55                     | 0.71              |
| 85:L5:2780:C:H2'   | 85:L5:2781:G:H8    | 1.55                     | 0.71              |
| 21:L8:67:U:H5''    | 55:Lj:86:PRO:HA    | 1.73                     | 0.71              |
| 77:SZ:102:LYS:HA   | 77:SZ:107:VAL:HG12 | 1.72                     | 0.71              |
| 79:S2:1144:A:H2'   | 79:S2:1145:A:C8    | 2.25                     | 0.71              |
| 82:PE:6:G:H1       | 82:PE:67:U:H3      | 1.37                     | 0.71              |
| 82:PE:41:U:H2'     | 82:PE:42:G:H8      | 1.55                     | 0.71              |
| 2:sE:15:PRO:HD3    | 2:sE:18:TRP:CZ3    | 2.25                     | 0.71              |
| 6:sG:132:ARG:CZ    | 79:s2:167:G:C2     | 2.73                     | 0.71              |
| 21:l8:138:C:H2'    | 21:l8:139:G:H8     | 1.56                     | 0.71              |
| 34:IN:115:VAL:HG21 | 34:IN:160:GLU:HB3  | 1.72                     | 0.71              |
| 52:lg:64:LEU:HA    | 52:lg:67:LEU:CD2   | 2.20                     | 0.71              |
| 57:ll:2:SER:N      | 85:l5:2406:G:N7    | 2.37                     | 0.71              |
| 77:sZ:47:LEU:HD13  | 77:sZ:79:ILE:HG13  | 1.72                     | 0.71              |
| 2:SE:118:GLU:HG2   | 2:SE:121:TYR:CE2   | 2.25                     | 0.71              |
| 12:SH:53:VAL:HG21  | 12:SH:175:GLY:HA3  | 1.71                     | 0.71              |
| 15:SC:183:LYS:HG2  | 18:SW:95:PRO:HA    | 1.73                     | 0.71              |
| 85:L5:2369:U:O2'   | 49:Ld:39:LYS:NZ    | 2.23                     | 0.71              |
| 85:L5:4110:C:O2'   | 85:L5:4111:U:OP1   | 2.07                     | 0.71              |
| 22:LA:107:MET:HB2  | 22:LA:111:THR:HG21 | 1.73                     | 0.71              |
| 25:LD:69:ILE:HD13  | 40:LT:31:MET:HG2   | 1.71                     | 0.71              |
| 26:LE:150:LEU:HD12 | 26:LE:151:ILE:N    | 2.06                     | 0.71              |
| 79:S2:878:G:H1     | 79:S2:908:A:H61    | 1.36                     | 0.71              |
| 79:S2:1277:C:H2'   | 79:S2:1278:A:H8    | 1.55                     | 0.71              |
| 79:S2:1401:A:H2'   | 79:S2:1402:A:C8    | 2.26                     | 0.71              |
| 9:se:31:ARG:NH2    | 79:s2:523:A:OP1    | 2.23                     | 0.71              |
| 24:lC:326:LEU:HD12 | 24:lC:330:PRO:HA   | 1.72                     | 0.71              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 31:IJ:90:ARG:O    | 31:IJ:93:GLU:HG2   | 1.91                     | 0.71              |
| 45:IZ:122:TYR:HB2 | 45:IZ:131:PHE:CE2  | 2.26                     | 0.71              |
| 64:sR:49:LYS:NZ   | 79:s2:1370:A:N7    | 2.34                     | 0.71              |
| 79:s2:1115:U:H3   | 79:s2:1118:C:H41   | 1.39                     | 0.71              |
| 79:s2:1171:G:O2'  | 79:s2:1187:G:O6    | 2.08                     | 0.71              |
| 80:CB:50:ARG:NH1  | 79:S2:463:C:O3'    | 2.21                     | 0.71              |
| 6:SG:76:LEU:HA    | 6:SG:94:ARG:HA     | 1.73                     | 0.71              |
| 85:L5:2519:U:O2'  | 85:L5:2530:U:O2    | 2.07                     | 0.71              |
| 85:L5:3956:G:H21  | 85:L5:3963:A:H1'   | 1.55                     | 0.71              |
| 75:Sg:76:GLN:NE2  | 75:Sg:91:ASP:OD1   | 2.24                     | 0.71              |
| 10:sA:41:ARG:NH1  | 10:sA:42:LYS:O     | 2.24                     | 0.71              |
| 26:lE:74:SER:O    | 47:lb:117:ARG:NH2  | 2.23                     | 0.71              |
| 36:lP:50:ASP:OD2  | 36:lP:55:LYS:HB2   | 1.91                     | 0.71              |
| 66:sF:44:LYS:NZ   | 69:sQ:114:GLN:HE22 | 1.89                     | 0.71              |
| 79:s2:878:G:H1    | 79:s2:908:A:H61    | 0.76                     | 0.71              |
| 85:l5:2045:G:N2   | 85:l5:2046:G:N7    | 2.38                     | 0.71              |
| 18:SW:51:GLU:HB2  | 18:SW:62:VAL:HG13  | 1.73                     | 0.71              |
| 85:L5:68:U:OP1    | 34:LN:178:HIS:ND1  | 2.22                     | 0.71              |
| 79:S2:165:G:OP2   | 79:S2:165:G:N2     | 2.19                     | 0.71              |
| 79:S2:526:A:H2'   | 79:S2:527:C:C6     | 2.26                     | 0.71              |
| 1:cH:46:ALA:HA    | 9:se:41:ARG:HG2    | 1.73                     | 0.71              |
| 3:sI:74:ARG:NH1   | 79:s2:302:A:O5'    | 2.22                     | 0.71              |
| 9:se:13:ARG:NH2   | 79:s2:634:A:OP1    | 2.24                     | 0.71              |
| 12:sH:30:LEU:O    | 12:sH:33:ASN:ND2   | 2.23                     | 0.71              |
| 30:II:86:HIS:HB3  | 30:II:139:ARG:HG3  | 1.73                     | 0.71              |
| 56:lk:35:LYS:NZ   | 85:l5:2695:A:OP1   | 2.22                     | 0.71              |
| 64:sR:32:LYS:HG2  | 79:s2:1453:C:H2'   | 1.73                     | 0.71              |
| 79:s2:1729:U:O2   | 79:s2:1805:G:N2    | 2.15                     | 0.71              |
| 85:l5:966:A:OP1   | 85:l5:967:C:N4     | 2.24                     | 0.71              |
| 85:l5:2599:G:N2   | 85:l5:2747:U:O4    | 2.24                     | 0.71              |
| 7:SJ:38:ARG:NH1   | 79:S2:643:A:OP1    | 2.24                     | 0.71              |
| 17:SO:135:ILE:O   | 79:S2:943:U:O2'    | 2.09                     | 0.71              |
| 85:L5:2702:C:OP1  | 41:LU:101:ARG:NH2  | 2.23                     | 0.71              |
| 85:L5:4095:G:H5'' | 85:L5:4110:C:N3    | 2.06                     | 0.71              |
| 63:Lz:55:LEU:HD11 | 63:Lz:183:ILE:HG12 | 1.73                     | 0.71              |
| 79:S2:1244:U:H2'  | 79:S2:1245:G:H8    | 1.54                     | 0.71              |
| 79:S2:1546:G:H21  | 79:S2:1670:C:H1'   | 1.56                     | 0.71              |
| 6:sG:175:LYS:NZ   | 79:s2:77:A:N3      | 2.39                     | 0.70              |
| 10:sA:85:ARG:NH2  | 10:sA:202:TYR:HA   | 2.04                     | 0.70              |
| 21:l8:67:U:H2'    | 21:l8:68:G:H8      | 1.56                     | 0.70              |
| 24:lC:325:MET:HE1 | 27:lF:155:TYR:CD1  | 2.26                     | 0.70              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:1F:96:ARG:NH2   | 85:15:1895:G:OP1   | 2.24                     | 0.70              |
| 27:1F:232:ASP:HB3  | 27:1F:236:ARG:HH22 | 1.57                     | 0.70              |
| 31:1J:95:ARG:HD3   | 31:1J:95:ARG:H     | 1.56                     | 0.70              |
| 36:1P:115:GLU:OE2  | 36:1P:151:THR:HG21 | 1.91                     | 0.70              |
| 36:1P:126:ARG:HG2  | 36:1P:140:MET:HE1  | 1.71                     | 0.70              |
| 41:1U:110:TYR:OH   | 85:15:2621:A:OP2   | 2.09                     | 0.70              |
| 47:1b:117:ARG:NH2  | 85:15:1273:G:O4'   | 2.24                     | 0.70              |
| 66:sF:124:ASP:OD2  | 66:sF:125:SER:N    | 2.22                     | 0.70              |
| 69:sQ:13:PHE:CD2   | 79:s2:1443:C:H5'   | 2.26                     | 0.70              |
| 78:sf:132:MET:HG3  | 78:sf:139:HIS:CE1  | 2.26                     | 0.70              |
| 79:s2:527:C:H2'    | 79:s2:528:A:C8     | 2.26                     | 0.70              |
| 79:s2:567:C:O2'    | 79:s2:583:A:N6     | 2.22                     | 0.70              |
| 79:s2:746:C:H2'    | 79:s2:747:U:C6     | 2.26                     | 0.70              |
| 79:s2:1550:G:H3'   | 79:s2:1579:A:H61   | 1.55                     | 0.70              |
| 85:15:3917:A:H2'   | 85:15:3918:G:H8    | 1.55                     | 0.70              |
| 80:CB:22:MET:HE1   | 80:CB:100:ILE:HG23 | 1.71                     | 0.70              |
| 85:L5:519:C:H1'    | 85:L5:643:C:C2     | 2.26                     | 0.70              |
| 1:CH:73:VAL:HG11   | 1:CH:114:ALA:HB3   | 1.73                     | 0.70              |
| 14:sa:43:ASN:HB3   | 14:sa:66:LYS:HD3   | 1.73                     | 0.70              |
| 23:1B:20:LYS:HD3   | 85:15:4717:A:H4'   | 1.71                     | 0.70              |
| 26:1E:161:ARG:NH1  | 26:1E:273:SER:OG   | 2.23                     | 0.70              |
| 52:lg:44:SER:OG    | 52:lg:46:CYS:SG    | 2.48                     | 0.70              |
| 64:sR:27:ASP:HB2   | 64:sR:55:THR:HG21  | 1.73                     | 0.70              |
| 71:sT:31:PRO:HD2   | 71:sT:53:PHE:HE2   | 1.56                     | 0.70              |
| 85:15:1933:G:H2'   | 85:15:1934:A:C8    | 2.27                     | 0.70              |
| 85:15:2484:A:H62   | 85:15:2494:U:H3    | 1.40                     | 0.70              |
| 2:SE:19:MET:HB3    | 2:SE:51:ARG:HH22   | 1.55                     | 0.70              |
| 85:L5:4095:G:H1'   | 85:L5:4109:G:H1'   | 1.72                     | 0.70              |
| 71:ST:75:MET:HE2   | 71:ST:75:MET:HA    | 1.71                     | 0.70              |
| 79:S2:830:A:OP2    | 79:S2:846:G:N2     | 2.21                     | 0.70              |
| 79:S2:1755:C:H2'   | 79:S2:1756:C:C6    | 2.26                     | 0.70              |
| 12:sH:144:ILE:HG13 | 12:sH:152:ARG:HD2  | 1.74                     | 0.70              |
| 19:sb:83:GLN:NE2   | 19:sb:84:HIS:O     | 2.24                     | 0.70              |
| 20:17:39:C:H2'     | 20:17:40:U:C6      | 2.27                     | 0.70              |
| 55:lj:67:LEU:HG    | 55:lj:71:TYR:HE2   | 1.54                     | 0.70              |
| 85:15:2749:C:H2'   | 85:15:2750:G:H8    | 1.56                     | 0.70              |
| 86:Se:28:LYS:NZ    | 79:S2:526:A:OP2    | 2.21                     | 0.70              |
| 86:Se:34:ARG:NH2   | 79:S2:642:U:OP2    | 2.25                     | 0.70              |
| 11:SB:101:HIS:HA   | 11:SB:217:MET:HE3  | 1.72                     | 0.70              |
| 85:L5:1333:A:H2'   | 85:L5:1334:A:H8    | 1.54                     | 0.70              |
| 85:L5:1514:U:H2'   | 85:L5:1515:A:H8    | 1.57                     | 0.70              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 85:L5:4096:C:H5''  | 85:L5:4108:G:N7   | 2.06                     | 0.70              |
| 45:LZ:124:THR:HG1  | 45:LZ:126:LYS:HZ2 | 1.39                     | 0.70              |
| 66:SF:179:ASN:HA   | 66:SF:182:LYS:HZ2 | 1.53                     | 0.70              |
| 71:ST:67:ARG:NH2   | 79:S2:1587:G:OP1  | 2.23                     | 0.70              |
| 83:LS:26:LYS:HD3   | 83:LS:194:ASP:HB3 | 1.73                     | 0.70              |
| 4:sL:7:GLU:HG3     | 4:sL:9:ALA:H      | 1.56                     | 0.70              |
| 24:IC:76:ILE:HD11  | 24:IC:96:CYS:SG   | 2.31                     | 0.70              |
| 26:IE:146:PRO:O    | 26:IE:200:LYS:NZ  | 2.22                     | 0.70              |
| 29:IH:95:VAL:HG12  | 58:Im:82:LEU:HD22 | 1.73                     | 0.70              |
| 53:Ih:101:ASN:O    | 53:Ih:103:LYS:NZ  | 2.23                     | 0.70              |
| 71:sT:101:ARG:NH2  | 79:s2:1566:G:N7   | 2.40                     | 0.70              |
| 75:sg:59:LEU:HD11  | 75:sg:90:TRP:CE3  | 2.27                     | 0.70              |
| 85:l5:1346:C:H2'   | 85:l5:1347:G:C8   | 2.25                     | 0.70              |
| 4:SL:80:MET:HA     | 4:SL:86:ILE:HD11  | 1.72                     | 0.70              |
| 85:L5:2475:G:N1    | 43:LX:51:THR:O    | 2.19                     | 0.70              |
| 64:SR:116:ASN:OD1  | 64:SR:117:LEU:N   | 2.24                     | 0.70              |
| 69:SQ:43:GLU:OE2   | 79:S2:1543:U:O2'  | 2.08                     | 0.70              |
| 73:Sc:23:SER:O     | 79:S2:1681:U:O2'  | 2.10                     | 0.70              |
| 2:sE:188:ASN:ND2   | 2:sE:220:THR:OG1  | 2.24                     | 0.70              |
| 10:sA:17:LYS:HA    | 10:sA:17:LYS:HE3  | 1.71                     | 0.70              |
| 22:IA:36:GLU:OE1   | 22:IA:163:ARG:NH1 | 2.25                     | 0.70              |
| 42:IV:139:ILE:HD12 | 42:IV:140:ALA:H   | 1.57                     | 0.70              |
| 51:lf:4:ARG:NH1    | 51:lf:6:TRP:O     | 2.24                     | 0.70              |
| 65:sD:175:VAL:HB   | 65:sD:182:LEU:HB2 | 1.74                     | 0.70              |
| 76:sM:36:ARG:NH1   | 79:s2:1310:U:OP2  | 2.22                     | 0.70              |
| 85:l5:1377:G:H4'   | 85:l5:1378:C:H3'  | 1.74                     | 0.70              |
| 85:l5:1972:G:H2'   | 85:l5:1973:G:C8   | 2.26                     | 0.70              |
| 2:SE:94:LYS:O      | 8:SY:16:ARG:NH2   | 2.25                     | 0.70              |
| 85:L5:2658:G:O2'   | 85:L5:2675:G:N2   | 2.23                     | 0.70              |
| 85:L5:3967:G:N2    | 85:L5:4055:U:O2   | 2.19                     | 0.70              |
| 85:L5:4184:G:H5'   | 22:LA:233:ARG:HB2 | 1.73                     | 0.70              |
| 75:Sg:283:PRO:O    | 75:Sg:285:GLN:NE2 | 2.24                     | 0.70              |
| 11:sB:26:SER:O     | 11:sB:51:ARG:NH2  | 2.24                     | 0.70              |
| 16:sN:107:LYS:NZ   | 79:s2:937:C:OP1   | 2.21                     | 0.70              |
| 18:sW:37:PHE:O     | 18:sW:41:MET:HG2  | 1.90                     | 0.70              |
| 29:IH:4:ILE:HG12   | 39:IS:144:GLN:NE2 | 2.06                     | 0.70              |
| 51:lf:91:ASN:O     | 85:l5:440:U:O2'   | 2.10                     | 0.70              |
| 54:li:68:ARG:NH1   | 85:l5:3723:A:OP2  | 2.24                     | 0.70              |
| 66:sF:87:LEU:HD11  | 79:s2:1592:C:H5'  | 1.72                     | 0.70              |
| 79:s2:1528:G:O2'   | 79:s2:1666:C:OP1  | 2.08                     | 0.70              |
| 84:lt:121:LEU:HD11 | 85:l5:1972:G:N3   | 2.07                     | 0.70              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 85:l5:179:G:H2'   | 85:l5:180:C:C6     | 2.26                     | 0.70              |
| 85:l5:2705:G:H1   | 85:l5:2710:C:H41   | 1.40                     | 0.70              |
| 85:l5:3948:C:HO2' | 85:l5:4065:G:H1    | 1.38                     | 0.70              |
| 2:SE:11:ARG:NH1   | 2:SE:21:ASP:OD1    | 2.25                     | 0.70              |
| 10:SA:63:ARG:HH21 | 13:SV:38:GLU:HA    | 1.56                     | 0.70              |
| 12:SH:70:LYS:O    | 12:SH:70:LYS:NZ    | 2.23                     | 0.70              |
| 85:L5:4101:C:H3'  | 85:L5:4106:G:C2'   | 2.21                     | 0.70              |
| 85:L5:4636:U:O4   | 49:Ld:78:ARG:NH1   | 2.24                     | 0.70              |
| 23:LB:282:LYS:HB3 | 23:LB:333:LEU:HD11 | 1.74                     | 0.70              |
| 75:Sg:60:ARG:HD2  | 75:Sg:61:GLY:N     | 2.06                     | 0.70              |
| 12:sH:10:LYS:O    | 12:sH:10:LYS:HG3   | 1.91                     | 0.70              |
| 13:sV:1:MET:HE2   | 13:sV:10:ASP:HB3   | 1.72                     | 0.70              |
| 21:l8:141:C:OP1   | 34:lN:38:ARG:NH1   | 2.24                     | 0.70              |
| 22:lA:208:GLU:OE1 | 85:l5:1629:G:N1    | 2.24                     | 0.70              |
| 26:lE:164:PHE:HA  | 26:lE:175:VAL:HG12 | 1.73                     | 0.70              |
| 31:lJ:35:ARG:HB3  | 31:lJ:123:ILE:CD1  | 2.20                     | 0.70              |
| 33:lM:90:ARG:HA   | 33:lM:93:LYS:HG2   | 1.74                     | 0.70              |
| 56:lk:23:VAL:HG13 | 56:lk:64:LEU:HD21  | 1.73                     | 0.70              |
| 79:s2:941:C:H2'   | 79:s2:942:G:C8     | 2.27                     | 0.70              |
| 80:CB:615:GLU:N   | 80:CB:615:GLU:OE1  | 2.22                     | 0.70              |
| 8:SY:21:LYS:NZ    | 79:S2:841:G:OP2    | 2.23                     | 0.70              |
| 11:SB:222:LYS:NZ  | 11:SB:224:GLU:OE1  | 2.25                     | 0.70              |
| 85:L5:2611:A:H5'  | 85:L5:2688:G:H4'   | 1.72                     | 0.70              |
| 85:L5:4689:U:OP1  | 29:LH:184:LYS:NZ   | 2.23                     | 0.70              |
| 71:ST:40:ALA:O    | 71:ST:43:LYS:N     | 2.21                     | 0.70              |
| 75:Sg:62:HIS:NE2  | 75:Sg:80:SER:OG    | 2.24                     | 0.70              |
| 76:SM:116:LYS:N   | 76:SM:116:LYS:HD3  | 2.06                     | 0.70              |
| 15:sC:196:ILE:HB  | 15:sC:223:TYR:HB2  | 1.72                     | 0.70              |
| 18:sW:87:GLU:N    | 18:sW:87:GLU:OE1   | 2.24                     | 0.70              |
| 24:lC:307:LYS:NZ  | 85:l5:2089:G:O2'   | 2.23                     | 0.70              |
| 28:lG:34:LYS:HE3  | 85:l5:4129:G:H1'   | 1.74                     | 0.70              |
| 44:lY:132:LYS:NZ  | 85:l5:246:G:OP2    | 2.20                     | 0.70              |
| 68:sP:31:GLU:OE1  | 68:sP:31:GLU:N     | 2.21                     | 0.70              |
| 72:sU:18:HIS:CE1  | 72:sU:94:PRO:HA    | 2.27                     | 0.70              |
| 75:sg:22:ALA:HB3  | 75:sg:32:LEU:HD11  | 1.74                     | 0.70              |
| 77:sZ:47:LEU:HD22 | 77:sZ:79:ILE:HG23  | 1.72                     | 0.70              |
| 80:cB:5:THR:O     | 80:cB:8:GLN:NE2    | 2.21                     | 0.70              |
| 85:L5:278:G:H5''  | 34:LN:8:GLN:HE22   | 1.56                     | 0.70              |
| 85:L5:2092:G:O2'  | 85:L5:2262:G:N2    | 2.24                     | 0.70              |
| 85:L5:2624:G:N7   | 41:LU:88:LYS:NZ    | 2.39                     | 0.70              |
| 85:L5:4076:G:OP1  | 28:LG:73:ARG:NH1   | 2.24                     | 0.70              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 85:L5:4888:U:O2   | 85:L5:4931:G:N1    | 2.20                     | 0.70              |
| 30:LI:171:TRP:HB2 | 30:LI:178:ALA:HA   | 1.74                     | 0.70              |
| 65:SD:103:GLU:O   | 65:SD:106:ARG:HG2  | 1.91                     | 0.70              |
| 66:SF:99:ILE:HA   | 66:SF:102:LEU:HG   | 1.73                     | 0.70              |
| 71:ST:32:GLU:OE1  | 71:ST:32:GLU:N     | 2.19                     | 0.70              |
| 71:ST:102:ARG:NH2 | 79:S2:1566:G:OP2   | 2.24                     | 0.70              |
| 87:IW:20:ARG:HH12 | 87:IW:30:GLN:HB2   | 1.57                     | 0.70              |
| 1:cH:126:ARG:NH2  | 79:s2:551:U:O2'    | 2.20                     | 0.70              |
| 33:IM:70:GLN:NE2  | 85:l5:736:C:OP2    | 2.25                     | 0.70              |
| 66:sF:88:MET:HE1  | 79:s2:1535:U:O3'   | 1.92                     | 0.70              |
| 69:sQ:15:ARG:NH2  | 79:s2:1444:U:OP1   | 2.25                     | 0.70              |
| 75:sg:8:ARG:HD3   | 75:sg:311:GLN:HG3  | 1.74                     | 0.70              |
| 79:s2:557:U:H3'   | 79:s2:558:G:H2'    | 1.73                     | 0.70              |
| 79:s2:677:G:N1    | 79:s2:1027:A:OP2   | 2.20                     | 0.70              |
| 79:s2:1757:G:O6   | 79:s2:1758:G:N2    | 2.25                     | 0.70              |
| 85:l5:3877:A:N3   | 85:l5:4401:G:O2'   | 2.22                     | 0.70              |
| 2:SE:134:LYS:N    | 79:S2:298:G:OP1    | 2.25                     | 0.70              |
| 5:SX:73:GLN:NE2   | 5:SX:78:GLY:O      | 2.24                     | 0.70              |
| 17:SO:56:VAL:HG13 | 17:SO:77:ALA:HB1   | 1.73                     | 0.70              |
| 26:LE:178:PRO:O   | 26:LE:181:LEU:N    | 2.16                     | 0.70              |
| 35:LO:157:GLU:OE1 | 35:LO:160:ARG:NE   | 2.24                     | 0.70              |
| 75:Sg:262:GLU:N   | 75:Sg:262:GLU:OE1  | 2.25                     | 0.70              |
| 6:sG:32:MET:HG2   | 6:sG:63:MET:HE1    | 1.72                     | 0.70              |
| 6:sG:44:GLU:HG2   | 6:sG:45:TRP:CZ3    | 2.27                     | 0.70              |
| 6:sG:48:TYR:OH    | 6:sG:116:LYS:NZ    | 2.24                     | 0.70              |
| 18:sW:111:MET:N   | 18:sW:111:MET:SD   | 2.65                     | 0.70              |
| 23:lB:174:ARG:NH1 | 85:l5:4985:U:O2    | 2.17                     | 0.70              |
| 30:II:43:VAL:HG21 | 30:II:192:PRO:HB3  | 1.73                     | 0.70              |
| 41:lU:52:LYS:NZ   | 41:lU:54:GLY:O     | 2.25                     | 0.70              |
| 52:lg:11:LEU:HD21 | 85:l5:2513:A:OP2   | 1.92                     | 0.70              |
| 66:sF:71:ARG:NH2  | 79:s2:1677:U:OP1   | 2.25                     | 0.70              |
| 72:sU:26:SER:HB3  | 72:sU:32:LEU:HD21  | 1.72                     | 0.70              |
| 80:CB:531:ASP:HB3 | 80:CB:534:VAL:HG12 | 1.73                     | 0.70              |
| 85:L5:1705:G:H2'  | 85:L5:1706:A:O4'   | 1.91                     | 0.70              |
| 85:L5:2801:U:O2'  | 55:Lj:12:ARG:NH1   | 2.25                     | 0.70              |
| 85:L5:4274:A:H2'  | 85:L5:4275:G:C8    | 2.27                     | 0.70              |
| 29:LH:86:LEU:O    | 29:LH:186:THR:OG1  | 2.10                     | 0.70              |
| 59:Ln:17:ARG:NH1  | 79:S2:1173:A:H5''  | 2.03                     | 0.70              |
| 65:SD:8:LYS:NZ    | 79:S2:1550:G:OP2   | 2.24                     | 0.70              |
| 69:SQ:10:VAL:HG12 | 69:SQ:95:TYR:HD1   | 1.55                     | 0.70              |
| 72:SU:22:ILE:HD13 | 72:SU:114:VAL:HG23 | 1.74                     | 0.70              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 6:sG:186:GLN:HG3   | 6:sG:189:ARG:HH21  | 1.57                     | 0.69              |
| 24:IC:103:ALA:HA   | 85:l5:1517:G:H22   | 1.56                     | 0.69              |
| 26:IE:99:ASP:OD1   | 26:IE:100:LYS:N    | 2.22                     | 0.69              |
| 26:IE:272:ARG:NH2  | 85:l5:4884:G:N7    | 2.39                     | 0.69              |
| 27:IF:85:ALA:HB2   | 40:IT:138:ALA:H    | 1.57                     | 0.69              |
| 28:IG:98:LEU:HD13  | 28:IG:214:ALA:HB1  | 1.74                     | 0.69              |
| 29:IH:60:TRP:CZ2   | 33:IM:6:PHE:HZ     | 2.10                     | 0.69              |
| 35:IO:54:TYR:OH    | 35:IO:73:PHE:O     | 2.09                     | 0.69              |
| 53:lh:32:ARG:NH1   | 53:lh:36:VAL:HB    | 2.07                     | 0.69              |
| 58:lm:97:ARG:HH21  | 85:l5:4423:U:H3'   | 1.56                     | 0.69              |
| 63:lz:204:LEU:HD12 | 63:lz:216:LEU:HB3  | 1.73                     | 0.69              |
| 64:sR:3:ARG:HH22   | 79:s2:1467:C:H1'   | 1.56                     | 0.69              |
| 67:sK:14:LEU:HA    | 67:sK:17:LYS:HG2   | 1.73                     | 0.69              |
| 71:sT:84:ARG:NH2   | 79:s2:1605:G:OP1   | 2.24                     | 0.69              |
| 75:sg:8:ARG:HB2    | 75:sg:311:GLN:HB2  | 1.72                     | 0.69              |
| 79:s2:1446:A:HO2'  | 79:s2:1447:G:H8    | 1.37                     | 0.69              |
| 80:cB:481:LYS:NZ   | 80:cB:528:ALA:O    | 2.23                     | 0.69              |
| 82:pE:42:G:H2'     | 82:pE:43:A:H8      | 1.57                     | 0.69              |
| 85:l5:2770:C:H2'   | 85:l5:2771:G:H8    | 1.57                     | 0.69              |
| 85:l5:4238:G:H2'   | 85:l5:4239:A:C8    | 2.27                     | 0.69              |
| 85:l5:4670:C:O2'   | 85:l5:4672:A:OP2   | 2.10                     | 0.69              |
| 80:CB:686:ALA:HB1  | 80:CB:729:LEU:HD22 | 1.74                     | 0.69              |
| 85:L5:4896:G:OP1   | 33:LM:132:LYS:NZ   | 2.25                     | 0.69              |
| 25:LD:200:MET:HE1  | 25:LD:240:TYR:HB2  | 1.74                     | 0.69              |
| 31:LJ:32:ARG:HA    | 31:LJ:35:ARG:HD3   | 1.73                     | 0.69              |
| 63:Lz:68:LEU:HD22  | 63:Lz:90:LEU:HD22  | 1.73                     | 0.69              |
| 74:Sd:10:HIS:NE2   | 79:S2:1261:C:O2    | 2.21                     | 0.69              |
| 79:S2:1854:U:H2'   | 79:S2:1855:G:H8    | 1.56                     | 0.69              |
| 6:sG:131:ARG:N     | 87:IW:81:ALA:O     | 2.23                     | 0.69              |
| 7:sJ:179:LYS:HD2   | 7:sJ:179:LYS:C     | 2.16                     | 0.69              |
| 8:sY:18:LEU:HG     | 8:sY:20:ARG:CD     | 2.15                     | 0.69              |
| 10:sA:183:LEU:O    | 10:sA:188:THR:OG1  | 2.09                     | 0.69              |
| 14:sa:71:LEU:HD11  | 14:sa:73:TYR:HE2   | 1.57                     | 0.69              |
| 24:IC:350:ARG:NH1  | 85:l5:725:G:OP2    | 2.25                     | 0.69              |
| 31:IJ:95:ARG:O     | 31:IJ:175:LEU:N    | 2.23                     | 0.69              |
| 39:IS:16:CYS:HA    | 39:IS:59:GLY:HA2   | 1.72                     | 0.69              |
| 50:le:77:PHE:HD2   | 62:lr:23:GLN:HE21  | 1.38                     | 0.69              |
| 51:lf:77:ALA:HA    | 51:lf:84:VAL:HG22  | 1.72                     | 0.69              |
| 52:lg:54:ARG:NH1   | 85:l5:2653:C:H1'   | 2.06                     | 0.69              |
| 74:sd:5:GLN:HE22   | 79:s2:1301:A:P     | 2.15                     | 0.69              |
| 76:sM:24:THR:HA    | 76:sM:27:ILE:HD12  | 1.73                     | 0.69              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 79:s2:1726:G:O6    | 79:s2:1809:A:N6    | 2.25                     | 0.69              |
| 85:l5:3589:G:N2    | 85:l5:3590:G:N7    | 2.39                     | 0.69              |
| 85:l5:4478:G:O2'   | 85:l5:4602:A:N1    | 2.24                     | 0.69              |
| 10:SA:23:THR:HG21  | 10:SA:173:LEU:HD13 | 1.74                     | 0.69              |
| 85:L5:1517:G:H22   | 24:LC:103:ALA:HA   | 1.57                     | 0.69              |
| 26:LE:223:ARG:NH2  | 26:LE:238:GLU:OE2  | 2.25                     | 0.69              |
| 29:LH:115:ARG:O    | 29:LH:124:ARG:NH2  | 2.24                     | 0.69              |
| 39:LS:93:MET:SD    | 39:LS:93:MET:N     | 2.65                     | 0.69              |
| 75:Sg:17:TRP:H     | 75:Sg:36:ARG:HB2   | 1.56                     | 0.69              |
| 75:Sg:165:ILE:HD11 | 75:Sg:179:LEU:HD23 | 1.73                     | 0.69              |
| 79:S2:149:A:H3'    | 79:S2:150:A:H8     | 1.57                     | 0.69              |
| 79:S2:1115:U:H3    | 79:S2:1118:C:H41   | 1.38                     | 0.69              |
| 7:sJ:63:LEU:O      | 7:sJ:70:ARG:NH1    | 2.24                     | 0.69              |
| 13:sV:34:MET:O     | 13:sV:52:THR:OG1   | 2.09                     | 0.69              |
| 27:lF:165:LYS:NZ   | 85:l5:2274:C:O2    | 2.25                     | 0.69              |
| 33:lM:8:GLU:OE2    | 39:lS:151:LYS:NZ   | 2.25                     | 0.69              |
| 65:sD:150:MET:CE   | 65:sD:152:PHE:CZ   | 2.75                     | 0.69              |
| 85:l5:3664:G:H2'   | 85:l5:3665:G:H8    | 1.58                     | 0.69              |
| 85:l5:3717:A:H2'   | 85:l5:3718:A:H8    | 1.55                     | 0.69              |
| 80:CB:28:VAL:HG21  | 85:L5:4606:G:H5''  | 1.74                     | 0.69              |
| 3:SI:10:LYS:NZ     | 79:S2:370:G:O2'    | 2.25                     | 0.69              |
| 18:SW:37:PHE:CE1   | 18:SW:41:MET:HE2   | 2.28                     | 0.69              |
| 85:L5:181:C:H3'    | 85:L5:182:G:H8     | 1.58                     | 0.69              |
| 85:L5:1269:G:O2'   | 85:L5:1440:U:O2'   | 2.10                     | 0.69              |
| 85:L5:1501:C:H2'   | 37:LQ:68:ARG:NH1   | 2.07                     | 0.69              |
| 85:L5:5055:G:N2    | 49:Ld:118:GLN:OE1  | 2.24                     | 0.69              |
| 79:S2:76:U:O2'     | 79:S2:78:C:OP1     | 2.10                     | 0.69              |
| 79:S2:1115:U:O2'   | 79:S2:1117:C:OP2   | 2.07                     | 0.69              |
| 79:S2:1677:U:H2'   | 79:S2:1678:A:H8    | 1.57                     | 0.69              |
| 8:sY:37:LYS:HA     | 8:sY:40:ILE:HD12   | 1.74                     | 0.69              |
| 9:se:33:LYS:HA     | 9:se:36:MET:HE1    | 1.74                     | 0.69              |
| 13:sV:16:LYS:HA    | 13:sV:23:ILE:HA    | 1.73                     | 0.69              |
| 22:lA:71:LYS:HE3   | 85:l5:2595:C:C5'   | 2.19                     | 0.69              |
| 69:sQ:13:PHE:CE2   | 79:s2:1443:C:H5'   | 2.28                     | 0.69              |
| 70:sS:88:LYS:NZ    | 79:s2:1613:G:OP1   | 2.24                     | 0.69              |
| 79:s2:1438:A:H2'   | 79:s2:1439:A:H8    | 1.56                     | 0.69              |
| 80:cB:822:GLY:H    | 80:cB:830:ARG:NH2  | 1.90                     | 0.69              |
| 85:l5:67:C:N4      | 85:l5:325:U:O2'    | 2.23                     | 0.69              |
| 85:l5:513:U:N3     | 85:l5:516:C:OP2    | 2.25                     | 0.69              |
| 85:l5:4260:U:H2'   | 85:l5:4261:C:C6    | 2.27                     | 0.69              |
| 4:SL:99:TYR:CD2    | 5:SX:13:LEU:HD13   | 2.27                     | 0.69              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 54:Li:61:LEU:HD12  | 54:Li:62:LYS:N     | 2.07                     | 0.69              |
| 61:Lp:42:CYS:SG    | 61:Lp:59:SER:OG    | 2.49                     | 0.69              |
| 64:SR:10:LYS:NZ    | 79:S2:1373:C:O2'   | 2.24                     | 0.69              |
| 64:SR:126:MET:HE1  | 79:S2:1125:C:H1'   | 1.74                     | 0.69              |
| 66:SF:91:ARG:HH22  | 77:SZ:105:ALA:HB3  | 1.57                     | 0.69              |
| 76:SM:62:VAL:O     | 76:SM:66:GLU:HG3   | 1.92                     | 0.69              |
| 84:Lt:114:ARG:NH1  | 84:Lt:130:LYS:HD2  | 2.07                     | 0.69              |
| 39:lS:127:MET:HG2  | 40:lT:153:PRO:HG2  | 1.74                     | 0.69              |
| 66:sF:100:ILE:HG21 | 66:sF:111:VAL:HG11 | 1.73                     | 0.69              |
| 85:l5:2041:A:N7    | 85:l5:4434:C:O2'   | 2.25                     | 0.69              |
| 85:l5:4896:G:H2'   | 85:l5:4897:G:C8    | 2.26                     | 0.69              |
| 16:SN:46:THR:OG1   | 16:SN:49:GLN:OE1   | 2.10                     | 0.69              |
| 16:SN:140:LYS:NZ   | 85:L5:1564:A:OP1   | 2.25                     | 0.69              |
| 85:L5:399:G:N2     | 36:LP:101:ASN:OD1  | 2.22                     | 0.69              |
| 85:L5:2486:G:O6    | 85:L5:2493:G:O6    | 2.09                     | 0.69              |
| 85:L5:4228:G:HO2'  | 85:L5:4373:G:H1    | 1.40                     | 0.69              |
| 85:L5:4911:A:OP1   | 23:LB:97:ARG:NH2   | 2.25                     | 0.69              |
| 21:L8:94:G:N3      | 55:Lj:82:THR:OG1   | 2.23                     | 0.69              |
| 26:LE:57:TYR:HB2   | 26:LE:62:MET:HE3   | 1.74                     | 0.69              |
| 30:LI:206:LEU:HG   | 30:LI:210:ARG:HH12 | 1.58                     | 0.69              |
| 69:SQ:72:VAL:HG11  | 69:SQ:80:GLN:HG2   | 1.75                     | 0.69              |
| 4:sL:110:SER:HG    | 4:sL:137:THR:HG1   | 1.34                     | 0.69              |
| 8:sY:19:GLN:CD     | 8:sY:81:TYR:HD1    | 2.00                     | 0.69              |
| 11:sB:68:GLU:OE1   | 11:sB:68:GLU:N     | 2.20                     | 0.69              |
| 13:sV:29:HIS:CE1   | 15:sC:87:PRO:HA    | 2.28                     | 0.69              |
| 19:sb:70:LYS:HZ1   | 79:s2:1107:G:P     | 2.14                     | 0.69              |
| 22:lA:53:GLY:O     | 22:lA:192:LYS:NZ   | 2.26                     | 0.69              |
| 41:lU:81:ARG:NH1   | 85:l5:2622:G:O6    | 2.23                     | 0.69              |
| 68:sP:134:GLY:H    | 79:s2:1236:G:H4'   | 1.58                     | 0.69              |
| 80:cB:822:GLY:HA3  | 80:cB:831:PRO:HG2  | 1.73                     | 0.69              |
| 85:l5:4139:G:H21   | 85:l5:4140:C:H41   | 1.39                     | 0.69              |
| 4:SL:103:GLU:OE1   | 5:SX:11:ARG:N      | 2.26                     | 0.69              |
| 16:SN:84:LEU:HG    | 16:SN:89:TYR:HB2   | 1.74                     | 0.69              |
| 85:L5:1750:G:N2    | 30:LI:193:ASP:OD2  | 2.25                     | 0.69              |
| 85:L5:1849:U:H3'   | 32:LL:5:ARG:HH12   | 1.57                     | 0.69              |
| 85:L5:4069:U:H2'   | 85:L5:4070:U:H6    | 1.58                     | 0.69              |
| 85:L5:4280:A:OP2   | 25:LD:23:ARG:NH2   | 2.21                     | 0.69              |
| 30:LI:52:MET:HA    | 30:LI:52:MET:HE2   | 1.74                     | 0.69              |
| 57:Ll:2:SER:O      | 57:Ll:5:LYS:NZ     | 2.24                     | 0.69              |
| 79:S2:90:G:OP1     | 79:S2:445:A:N6     | 2.23                     | 0.69              |
| 82:PE:18:U:N3      | 82:PE:55:U:O2      | 2.19                     | 0.69              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CH:133:ARG:HH12  | 79:S2:534:G:H5'    | 1.58                     | 0.69              |
| 26:IE:128:HIS:HD2  | 85:l5:1281:G:C5    | 2.10                     | 0.69              |
| 29:IH:104:VAL:HB   | 29:lH:113:GLU:HB2  | 1.74                     | 0.69              |
| 62:lr:66:ARG:NH1   | 62:lr:75:THR:O     | 2.24                     | 0.69              |
| 78:sf:95:ARG:NH1   | 79:s2:1302:G:N3    | 2.41                     | 0.69              |
| 79:s2:693:A:N6     | 79:s2:738:C:O2'    | 2.23                     | 0.69              |
| 80:cB:3:ASN:N      | 80:cB:44:GLY:O     | 2.25                     | 0.69              |
| 85:l5:382:G:N1     | 85:l5:385:A:OP2    | 2.26                     | 0.69              |
| 80:CB:155:LEU:HD22 | 80:CB:185:VAL:HG21 | 1.75                     | 0.69              |
| 7:SJ:176:LYS:HA    | 7:SJ:179:LYS:HE2   | 1.72                     | 0.69              |
| 15:SC:80:GLU:N     | 15:SC:80:GLU:OE1   | 2.25                     | 0.69              |
| 85:L5:1480:C:O2'   | 85:L5:1482:G:OP2   | 2.11                     | 0.69              |
| 85:L5:4092:G:N2    | 85:L5:4094:G:O6    | 2.26                     | 0.69              |
| 85:L5:4989:U:H1'   | 85:L5:4990:C:H5    | 1.56                     | 0.69              |
| 85:L5:4997:G:H1    | 85:L5:5053:U:H3    | 1.40                     | 0.69              |
| 33:LM:62:LEU:HD12  | 33:LM:76:ALA:HB1   | 1.75                     | 0.69              |
| 77:SZ:50:PHE:CE1   | 77:SZ:55:TYR:HA    | 2.27                     | 0.69              |
| 79:S2:696:G:O2'    | 79:S2:736:C:O2     | 2.10                     | 0.69              |
| 79:S2:1407:U:H2'   | 79:S2:1408:U:C6    | 2.28                     | 0.69              |
| 6:sG:190:ARG:NH2   | 79:s2:334:C:OP2    | 2.26                     | 0.69              |
| 8:sY:80:ASP:OD1    | 28:LG:224:THR:HG23 | 1.92                     | 0.69              |
| 11:sB:75:GLN:HB3   | 11:sB:78:GLU:CD    | 2.17                     | 0.69              |
| 15:sC:114:LYS:HE2  | 79:s2:1357:A:O3'   | 1.92                     | 0.69              |
| 17:sO:138:ASP:OD1  | 79:s2:984:C:O2'    | 2.11                     | 0.69              |
| 23:IB:210:VAL:O    | 23:IB:349:LYS:NZ   | 2.22                     | 0.69              |
| 25:ID:223:PHE:HB3  | 25:ID:226:TYR:HB2  | 1.74                     | 0.69              |
| 32:IL:184:MET:O    | 32:IL:188:ASN:ND2  | 2.24                     | 0.69              |
| 34:IN:195:ARG:NH1  | 85:l5:98:A:H4'     | 2.08                     | 0.69              |
| 38:IR:176:ARG:O    | 38:IR:176:ARG:NH1  | 2.25                     | 0.69              |
| 39:IS:45:TRP:HE1   | 39:IS:61:ILE:HD11  | 1.56                     | 0.69              |
| 41:IU:40:GLU:O     | 41:IU:44:GLN:HG3   | 1.91                     | 0.69              |
| 41:IU:41:GLN:C     | 41:IU:44:GLN:HE21  | 2.01                     | 0.69              |
| 48:lc:20:LEU:O     | 48:lc:24:SER:OG    | 2.06                     | 0.69              |
| 49:ld:39:LYS:NZ    | 85:l5:2369:U:O2'   | 2.26                     | 0.69              |
| 64:sR:27:ASP:HB3   | 79:s2:1455:A:H5''  | 1.74                     | 0.69              |
| 64:sR:53:TYR:HB3   | 79:s2:1465:A:O5'   | 1.91                     | 0.69              |
| 70:sS:73:ASN:O     | 70:sS:76:GLN:NE2   | 2.23                     | 0.69              |
| 71:sT:9:VAL:O      | 71:sT:11:GLN:NE2   | 2.26                     | 0.69              |
| 75:sg:15:ASN:ND2   | 79:s2:1472:C:H4'   | 2.07                     | 0.69              |
| 77:sZ:98:LYS:CE    | 77:sZ:112:ASN:HA   | 2.22                     | 0.69              |
| 79:s2:1286:G:N2    | 79:s2:1312:G:O2'   | 2.23                     | 0.69              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 81:aP:21:A:H61     | 81:aP:46:G:H2'     | 1.57                     | 0.69              |
| 83:ls:47:LEU:HA    | 83:ls:50:LYS:NZ    | 2.07                     | 0.69              |
| 85:l5:189:G:H2'    | 85:l5:190:G:C8     | 2.28                     | 0.69              |
| 80:CB:116:THR:OG1  | 80:CB:497:MET:SD   | 2.50                     | 0.69              |
| 80:CB:590:LEU:HD21 | 80:CB:603:TYR:HB3  | 1.74                     | 0.69              |
| 80:CB:744:ILE:HD11 | 80:CB:787:TYR:HB3  | 1.74                     | 0.69              |
| 11:SB:105:LEU:HD21 | 11:SB:110:MET:HB2  | 1.73                     | 0.69              |
| 12:SH:101:LEU:HD12 | 12:SH:102:PRO:HD2  | 1.74                     | 0.69              |
| 17:SO:55:ARG:NH1   | 79:S2:973:C:N3     | 2.40                     | 0.69              |
| 19:Sb:18:LYS:HD3   | 19:Sb:19:HIS:H     | 1.58                     | 0.69              |
| 85:L5:920:C:H2'    | 85:L5:921:C:C6     | 2.26                     | 0.69              |
| 85:L5:1667:G:N1    | 85:L5:2281:U:OP2   | 2.24                     | 0.69              |
| 85:L5:2457:G:OP1   | 34:LN:65:ARG:NH2   | 2.23                     | 0.69              |
| 85:L5:2870:A:OP2   | 85:L5:2879:A:N6    | 2.24                     | 0.69              |
| 85:L5:4129:G:O6    | 85:L5:4156:G:N2    | 2.25                     | 0.69              |
| 85:L5:4195:G:OP1   | 30:LI:116:ARG:NE   | 2.24                     | 0.69              |
| 47:Lb:40:LEU:HA    | 47:Lb:43:MET:HG2   | 1.73                     | 0.69              |
| 53:Lh:27:GLU:O     | 53:Lh:30:GLN:NE2   | 2.26                     | 0.69              |
| 79:S2:925:G:N2     | 79:S2:1017:U:O2    | 2.19                     | 0.69              |
| 19:sb:70:LYS:HZ3   | 79:s2:1107:G:P     | 2.16                     | 0.69              |
| 21:l8:67:U:H5''    | 55:lj:86:PRO:HA    | 1.75                     | 0.69              |
| 24:lC:242:PRO:HB2  | 85:l5:2297:G:H4'   | 1.75                     | 0.69              |
| 34:lN:124:ASP:OD1  | 34:lN:125:SER:N    | 2.25                     | 0.69              |
| 54:li:69:ALA:O     | 54:li:73:ILE:HD12  | 1.93                     | 0.69              |
| 64:sR:30:THR:N     | 79:s2:1455:A:OP1   | 2.26                     | 0.69              |
| 67:sK:80:ARG:NH1   | 67:sK:89:ILE:O     | 2.25                     | 0.69              |
| 79:s2:851:C:H5''   | 79:s2:852:G:H5'    | 1.74                     | 0.69              |
| 85:l5:2098:G:H2'   | 85:l5:2099:G:C8    | 2.28                     | 0.69              |
| 85:l5:2568:C:H2'   | 85:l5:2569:G:C8    | 2.28                     | 0.69              |
| 80:CB:20:ARG:HG3   | 80:CB:358:LEU:HD22 | 1.74                     | 0.69              |
| 80:CB:692:LEU:O    | 80:CB:839:ARG:NH1  | 2.26                     | 0.69              |
| 3:SI:81:VAL:HB     | 3:SI:102:VAL:HG22  | 1.75                     | 0.69              |
| 8:SY:7:ILE:HB      | 8:SY:43:LYS:HE2    | 1.74                     | 0.69              |
| 85:L5:326:C:OP1    | 32:LL:103:ARG:NH1  | 2.25                     | 0.69              |
| 85:L5:2072:C:OP1   | 37:LQ:2:GLY:N      | 2.26                     | 0.69              |
| 85:L5:2622:G:O6    | 41:LU:81:ARG:NH2   | 2.26                     | 0.69              |
| 23:LB:84:MET:SD    | 23:LB:164:ALA:HB1  | 2.33                     | 0.69              |
| 28:LG:159:HIS:CD2  | 28:LG:185:LYS:HD3  | 2.28                     | 0.69              |
| 66:SF:49:LEU:HD12  | 69:SQ:49:TYR:HB2   | 1.75                     | 0.69              |
| 67:SK:5:LYS:HE3    | 79:S2:1313:A:H5''  | 1.74                     | 0.69              |
| 67:SK:76:ILE:O     | 67:SK:80:ARG:HG2   | 1.93                     | 0.69              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 16:sN:102:LEU:HD11 | 16:sN:112:LYS:HB2  | 1.73                     | 0.69              |
| 16:sN:119:GLU:HA   | 16:sN:122:ILE:HG12 | 1.75                     | 0.69              |
| 39:IS:130:GLU:OE2  | 39:IS:130:GLU:N    | 2.26                     | 0.69              |
| 44:IY:47:MET:HE3   | 44:IY:48:PRO:HD2   | 1.75                     | 0.69              |
| 64:sR:28:PHE:HB3   | 79:s2:1455:A:H8    | 1.58                     | 0.69              |
| 65:sD:168:VAL:HG12 | 65:sD:189:MET:HB3  | 1.75                     | 0.69              |
| 65:sD:194:PRO:HB3  | 65:sD:197:LYS:HB2  | 1.75                     | 0.69              |
| 79:s2:1693:G:O2'   | 79:s2:1694:U:O5'   | 2.09                     | 0.69              |
| 85:l5:2459:G:N2    | 85:l5:2462:C:OP2   | 2.24                     | 0.69              |
| 85:l5:5057:C:H2'   | 85:l5:5058:A:C8    | 2.28                     | 0.69              |
| 2:SE:10:LYS:NZ     | 79:S2:95:G:OP1     | 2.25                     | 0.69              |
| 2:SE:19:MET:HE1    | 79:S2:846:G:C5     | 2.28                     | 0.69              |
| 15:SC:202:THR:N    | 15:SC:221:ASP:OD2  | 2.24                     | 0.69              |
| 17:SO:146:ARG:NH2  | 79:S2:1858:G:OP2   | 2.23                     | 0.69              |
| 85:L5:1070:G:N7    | 26:LE:46:ARG:NH1   | 2.41                     | 0.69              |
| 85:L5:4951:G:H2'   | 85:L5:4952:G:H8    | 1.58                     | 0.69              |
| 21:L8:84:A:OP1     | 44:LY:113:LYS:NZ   | 2.25                     | 0.69              |
| 41:LU:114:TYR:HD1  | 41:LU:115:PHE:H    | 1.39                     | 0.69              |
| 54:Li:50:PHE:O     | 54:Li:55:ARG:NH2   | 2.25                     | 0.69              |
| 63:Lz:214:GLN:H    | 63:Lz:215:ARG:NH2  | 1.87                     | 0.69              |
| 79:S2:1601:A:OP2   | 79:S2:1636:G:N2    | 2.26                     | 0.69              |
| 10:sA:19:LEU:HD23  | 64:sR:96:ILE:HD13  | 1.74                     | 0.68              |
| 13:sV:74:LYS:HZ1   | 13:sV:83:PHE:HB2   | 1.56                     | 0.68              |
| 23:lB:43:LEU:HD12  | 23:lB:183:ILE:HG21 | 1.76                     | 0.68              |
| 45:lZ:21:ARG:NH1   | 45:lZ:47:ASP:OD1   | 2.25                     | 0.68              |
| 45:lZ:112:ARG:HH21 | 85:l5:2573:A:H1'   | 1.56                     | 0.68              |
| 52:lg:85:LYS:NZ    | 85:l5:2653:C:O3'   | 2.23                     | 0.68              |
| 54:li:70:LEU:HB2   | 54:li:87:ARG:HH21  | 1.56                     | 0.68              |
| 59:ln:2:ARG:NH1    | 79:s2:1841:C:OP2   | 2.26                     | 0.68              |
| 60:lo:39:ARG:NH1   | 85:l5:295:A:OP2    | 2.25                     | 0.68              |
| 60:lo:92:GLU:OE2   | 60:lo:95:GLY:N     | 2.25                     | 0.68              |
| 70:sS:24:ARG:HH21  | 70:sS:28:PHE:HB3   | 1.57                     | 0.68              |
| 79:s2:925:G:O6     | 79:s2:1017:U:O4    | 2.11                     | 0.68              |
| 81:aP:23:C:H2'     | 81:aP:24:A:H8      | 1.57                     | 0.68              |
| 85:l5:138:G:H2'    | 85:l5:139:G:C8     | 2.28                     | 0.68              |
| 85:l5:502:C:H3'    | 85:l5:503:C:H3'    | 1.74                     | 0.68              |
| 85:l5:909:A:H2'    | 85:l5:910:G:C8     | 2.28                     | 0.68              |
| 6:SG:66:GLY:HA2    | 79:S2:1745:A:H1'   | 1.75                     | 0.68              |
| 14:Sa:13:LYS:NZ    | 79:S2:1133:A:O4'   | 2.24                     | 0.68              |
| 85:L5:1514:U:H2'   | 85:L5:1515:A:C8    | 2.27                     | 0.68              |
| 85:L5:4096:C:H4'   | 85:L5:4110:C:H5''  | 1.75                     | 0.68              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:LA:28:ARG:HH11  | 22:LA:123:ARG:HG3  | 1.57                     | 0.68              |
| 30:LI:76:MET:HA    | 30:LI:76:MET:HE3   | 1.74                     | 0.68              |
| 54:LI:70:LEU:HD13  | 54:LI:87:ARG:HD2   | 1.74                     | 0.68              |
| 64:SR:59:LYS:O     | 64:SR:62:GLN:NE2   | 2.26                     | 0.68              |
| 67:SK:90:VAL:HB    | 67:SK:95:ARG:HE    | 1.57                     | 0.68              |
| 10:sA:55:TRP:HD1   | 10:sA:58:LEU:HD11  | 1.58                     | 0.68              |
| 20:17:7:G:OP1      | 25:1D:33:ARG:NH1   | 2.27                     | 0.68              |
| 26:1E:110:ARG:NH2  | 85:15:967:C:O2     | 2.22                     | 0.68              |
| 34:1N:157:LYS:O    | 34:1N:162:ARG:NH2  | 2.26                     | 0.68              |
| 47:1b:6:ASN:ND2    | 85:15:4220:A:H5'   | 2.08                     | 0.68              |
| 64:sR:51:ALA:HA    | 64:sR:54:VAL:HG21  | 1.76                     | 0.68              |
| 85:15:4947:U:H2'   | 85:15:4948:C:C6    | 2.27                     | 0.68              |
| 10:SA:196:GLU:OE1  | 10:SA:196:GLU:N    | 2.21                     | 0.68              |
| 11:SB:125:VAL:HB   | 11:SB:169:MET:SD   | 2.32                     | 0.68              |
| 13:SV:1:MET:SD     | 13:SV:1:MET:N      | 2.62                     | 0.68              |
| 13:SV:32:ILE:HG22  | 13:SV:55:ILE:HB    | 1.75                     | 0.68              |
| 85:L5:268:G:H2'    | 85:L5:269:G:H8     | 1.59                     | 0.68              |
| 85:L5:499:G:N2     | 85:L5:504:G:O6     | 2.26                     | 0.68              |
| 85:L5:1683:U:H2'   | 85:L5:1684:A:H8    | 1.57                     | 0.68              |
| 85:L5:4093:G:H2'   | 85:L5:4094:G:H5''  | 1.75                     | 0.68              |
| 85:L5:4324:A:H2'   | 85:L5:4325:A:C8    | 2.28                     | 0.68              |
| 33:LM:47:ARG:HD2   | 39:LS:73:LEU:HD11  | 1.75                     | 0.68              |
| 45:LZ:41:ALA:HB2   | 45:LZ:77:TYR:HE1   | 1.58                     | 0.68              |
| 65:SD:136:VAL:HG12 | 65:SD:186:VAL:HG13 | 1.75                     | 0.68              |
| 2:sE:182:MET:HB3   | 2:sE:226:PHE:HB3   | 1.74                     | 0.68              |
| 8:sY:102:THR:OG1   | 8:sY:106:GLN:OE1   | 2.10                     | 0.68              |
| 13:sV:68:SER:O     | 13:sV:72:LEU:HG    | 1.92                     | 0.68              |
| 15:sC:210:PRO:HB3  | 15:sC:240:THR:HG21 | 1.75                     | 0.68              |
| 51:1f:29:LYS:NZ    | 85:15:1919:G:O6    | 2.24                     | 0.68              |
| 75:sg:72:SER:OG    | 75:sg:74:ASP:OD1   | 2.09                     | 0.68              |
| 76:sM:33:ARG:CZ    | 79:s2:1284:A:N7    | 2.56                     | 0.68              |
| 77:sZ:47:LEU:HD11  | 77:sZ:83:LEU:HD23  | 1.74                     | 0.68              |
| 79:s2:868:G:OP2    | 79:s2:868:G:N2     | 2.14                     | 0.68              |
| 80:cB:209:LEU:H    | 80:cB:209:LEU:HD23 | 1.57                     | 0.68              |
| 80:cB:654:PRO:HA   | 80:cB:684:GLN:HE22 | 1.59                     | 0.68              |
| 81:aP:51:C:H2'     | 81:aP:52:G:H8      | 1.58                     | 0.68              |
| 85:15:753:C:H5     | 85:15:910:G:H1     | 1.41                     | 0.68              |
| 85:15:2108:G:H2'   | 85:15:2109:G:C8    | 2.29                     | 0.68              |
| 85:15:3599:A:H2'   | 85:15:3600:G:C8    | 2.29                     | 0.68              |
| 80:CB:313:ALA:O    | 80:CB:317:GLU:OE1  | 2.11                     | 0.68              |
| 6:SG:151:ASP:OD1   | 87:LW:105:ARG:NH1  | 2.25                     | 0.68              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 17:SO:149:ARG:NH1 | 79:S2:1064:C:O3'   | 2.26                     | 0.68              |
| 85:L5:1501:C:H5'  | 37:LQ:68:ARG:HH12  | 1.57                     | 0.68              |
| 85:L5:2068:C:OP1  | 51:Lf:85:ARG:NH2   | 2.26                     | 0.68              |
| 85:L5:3644:U:N3   | 85:L5:4532:U:O4    | 2.18                     | 0.68              |
| 85:L5:3672:G:OP2  | 85:L5:3672:G:N2    | 2.22                     | 0.68              |
| 85:L5:4195:G:C6   | 30:LI:115:MET:HE1  | 2.27                     | 0.68              |
| 85:L5:4459:U:H2'  | 85:L5:4460:U:C6    | 2.28                     | 0.68              |
| 85:L5:4527:G:OP2  | 85:L5:4527:G:N2    | 2.27                     | 0.68              |
| 51:Lf:29:LYS:HD3  | 51:Lf:83:MET:SD    | 2.33                     | 0.68              |
| 53:Lh:10:ARG:NH2  | 53:Lh:63:GLN:OE1   | 2.27                     | 0.68              |
| 66:SF:121:PRO:HD3 | 66:SF:193:LYS:HG3  | 1.76                     | 0.68              |
| 79:S2:557:U:H5'   | 79:S2:558:G:H8     | 1.56                     | 0.68              |
| 79:S2:1259:A:H62  | 79:S2:1518:C:H3'   | 1.59                     | 0.68              |
| 16:sN:83:ASP:OD1  | 16:sN:84:LEU:N     | 2.26                     | 0.68              |
| 21:l8:145:C:N3    | 85:l5:11:G:N1      | 2.33                     | 0.68              |
| 28:lG:34:LYS:HE2  | 28:lG:34:LYS:HA    | 1.76                     | 0.68              |
| 43:IX:98:PHE:O    | 43:IX:136:ALA:N    | 2.25                     | 0.68              |
| 79:s2:588:G:OP2   | 79:s2:588:G:N2     | 2.26                     | 0.68              |
| 85:l5:1444:G:N2   | 85:l5:2103:G:H1    | 1.91                     | 0.68              |
| 85:l5:5006:U:H4'  | 85:l5:5007:A:H5'   | 1.74                     | 0.68              |
| 6:SG:2:LYS:HB3    | 6:SG:15:LEU:HD11   | 1.75                     | 0.68              |
| 8:SY:122:LYS:NZ   | 79:S2:151:C:OP1    | 2.27                     | 0.68              |
| 14:Sa:13:LYS:HZ3  | 79:S2:1132:C:C2'   | 2.02                     | 0.68              |
| 85:L5:1178:G:OP1  | 85:L5:1178:G:N2    | 2.21                     | 0.68              |
| 85:L5:1663:C:H1'  | 85:L5:2320:G:H21   | 1.57                     | 0.68              |
| 85:L5:3948:C:HO2' | 85:L5:4065:G:H1    | 1.40                     | 0.68              |
| 85:L5:3964:U:O2'  | 85:L5:4048:A:N1    | 2.27                     | 0.68              |
| 85:L5:4102:C:H6   | 85:L5:4106:G:N3    | 1.90                     | 0.68              |
| 54:Li:61:LEU:HD11 | 54:Li:94:LEU:HD23  | 1.75                     | 0.68              |
| 61:Lp:47:MET:SD   | 61:Lp:55:TRP:HB3   | 2.33                     | 0.68              |
| 70:SS:24:ARG:NH1  | 70:SS:28:PHE:O     | 2.27                     | 0.68              |
| 79:S2:1215:C:O2   | 79:S2:1219:C:N4    | 2.25                     | 0.68              |
| 1:cH:44:TRP:CD1   | 9:se:53:LYS:HZ3    | 2.11                     | 0.68              |
| 8:sY:11:LYS:NZ    | 79:s2:832:G:N7     | 2.41                     | 0.68              |
| 12:sH:6:ALA:O     | 12:sH:25:GLN:NE2   | 2.19                     | 0.68              |
| 25:lD:287:PHE:HD2 | 25:lD:288:LEU:HD22 | 1.58                     | 0.68              |
| 41:lU:23:LEU:HB2  | 41:lU:83:LEU:HD21  | 1.76                     | 0.68              |
| 48:lc:36:LYS:HE2  | 48:lc:36:LYS:HA    | 1.75                     | 0.68              |
| 79:s2:44:U:OP1    | 79:s2:407:G:N2     | 2.26                     | 0.68              |
| 79:s2:106:C:H2'   | 79:s2:107:A:H8     | 1.56                     | 0.68              |
| 79:s2:1396:A:N7   | 79:s2:1449:G:O6    | 2.27                     | 0.68              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 85:L5:1336:G:H2'   | 85:L5:2346:C:H42   | 1.59                     | 0.68              |
| 85:L5:3967:G:O2'   | 85:L5:4047:A:N6    | 2.26                     | 0.68              |
| 85:L5:4195:G:N2    | 85:L5:4221:C:O2'   | 2.27                     | 0.68              |
| 3:SI:81:VAL:O      | 3:SI:94:LYS:NZ     | 2.24                     | 0.68              |
| 85:L5:1273:G:O6    | 47:Lb:117:ARG:NH2  | 2.26                     | 0.68              |
| 85:L5:4935:C:H2'   | 85:L5:4936:G:C8    | 2.29                     | 0.68              |
| 34:LN:51:LEU:HD13  | 34:LN:117:ASN:HB3  | 1.76                     | 0.68              |
| 65:SD:29:LEU:HB3   | 65:SD:32:ASP:HB2   | 1.76                     | 0.68              |
| 2:sE:3:ARG:NH1     | 79:s2:449:A:O3'    | 2.27                     | 0.68              |
| 23:lB:374:PHE:HE2  | 85:l5:5050:C:C2    | 2.11                     | 0.68              |
| 29:lH:4:ILE:HD13   | 29:lH:61:TRP:HE1   | 1.58                     | 0.68              |
| 33:lM:108:ASP:HB3  | 35:lO:199:HIS:CD2  | 2.28                     | 0.68              |
| 45:lZ:89:ILE:HD11  | 45:lZ:117:LYS:HB3  | 1.76                     | 0.68              |
| 47:lB:107:ARG:HH22 | 85:l5:1268:G:H3'   | 1.57                     | 0.68              |
| 65:sD:159:HIS:HB2  | 79:s2:1385:G:H5'   | 1.76                     | 0.68              |
| 76:sM:35:ILE:HD12  | 78:sf:103:LEU:HD22 | 1.76                     | 0.68              |
| 79:s2:1560:U:O2    | 79:s2:1575:G:O6    | 2.10                     | 0.68              |
| 80:CB:56:PHE:HD2   | 80:CB:456:ARG:H    | 1.42                     | 0.68              |
| 80:CB:401:MET:CE   | 80:CB:410:PHE:HB2  | 2.24                     | 0.68              |
| 2:SE:64:ILE:HD11   | 8:SY:18:LEU:HG     | 1.75                     | 0.68              |
| 6:SG:175:LYS:NZ    | 79:S2:78:C:O2      | 2.26                     | 0.68              |
| 13:SV:51:LYS:HD2   | 13:SV:52:THR:H     | 1.58                     | 0.68              |
| 17:SO:14:VAL:H     | 17:SO:15:ILE:HA    | 1.57                     | 0.68              |
| 85:L5:679:C:H2'    | 85:L5:680:G:H8     | 1.57                     | 0.68              |
| 85:L5:1444:G:N2    | 85:L5:2103:G:H1    | 1.91                     | 0.68              |
| 85:L5:2338:C:OP1   | 62:Lr:19:LYS:NZ    | 2.26                     | 0.68              |
| 85:L5:4095:G:O2'   | 85:L5:4110:C:O5'   | 2.12                     | 0.68              |
| 85:L5:4105:A:N9    | 85:L5:4105:A:H1'   | 2.03                     | 0.68              |
| 85:L5:5006:U:H4'   | 85:L5:5007:A:H5'   | 1.76                     | 0.68              |
| 22:LA:131:GLY:H    | 22:LA:169:VAL:HG23 | 1.56                     | 0.68              |
| 25:LD:65:ALA:HB2   | 25:LD:74:ILE:HD13  | 1.75                     | 0.68              |
| 26:LE:223:ARG:NH2  | 26:LE:234:ASP:O    | 2.27                     | 0.68              |
| 27:LF:115:ARG:NH1  | 37:LQ:4:ASP:O      | 2.26                     | 0.68              |
| 45:LZ:16:GLY:O     | 45:LZ:19:SER:OG    | 2.11                     | 0.68              |
| 67:SK:15:LEU:HD12  | 67:SK:71:LEU:HD21  | 1.76                     | 0.68              |
| 79:S2:1354:G:N1    | 79:S2:1357:A:OP2   | 2.23                     | 0.68              |
| 25:ID:91:GLY:O     | 25:ID:94:ASN:ND2   | 2.25                     | 0.68              |
| 29:lH:82:LYS:HA    | 29:lH:85:THR:HG22  | 1.76                     | 0.68              |
| 39:IS:80:ILE:HG23  | 39:IS:126:ILE:HD11 | 1.76                     | 0.68              |
| 41:lU:107:LYS:NZ   | 85:l5:2716:C:O2'   | 2.27                     | 0.68              |
| 43:IX:51:THR:O     | 85:l5:2475:G:N1    | 2.23                     | 0.68              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 46:la:26:ARG:NH2  | 85:l5:1656:U:OP2   | 2.27                     | 0.68              |
| 68:sP:108:LYS:H   | 68:sP:111:MET:HE1  | 1.57                     | 0.68              |
| 79:s2:1373:C:H2'  | 79:s2:1374:C:H6    | 1.58                     | 0.68              |
| 82:pE:21:A:H2'    | 82:pE:22:G:C8      | 2.28                     | 0.68              |
| 80:CB:311:GLU:HA  | 80:CB:314:LYS:HG2  | 1.76                     | 0.68              |
| 3:SI:7:ASN:ND2    | 79:S2:351:G:OP1    | 2.26                     | 0.68              |
| 12:SH:50:GLU:HA   | 12:SH:60:ILE:HA    | 1.75                     | 0.68              |
| 85:L5:418:A:H4'   | 85:L5:2311:C:H5'   | 1.75                     | 0.68              |
| 85:L5:2737:C:OP1  | 61:Lp:34:HIS:NE2   | 2.27                     | 0.68              |
| 85:L5:3717:A:OP2  | 85:L5:3735:G:N2    | 2.26                     | 0.68              |
| 85:L5:3727:A:OP1  | 54:Li:67:LYS:NZ    | 2.26                     | 0.68              |
| 85:L5:4301:U:H1'  | 40:LT:7:LYS:HE3    | 1.75                     | 0.68              |
| 79:S2:1064:C:H2'  | 79:S2:1065:G:H8    | 1.59                     | 0.68              |
| 1:cH:47:GLY:H     | 9:se:55:PRO:HG3    | 1.58                     | 0.68              |
| 5:sX:21:LYS:NZ    | 79:s2:658:U:O2'    | 2.26                     | 0.68              |
| 10:sA:9:GLN:C     | 10:sA:55:TRP:HH2   | 2.01                     | 0.68              |
| 22:lA:124:GLY:O   | 22:lA:128:ARG:NH1  | 2.26                     | 0.68              |
| 23:lB:50:LYS:HB2  | 23:lB:345:LEU:HD11 | 1.76                     | 0.68              |
| 24:lC:219:LYS:NZ  | 85:l5:224:U:O2     | 2.27                     | 0.68              |
| 42:lV:97:TYR:HE1  | 87:lW:19:ARG:HE    | 1.39                     | 0.68              |
| 65:sD:134:CYS:SG  | 65:sD:135:GLU:N    | 2.66                     | 0.68              |
| 66:sF:158:ALA:HA  | 66:sF:176:GLU:OE1  | 1.94                     | 0.68              |
| 67:sK:74:GLU:OE2  | 67:sK:74:GLU:N     | 2.22                     | 0.68              |
| 69:sQ:34:VAL:HG23 | 69:sQ:70:VAL:HG13  | 1.75                     | 0.68              |
| 79:s2:1839:U:O4'  | 79:s2:1863:A:N6    | 2.27                     | 0.68              |
| 85:l5:1683:U:H2'  | 85:l5:1684:A:H8    | 1.59                     | 0.68              |
| 85:l5:4459:U:H2'  | 85:l5:4460:U:C6    | 2.29                     | 0.68              |
| 85:l5:4954:G:H2'  | 85:l5:4955:A:C8    | 2.28                     | 0.68              |
| 80:CB:204:MET:HA  | 80:CB:204:MET:HE3  | 1.76                     | 0.68              |
| 10:SA:210:ILE:H   | 10:SA:210:ILE:HD12 | 1.58                     | 0.68              |
| 85:L5:351:C:OP2   | 24:LC:197:ARG:NH1  | 2.24                     | 0.68              |
| 85:L5:1535:C:OP1  | 55:Lj:11:ARG:NH1   | 2.26                     | 0.68              |
| 85:L5:4928:C:H2'  | 33:LM:118:MET:CE   | 2.22                     | 0.68              |
| 22:LA:116:LEU:HB2 | 22:LA:126:LEU:HB2  | 1.75                     | 0.68              |
| 24:LC:331:TYR:OH  | 27:LF:55:LYS:HD2   | 1.94                     | 0.68              |
| 70:SS:21:ASP:OD2  | 70:SS:23:ARG:NH1   | 2.26                     | 0.68              |
| 79:S2:191:A:N6    | 79:S2:208:G:O2'    | 2.26                     | 0.68              |
| 79:S2:1277:C:H2'  | 79:S2:1278:A:C8    | 2.28                     | 0.68              |
| 79:S2:1588:A:H2'  | 79:S2:1589:A:C8    | 2.28                     | 0.68              |
| 1:cH:43:LYS:HD2   | 1:cH:44:TRP:H      | 1.59                     | 0.68              |
| 34:lN:172:ARG:NH1 | 85:l5:62:A:OP1     | 2.27                     | 0.68              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 41:IU:80:LYS:HE2   | 41:IU:110:TYR:CD2  | 2.29                     | 0.68              |
| 50:le:113:GLU:OE2  | 50:le:113:GLU:N    | 2.26                     | 0.68              |
| 55:lj:36:LYS:NZ    | 85:l5:372:A:OP1    | 2.23                     | 0.68              |
| 79:s2:1410:C:H2'   | 79:s2:1411:G:C8    | 2.29                     | 0.68              |
| 85:L5:1976:G:H21   | 84:Lt:139:VAL:HG12 | 1.58                     | 0.68              |
| 85:L5:1992:U:H4'   | 85:L5:1993:C:H5''  | 1.75                     | 0.68              |
| 85:L5:2579:G:N2    | 85:L5:2582:A:OP2   | 2.18                     | 0.68              |
| 85:L5:2856:C:O2    | 23:LB:242:ARG:NH2  | 2.26                     | 0.68              |
| 85:L5:4101:C:H6    | 85:L5:4105:A:P     | 2.15                     | 0.68              |
| 22:LA:80:GLU:OE1   | 22:LA:170:ALA:HA   | 1.92                     | 0.68              |
| 29:LH:134:CYS:HA   | 29:LH:146:LEU:HA   | 1.75                     | 0.68              |
| 39:LS:101:THR:HG23 | 39:LS:104:GLY:H    | 1.58                     | 0.68              |
| 58:Lm:98:LYS:HG3   | 58:Lm:120:ASN:HD21 | 1.59                     | 0.68              |
| 61:Lp:37:TYR:HB2   | 61:Lp:47:MET:HB3   | 1.76                     | 0.68              |
| 62:Lr:81:THR:C     | 62:Lr:82:ILE:HD13  | 2.18                     | 0.68              |
| 70:SS:6:PRO:HD3    | 77:SZ:49:LEU:HD13  | 1.76                     | 0.68              |
| 79:S2:140:C:H42    | 79:S2:313:A:H61    | 1.42                     | 0.68              |
| 87:LW:20:ARG:HD3   | 87:LW:30:GLN:HG3   | 1.75                     | 0.68              |
| 3:sI:53:LYS:HD3    | 3:sI:55:TYR:HE1    | 1.57                     | 0.68              |
| 6:sG:164:LYS:HD2   | 6:sG:167:LYS:HD3   | 1.76                     | 0.68              |
| 25:ID:35:ARG:NH1   | 85:l5:4326:G:H1'   | 2.09                     | 0.68              |
| 39:IS:83:ARG:HD2   | 39:IS:125:GLN:NE2  | 2.08                     | 0.68              |
| 76:sM:52:LEU:HD12  | 76:sM:53:ALA:N     | 2.09                     | 0.68              |
| 78:sf:118:ARG:HD3  | 78:sf:131:PHE:HE1  | 1.59                     | 0.68              |
| 79:s2:1259:A:H62   | 79:s2:1518:C:H3'   | 1.59                     | 0.68              |
| 85:l5:1095:A:N1    | 85:l5:1200:G:C6    | 2.62                     | 0.68              |
| 85:l5:2745:A:H2'   | 85:l5:2746:A:H8    | 1.58                     | 0.68              |
| 85:l5:4989:U:H1'   | 85:l5:4990:C:H5    | 1.59                     | 0.68              |
| 85:L5:3658:C:H2'   | 85:L5:3659:G:H8    | 1.56                     | 0.68              |
| 85:L5:4691:A:H5'   | 29:LH:71:ARG:HE    | 1.58                     | 0.68              |
| 20:L7:23:A:N3      | 20:L7:118:C:O2'    | 2.22                     | 0.68              |
| 48:Lc:26:LYS:HB2   | 48:Lc:97:ILE:HB    | 1.75                     | 0.68              |
| 71:ST:20:ALA:C     | 71:ST:24:LYS:HZ2   | 2.01                     | 0.68              |
| 7:sJ:125:HIS:HB2   | 79:s2:527:C:H5'    | 1.77                     | 0.67              |
| 24:lC:190:ARG:NH2  | 85:l5:2296:G:OP2   | 2.28                     | 0.67              |
| 40:IT:111:GLU:O    | 40:IT:114:GLN:NE2  | 2.26                     | 0.67              |
| 57:ll:5:LYS:HB2    | 57:ll:9:ILE:HD11   | 1.75                     | 0.67              |
| 75:sg:189:ILE:HG22 | 75:sg:190:GLY:H    | 1.57                     | 0.67              |
| 79:s2:1461:G:H21   | 79:s2:1465:A:N6    | 1.91                     | 0.67              |
| 79:s2:1601:A:OP2   | 79:s2:1636:G:N2    | 2.27                     | 0.67              |
| 80:cB:142:VAL:HA   | 80:cB:145:GLN:OE1  | 1.94                     | 0.67              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 85:l5:679:C:H2'    | 85:l5:680:G:H8     | 1.59                     | 0.67              |
| 80:CB:75:ILE:HA    | 80:CB:454:MET:HA   | 1.74                     | 0.67              |
| 85:L5:950:G:H2'    | 85:L5:951:G:H8     | 1.59                     | 0.67              |
| 85:L5:4208:U:OP2   | 40:LT:4:THR:OG1    | 2.12                     | 0.67              |
| 59:Ln:9:ARG:HA     | 59:Ln:12:ARG:HH11  | 1.58                     | 0.67              |
| 61:Lp:75:SER:O     | 61:Lp:79:VAL:HG22  | 1.94                     | 0.67              |
| 63:Lz:33:GLU:H     | 63:Lz:206:ILE:HG23 | 1.58                     | 0.67              |
| 79:S2:1723:G:H1    | 79:S2:1810:U:H3    | 1.41                     | 0.67              |
| 81:AP:23:C:H2'     | 81:AP:24:A:H8      | 1.58                     | 0.67              |
| 32:lL:158:ARG:CZ   | 85:l5:1378:C:N3    | 2.57                     | 0.67              |
| 45:lZ:14:LEU:HD21  | 45:lZ:81:MET:HB3   | 1.75                     | 0.67              |
| 56:lk:6:GLU:OE2    | 56:lk:6:GLU:N      | 2.27                     | 0.67              |
| 56:lk:7:GLU:OE2    | 56:lk:10:ASP:N     | 2.26                     | 0.67              |
| 79:s2:902:G:O2'    | 79:s2:903:A:O4'    | 2.12                     | 0.67              |
| 79:s2:1302:G:N2    | 79:s2:1307:U:O4    | 2.27                     | 0.67              |
| 80:cB:830:ARG:O    | 80:cB:834:VAL:HG23 | 1.93                     | 0.67              |
| 85:l5:2092:G:O2'   | 85:l5:2262:G:N2    | 2.27                     | 0.67              |
| 80:CB:205:ILE:HG23 | 80:CB:211:THR:HG23 | 1.75                     | 0.67              |
| 2:SE:18:TRP:HH2    | 2:SE:31:PRO:HD3    | 1.59                     | 0.67              |
| 5:SX:76:LYS:HG3    | 79:S2:482:G:H5'    | 1.75                     | 0.67              |
| 12:SH:145:ARG:NE   | 18:SW:51:GLU:OE2   | 2.27                     | 0.67              |
| 14:Sa:95:ARG:HG2   | 79:S2:1866:A:H5'   | 1.76                     | 0.67              |
| 20:L7:54:A:C2      | 31:LJ:12:MET:HE1   | 2.27                     | 0.67              |
| 24:LC:192:GLY:O    | 24:LC:195:LYS:NZ   | 2.27                     | 0.67              |
| 60:Lo:26:TYR:HB3   | 60:Lo:67:VAL:HG23  | 1.76                     | 0.67              |
| 65:SD:222:PRO:HA   | 75:Sg:190:GLY:HA3  | 1.75                     | 0.67              |
| 66:SF:164:ARG:NH1  | 79:S2:1533:A:OP1   | 2.27                     | 0.67              |
| 67:SK:95:ARG:O     | 67:SK:97:SER:N     | 2.28                     | 0.67              |
| 76:SM:115:GLY:C    | 76:SM:116:LYS:HD3  | 2.19                     | 0.67              |
| 79:S2:634:A:H2'    | 79:S2:635:G:H8     | 1.59                     | 0.67              |
| 1:cH:72:ARG:CZ     | 1:cH:113:ARG:HB3   | 2.24                     | 0.67              |
| 18:sW:90:GLN:HE22  | 18:sW:113:HIS:CG   | 2.11                     | 0.67              |
| 19:sb:13:GLU:O     | 19:sb:17:ARG:HB3   | 1.94                     | 0.67              |
| 22:lA:229:ALA:HB3  | 22:lA:234:LYS:HB3  | 1.75                     | 0.67              |
| 27:lF:217:ARG:O    | 27:lF:246:ARG:NH1  | 2.27                     | 0.67              |
| 37:lQ:69:LYS:NZ    | 85:l5:1458:C:OP1   | 2.26                     | 0.67              |
| 42:lV:57:VAL:HA    | 42:lV:81:VAL:HG12  | 1.76                     | 0.67              |
| 65:sD:25:LEU:HB3   | 65:sD:29:LEU:HD13  | 1.75                     | 0.67              |
| 75:sg:88:ARG:HD2   | 75:sg:90:TRP:CH2   | 2.29                     | 0.67              |
| 79:s2:463:C:O3'    | 80:cB:50:ARG:NH1   | 2.27                     | 0.67              |
| 80:cB:654:PRO:HD2  | 80:cB:658:GLY:HA3  | 1.76                     | 0.67              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 85:l5:1405:C:N4   | 85:l5:1408:G:N3    | 2.39                     | 0.67              |
| 80:CB:121:VAL:O   | 80:CB:415:ARG:HD3  | 1.94                     | 0.67              |
| 80:CB:200:MET:HB3 | 80:CB:203:ILE:HD11 | 1.77                     | 0.67              |
| 3:SI:57:ALA:HB1   | 3:SI:60:LEU:HD11   | 1.77                     | 0.67              |
| 17:SO:55:ARG:NH2  | 79:S2:972:A:N1     | 2.41                     | 0.67              |
| 85:L5:512:U:O4    | 85:L5:647:G:O6     | 2.11                     | 0.67              |
| 85:L5:1100:U:O4   | 85:L5:1194:G:O6    | 2.10                     | 0.67              |
| 85:L5:1855:G:O6   | 85:L5:1880:G:N2    | 2.27                     | 0.67              |
| 71:ST:120:GLY:H   | 79:S2:1562:C:H4'   | 1.58                     | 0.67              |
| 79:S2:1712:A:H2'  | 79:S2:1713:C:C6    | 2.29                     | 0.67              |
| 13:sV:64:GLU:HG3  | 19:sb:3:LEU:HD21   | 1.77                     | 0.67              |
| 26:lE:270:TYR:CE1 | 33:lM:107:PHE:HA   | 2.29                     | 0.67              |
| 39:lS:29:ARG:HE   | 40:lT:150:LEU:HG   | 1.58                     | 0.67              |
| 81:aP:3:C:H42     | 81:aP:70:A:H61     | 1.41                     | 0.67              |
| 85:l5:1406:G:H1   | 85:l5:1411:C:HO2'  | 1.41                     | 0.67              |
| 85:l5:3967:G:O6   | 85:l5:4055:U:O4    | 2.13                     | 0.67              |
| 85:l5:4922:C:H2'  | 85:l5:4923:C:C6    | 2.30                     | 0.67              |
| 80:CB:180:ARG:HE  | 80:CB:183:GLU:CD   | 2.02                     | 0.67              |
| 80:CB:227:GLN:O   | 80:CB:230:GLU:N    | 2.28                     | 0.67              |
| 80:CB:561:LEU:HA  | 80:CB:565:HIS:HB2  | 1.76                     | 0.67              |
| 3:SI:66:SER:HA    | 3:SI:73:THR:HG22   | 1.75                     | 0.67              |
| 85:L5:907:C:H2'   | 85:L5:908:G:H8     | 1.59                     | 0.67              |
| 85:L5:4274:A:H2'  | 85:L5:4275:G:H8    | 1.59                     | 0.67              |
| 24:LC:135:ALA:HA  | 62:Lr:43:LEU:HD11  | 1.76                     | 0.67              |
| 33:LM:136:LEU:O   | 33:LM:137:LYS:NZ   | 2.24                     | 0.67              |
| 78:Sf:135:HIS:ND1 | 79:S2:1307:U:O2'   | 2.26                     | 0.67              |
| 79:S2:207:G:H3'   | 79:S2:208:G:H8     | 1.59                     | 0.67              |
| 3:sI:5:ARG:NH1    | 79:s2:380:G:N3     | 2.43                     | 0.67              |
| 24:lC:155:GLU:OE1 | 24:lC:155:GLU:N    | 2.20                     | 0.67              |
| 31:lJ:9:GLU:OE2   | 31:lJ:10:ASN:ND2   | 2.27                     | 0.67              |
| 65:sD:27:ARG:HB2  | 67:sK:61:GLN:HE21  | 1.60                     | 0.67              |
| 66:sF:126:THR:HA  | 66:sF:135:ARG:HG3  | 1.77                     | 0.67              |
| 75:sg:149:GLU:HB2 | 75:sg:170:TRP:HB3  | 1.76                     | 0.67              |
| 79:s2:1277:C:H2'  | 79:s2:1278:A:C8    | 2.27                     | 0.67              |
| 80:cB:259:LYS:HD2 | 80:cB:264:ARG:HD3  | 1.76                     | 0.67              |
| 85:l5:4324:A:H2'  | 85:l5:4325:A:C8    | 2.29                     | 0.67              |
| 11:SB:85:LYS:NZ   | 11:SB:104:ASP:OD1  | 2.28                     | 0.67              |
| 14:Sa:15:ARG:HH22 | 79:S2:992:A:H3'    | 1.59                     | 0.67              |
| 85:L5:3667:C:P    | 22:LA:234:LYS:HE3  | 2.35                     | 0.67              |
| 85:L5:4896:G:H2'  | 85:L5:4897:G:C8    | 2.30                     | 0.67              |
| 85:L5:4928:C:H2'  | 33:LM:118:MET:HE1  | 1.76                     | 0.67              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 34:LN:61:ILE:HD11  | 34:LN:131:GLU:HB3 | 1.75                     | 0.67              |
| 82:PE:42:G:H2'     | 82:PE:43:A:C8     | 2.29                     | 0.67              |
| 10:sA:22:GLY:O     | 10:sA:24:HIS:ND1  | 2.28                     | 0.67              |
| 40:IT:4:THR:OG1    | 85:l5:4208:U:OP2  | 2.12                     | 0.67              |
| 67:sK:49:MET:HA    | 67:sK:52:LEU:HG   | 1.77                     | 0.67              |
| 85:l5:1271:G:OP2   | 85:l5:1271:G:N2   | 2.23                     | 0.67              |
| 85:l5:4088:C:H2'   | 85:l5:4089:G:H8   | 1.59                     | 0.67              |
| 12:SH:173:PHE:HB2  | 12:SH:187:PHE:CE1 | 2.29                     | 0.67              |
| 18:SW:4:MET:O      | 18:SW:4:MET:HE3   | 1.94                     | 0.67              |
| 85:L5:88:A:N7      | 37:LQ:173:LYS:NZ  | 2.42                     | 0.67              |
| 85:L5:4301:U:OP2   | 85:L5:4303:C:N4   | 2.26                     | 0.67              |
| 20:L7:28:C:OP2     | 25:LD:57:ASN:ND2  | 2.27                     | 0.67              |
| 63:Lz:32:VAL:N     | 63:Lz:170:GLY:O   | 2.28                     | 0.67              |
| 66:SF:78:MET:O     | 66:SF:159:ARG:NH2 | 2.27                     | 0.67              |
| 14:sa:85:ARG:NH1   | 79:s2:1209:A:O2'  | 2.26                     | 0.67              |
| 23:IB:145:GLN:HA   | 23:IB:148:LYS:NZ  | 2.10                     | 0.67              |
| 30:II:87:MET:HE3   | 30:II:88:ARG:N    | 2.10                     | 0.67              |
| 51:lf:83:MET:O     | 51:lf:83:MET:HG3  | 1.93                     | 0.67              |
| 67:sK:80:ARG:HH22  | 67:sK:90:VAL:HA   | 1.59                     | 0.67              |
| 80:cB:19:ILE:HD13  | 80:cB:468:ASN:ND2 | 2.10                     | 0.67              |
| 85:l5:1751:A:H2'   | 85:l5:1752:G:H8   | 1.59                     | 0.67              |
| 5:SX:107:ARG:HH21  | 79:S2:19:A:H5'    | 1.60                     | 0.67              |
| 7:SJ:122:SER:O     | 7:SJ:125:HIS:N    | 2.28                     | 0.67              |
| 85:L5:93:G:H2'     | 85:L5:94:A:C8     | 2.30                     | 0.67              |
| 85:L5:513:U:O2'    | 85:L5:646:G:O6    | 2.13                     | 0.67              |
| 85:L5:1187:G:OP2   | 85:L5:1187:G:N2   | 2.27                     | 0.67              |
| 85:L5:1708:G:N7    | 47:Lb:103:LYS:NZ  | 2.42                     | 0.67              |
| 24:LC:315:LYS:NZ   | 27:LF:156:LYS:O   | 2.27                     | 0.67              |
| 38:LR:99:MET:SD    | 38:LR:103:ARG:NH1 | 2.67                     | 0.67              |
| 65:SD:49:ILE:HG22  | 65:SD:87:TYR:HB2  | 1.77                     | 0.67              |
| 77:SZ:85:ARG:NH2   | 79:S2:1597:C:OP2  | 2.23                     | 0.67              |
| 79:S2:864:A:H2'    | 79:S2:865:A:H8    | 1.59                     | 0.67              |
| 83:Ls:44:ARG:NH1   | 83:Ls:53:VAL:O    | 2.28                     | 0.67              |
| 2:sE:42:LEU:HD21   | 2:sE:47:PHE:HB2   | 1.75                     | 0.67              |
| 11:sB:151:ARG:H    | 64:sR:132:ARG:HA  | 1.59                     | 0.67              |
| 25:ID:153:THR:HG21 | 85:l5:4323:A:N6   | 2.09                     | 0.67              |
| 27:IF:147:LEU:HD23 | 27:IF:147:LEU:C   | 2.20                     | 0.67              |
| 35:IO:62:MET:SD    | 85:l5:2045:G:C6   | 2.88                     | 0.67              |
| 35:IO:170:LYS:O    | 35:IO:173:GLN:HG3 | 1.94                     | 0.67              |
| 65:sD:66:ILE:HD11  | 65:sD:86:LEU:HB3  | 1.76                     | 0.67              |
| 79:s2:1266:C:N3    | 79:s2:1517:G:N2   | 2.42                     | 0.67              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 80:cB:59:THR:HG23  | 80:cB:456:ARG:HG3  | 1.77                     | 0.67              |
| 80:cB:141:THR:HG22 | 80:cB:145:GLN:HE22 | 1.59                     | 0.67              |
| 82:pE:55:U:N3      | 82:pE:58:A:OP2     | 2.27                     | 0.67              |
| 85:l5:1751:A:H2'   | 85:l5:1752:G:C8    | 2.29                     | 0.67              |
| 3:SI:5:ARG:HG3     | 79:S2:386:C:H1'    | 1.75                     | 0.67              |
| 6:SG:159:ARG:NH1   | 79:S2:76:U:O2'     | 2.26                     | 0.67              |
| 85:L5:1092:G:H2'   | 85:L5:1093:C:C6    | 2.30                     | 0.67              |
| 85:L5:1346:C:H2'   | 85:L5:1347:G:C8    | 2.29                     | 0.67              |
| 85:L5:4894:A:H3'   | 85:L5:4895:C:H5'   | 1.75                     | 0.67              |
| 28:LG:209:SER:HA   | 28:LG:212:LYS:HD2  | 1.76                     | 0.67              |
| 31:LJ:20:LEU:HD21  | 31:LJ:22:LEU:HD13  | 1.77                     | 0.67              |
| 72:SU:66:ARG:HH22  | 72:SU:75:LYS:HA    | 1.58                     | 0.67              |
| 79:S2:1560:U:O2    | 79:S2:1575:G:O6    | 2.13                     | 0.67              |
| 83:Ls:117:ALA:O    | 83:Ls:164:GLY:N    | 2.28                     | 0.67              |
| 24:lC:46:LYS:NZ    | 85:l5:2341:A:OP1   | 2.28                     | 0.67              |
| 29:IH:128:MET:HB2  | 29:IH:157:SER:HB3  | 1.77                     | 0.67              |
| 51:lF:74:VAL:HG13  | 51:lF:84:VAL:HG11  | 1.75                     | 0.67              |
| 81:aP:40:C:H2'     | 81:aP:41:G:C8      | 2.29                     | 0.67              |
| 80:CB:636:ALA:HA   | 80:CB:641:TRP:HB2  | 1.75                     | 0.67              |
| 80:CB:653:GLY:O    | 80:CB:684:GLN:NE2  | 2.27                     | 0.67              |
| 10:SA:30:LEU:HB2   | 10:SA:47:TYR:CE2   | 2.30                     | 0.67              |
| 11:SB:117:TRP:HB3  | 11:SB:153:THR:HA   | 1.77                     | 0.67              |
| 85:L5:3967:G:O2'   | 85:L5:4047:A:N6    | 2.27                     | 0.67              |
| 85:L5:4122:G:O2'   | 45:LZ:136:PHE:OXT  | 2.13                     | 0.67              |
| 85:L5:4263:C:O3'   | 25:LD:8:LYS:NZ     | 2.28                     | 0.67              |
| 85:L5:4615:C:H5''  | 23:LB:357:ARG:HD2  | 1.77                     | 0.67              |
| 20:L7:47:G:OP2     | 25:LD:158:LYS:NZ   | 2.23                     | 0.67              |
| 27:LF:55:LYS:O     | 27:LF:55:LYS:NZ    | 2.27                     | 0.67              |
| 38:LR:7:GLN:HG2    | 38:LR:32:ILE:HG22  | 1.77                     | 0.67              |
| 49:Ld:19:GLU:OE2   | 49:Ld:92:ARG:NH1   | 2.27                     | 0.67              |
| 51:Lf:88:PHE:CG    | 51:Lf:92:LEU:HD21  | 2.30                     | 0.67              |
| 66:SF:74:ASN:HD21  | 79:S2:1676:U:P     | 2.18                     | 0.67              |
| 79:S2:1048:G:N1    | 79:S2:1069:U:OP2   | 2.25                     | 0.67              |
| 2:sE:94:LYS:HD3    | 8:sY:16:ARG:HG2    | 1.77                     | 0.67              |
| 6:sG:51:ARG:NH2    | 79:s2:1747:C:OP1   | 2.28                     | 0.67              |
| 18:sW:111:MET:HB2  | 18:sW:115:GLU:OE2  | 1.95                     | 0.67              |
| 20:l7:8:G:O6       | 25:ID:21:ARG:NH2   | 2.27                     | 0.67              |
| 23:lB:168:MET:HA   | 23:lB:171:LEU:HD23 | 1.76                     | 0.67              |
| 27:lF:71:MET:HA    | 27:lF:74:MET:HG2   | 1.76                     | 0.67              |
| 39:IS:28:TYR:HD2   | 40:lT:151:LEU:HD11 | 1.59                     | 0.67              |
| 39:IS:71:SER:OG    | 39:IS:76:LYS:NZ    | 2.28                     | 0.67              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 50:le:92:ASN:O     | 50:le:93:LYS:NZ   | 2.23                     | 0.67              |
| 66:sF:34:SER:HA    | 73:sc:55:VAL:HG13 | 1.76                     | 0.67              |
| 75:sg:145:GLU:O    | 75:sg:175:LYS:NZ  | 2.26                     | 0.67              |
| 3:SI:138:ASN:OD1   | 3:SI:139:LYS:N    | 2.27                     | 0.67              |
| 6:SG:48:TYR:OH     | 6:SG:119:LYS:O    | 2.13                     | 0.67              |
| 13:SV:40:ASP:OD1   | 13:SV:45:ARG:N    | 2.28                     | 0.67              |
| 16:SN:132:LYS:NZ   | 79:S2:1021:U:OP1  | 2.27                     | 0.67              |
| 18:SW:24:GLN:HB3   | 18:SW:64:ASN:HA   | 1.76                     | 0.67              |
| 85:L5:65:A:OP2     | 32:LL:101:ARG:NH1 | 2.28                     | 0.67              |
| 85:L5:1333:A:H2'   | 85:L5:1334:A:C8   | 2.30                     | 0.67              |
| 85:L5:1433:A:H3'   | 85:L5:1434:G:H8   | 1.58                     | 0.67              |
| 85:L5:1781:U:H1'   | 30:LI:198:LYS:HE2 | 1.77                     | 0.67              |
| 85:L5:2088:A:OP2   | 37:LQ:37:ARG:NH2  | 2.28                     | 0.67              |
| 24:LC:302:LEU:HD11 | 37:LQ:38:ARG:HB3  | 1.77                     | 0.67              |
| 33:LM:25:VAL:HG13  | 33:LM:38:VAL:CG1  | 2.24                     | 0.67              |
| 35:LO:76:PRO:HA    | 35:LO:79:ILE:HD12 | 1.77                     | 0.67              |
| 36:LP:52:THR:O     | 36:LP:54:GLN:NE2  | 2.28                     | 0.67              |
| 38:LR:76:MET:SD    | 38:LR:81:ARG:NH2  | 2.63                     | 0.67              |
| 39:LS:27:LEU:HD23  | 39:LS:27:LEU:H    | 1.60                     | 0.67              |
| 79:S2:1513:C:H2'   | 79:S2:1514:G:H8   | 1.59                     | 0.67              |
| 12:sH:145:ARG:NH2  | 18:sW:52:ILE:H    | 1.93                     | 0.66              |
| 43:IX:60:TYR:CD1   | 53:lh:78:TYR:HD2  | 2.13                     | 0.66              |
| 68:sP:47:ARG:NE    | 79:s2:1619:A:OP1  | 2.27                     | 0.66              |
| 68:sP:118:GLU:OE1  | 79:s2:1621:U:H4'  | 1.95                     | 0.66              |
| 70:sS:87:GLN:HA    | 70:sS:95:TYR:HA   | 1.76                     | 0.66              |
| 79:s2:463:C:O2'    | 79:s2:466:G:O6    | 2.12                     | 0.66              |
| 85:l5:1179:U:H3'   | 85:l5:1180:C:H5'' | 1.76                     | 0.66              |
| 85:l5:2275:G:H2'   | 85:l5:2276:A:C8   | 2.30                     | 0.66              |
| 4:SL:99:TYR:CG     | 5:SX:13:LEU:HD13  | 2.29                     | 0.66              |
| 10:SA:85:ARG:O     | 10:SA:89:LYS:HG2  | 1.95                     | 0.66              |
| 85:L5:1338:G:H2'   | 46:La:17:HIS:HE1  | 1.59                     | 0.66              |
| 85:L5:1493:G:OP2   | 47:Lb:44:ARG:NH1  | 2.27                     | 0.66              |
| 85:L5:1786:A:H2'   | 85:L5:1789:C:C5   | 2.30                     | 0.66              |
| 26:LE:278:THR:O    | 51:Lf:4:ARG:NH2   | 2.28                     | 0.66              |
| 84:Lt:59:THR:HA    | 84:Lt:80:LEU:HD21 | 1.75                     | 0.66              |
| 6:sG:199:THR:HG21  | 79:s2:126:G:H8    | 1.60                     | 0.66              |
| 14:sa:27:ALA:HB3   | 17:sO:149:ARG:H   | 1.61                     | 0.66              |
| 33:IM:6:PHE:CD1    | 39:IS:151:LYS:NZ  | 2.62                     | 0.66              |
| 33:IM:16:SER:HB3   | 33:IM:56:GLN:HE21 | 1.59                     | 0.66              |
| 34:IN:2:GLY:N      | 85:l5:115:C:OP1   | 2.28                     | 0.66              |
| 45:IZ:90:PRO:HD2   | 45:IZ:117:LYS:HD3 | 1.78                     | 0.66              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 53:lh:32:ARG:HH12  | 53:lh:36:VAL:HB    | 1.59                     | 0.66              |
| 62:lr:96:MET:O     | 62:lr:100:ASN:HB2  | 1.95                     | 0.66              |
| 63:lz:103:LEU:HG   | 63:lz:105:LYS:H    | 1.59                     | 0.66              |
| 69:sQ:86:GLN:HE21  | 69:sQ:90:LYS:HG3   | 1.60                     | 0.66              |
| 71:sT:101:ARG:NH1  | 79:s2:1566:G:O6    | 2.27                     | 0.66              |
| 73:sc:18:LEU:HB3   | 73:sc:29:GLN:HB2   | 1.78                     | 0.66              |
| 79:s2:106:C:OP1    | 79:s2:431:G:O2'    | 2.12                     | 0.66              |
| 80:cB:369:CYS:HA   | 80:cB:372:LEU:HB2  | 1.76                     | 0.66              |
| 85:L5:2669:C:OP2   | 38:LR:128:LYS:NZ   | 2.25                     | 0.66              |
| 85:L5:4966:A:OP1   | 23:LB:128:LYS:NZ   | 2.29                     | 0.66              |
| 85:L5:4995:U:O3'   | 49:Ld:32:ARG:NH2   | 2.27                     | 0.66              |
| 23:LB:58:ARG:NH1   | 23:LB:59:GLU:O     | 2.27                     | 0.66              |
| 37:LQ:17:GLU:OE2   | 37:LQ:26:ARG:NH1   | 2.28                     | 0.66              |
| 46:La:78:LEU:HD11  | 46:La:117:LEU:HD11 | 1.77                     | 0.66              |
| 70:SS:63:GLU:OE1   | 70:SS:63:GLU:N     | 2.20                     | 0.66              |
| 72:SU:30:LYS:HD3   | 72:SU:30:LYS:H     | 1.60                     | 0.66              |
| 76:SM:45:ARG:HH12  | 76:SM:72:HIS:HA    | 1.61                     | 0.66              |
| 87:IW:113:LYS:HA   | 87:IW:116:LYS:HE3  | 1.76                     | 0.66              |
| 4:sL:11:GLN:HB2    | 4:sL:56:ILE:HG21   | 1.76                     | 0.66              |
| 11:sB:121:ILE:HD11 | 11:sB:161:VAL:HG22 | 1.76                     | 0.66              |
| 34:IN:119:TYR:OH   | 34:IN:131:GLU:OE1  | 2.11                     | 0.66              |
| 58:lm:99:CYS:HB3   | 58:lm:115:CYS:HB3  | 1.76                     | 0.66              |
| 59:ln:10:MET:CE    | 79:s2:1172:U:H4'   | 2.25                     | 0.66              |
| 61:lp:85:ARG:NH2   | 79:s2:940:U:OP2    | 2.29                     | 0.66              |
| 67:sK:25:LYS:N     | 67:sK:65:ARG:O     | 2.24                     | 0.66              |
| 75:sg:132:TRP:HA   | 75:sg:138:CYS:HA   | 1.78                     | 0.66              |
| 79:s2:1377:U:O2'   | 79:s2:1379:A:O5'   | 2.10                     | 0.66              |
| 85:l5:907:C:H2'    | 85:l5:908:G:H8     | 1.60                     | 0.66              |
| 85:l5:2775:C:H2'   | 85:l5:2776:G:H8    | 1.59                     | 0.66              |
| 85:l5:4069:U:H2'   | 85:l5:4070:U:H6    | 1.60                     | 0.66              |
| 3:SI:42:ARG:HH21   | 3:SI:59:ARG:HH22   | 1.42                     | 0.66              |
| 13:SV:38:GLU:OE1   | 13:SV:49:GLN:NE2   | 2.28                     | 0.66              |
| 13:SV:44:GLY:O     | 13:SV:45:ARG:NH1   | 2.26                     | 0.66              |
| 14:Sa:70:LYS:HD3   | 79:S2:987:A:H4'    | 1.76                     | 0.66              |
| 85:L5:128:C:H2'    | 85:L5:129:C:C6     | 2.30                     | 0.66              |
| 85:L5:1382:G:H2'   | 85:L5:1383:G:H8    | 1.59                     | 0.66              |
| 85:L5:1919:G:N2    | 39:LS:163:HIS:O    | 2.23                     | 0.66              |
| 21:L8:41:A:HO2'    | 55:Lj:59:THR:HG1   | 1.43                     | 0.66              |
| 24:LC:218:ILE:HG22 | 24:LC:229:LEU:HG   | 1.78                     | 0.66              |
| 25:LD:134:SER:HB3  | 25:LD:141:ALA:H    | 1.60                     | 0.66              |
| 68:SP:22:LEU:HA    | 68:SP:25:LEU:HD12  | 1.78                     | 0.66              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 79:S2:982:G:H2'    | 79:S2:983:A:H8     | 1.59                     | 0.66              |
| 3:sI:74:ARG:NH2    | 79:s2:301:A:O2'    | 2.29                     | 0.66              |
| 10:sA:55:TRP:CD1   | 10:sA:58:LEU:HD11  | 2.31                     | 0.66              |
| 32:IL:49:ARG:O     | 32:IL:149:GLN:NE2  | 2.23                     | 0.66              |
| 48:lc:36:LYS:NZ    | 48:lc:39:ARG:HD2   | 2.10                     | 0.66              |
| 62:lr:89:THR:O     | 62:lr:93:ILE:HG12  | 1.95                     | 0.66              |
| 64:sR:27:ASP:CB    | 79:s2:1455:A:H5''  | 2.25                     | 0.66              |
| 66:sF:122:ARG:HB3  | 66:sF:146:ARG:HH21 | 1.61                     | 0.66              |
| 79:s2:822:U:H3     | 79:s2:826:A:N6     | 1.94                     | 0.66              |
| 79:s2:928:G:H1     | 79:s2:1013:U:H3    | 1.40                     | 0.66              |
| 85:l5:1942:A:H2'   | 85:l5:1943:A:C8    | 2.30                     | 0.66              |
| 85:l5:2375:A:H2'   | 85:l5:2376:A:H8    | 1.60                     | 0.66              |
| 85:l5:2386:U:H2'   | 85:l5:2387:G:C8    | 2.30                     | 0.66              |
| 85:l5:2443:G:OP2   | 85:l5:2516:G:N2    | 2.24                     | 0.66              |
| 80:CB:409:ARG:HH12 | 79:S2:478:G:H4'    | 1.60                     | 0.66              |
| 2:SE:181:CYS:HA    | 2:SE:227:VAL:HA    | 1.77                     | 0.66              |
| 85:L5:1645:C:H2'   | 85:L5:1646:A:C8    | 2.30                     | 0.66              |
| 85:L5:1724:G:OP1   | 27:LF:107:LYS:NZ   | 2.28                     | 0.66              |
| 85:L5:1837:A:OP2   | 40:LT:130:ARG:NE   | 2.28                     | 0.66              |
| 21:L8:74:U:O4      | 44:LY:72:GLN:NE2   | 2.29                     | 0.66              |
| 79:S2:690:G:OP2    | 79:S2:690:G:N2     | 2.20                     | 0.66              |
| 79:S2:1656:G:O6    | 79:S2:1668:U:O4    | 2.13                     | 0.66              |
| 79:S2:1693:G:H4'   | 79:S2:1694:U:H5'   | 1.77                     | 0.66              |
| 10:sA:10:MET:HE3   | 10:sA:15:VAL:HG11  | 1.76                     | 0.66              |
| 10:sA:143:PRO:HD3  | 13:sV:32:ILE:HD11  | 1.78                     | 0.66              |
| 11:sB:209:ASP:CG   | 11:sB:211:PHE:HE1  | 2.03                     | 0.66              |
| 15:sC:72:ASP:OD2   | 15:sC:272:HIS:NE2  | 2.27                     | 0.66              |
| 16:sN:76:LYS:NZ    | 79:s2:871:U:OP2    | 2.29                     | 0.66              |
| 16:sN:109:LYS:NZ   | 79:s2:1033:G:OP1   | 2.26                     | 0.66              |
| 22:lA:204:MET:HE2  | 22:lA:208:GLU:HB2  | 1.77                     | 0.66              |
| 24:lC:204:ARG:NH2  | 24:lC:205:ARG:O    | 2.29                     | 0.66              |
| 28:lG:209:SER:HA   | 28:lG:212:LYS:HG2  | 1.76                     | 0.66              |
| 33:IM:34:ASN:ND2   | 85:l5:1925:G:OP2   | 2.25                     | 0.66              |
| 34:lN:189:ARG:NH2  | 85:l5:28:C:OP2     | 2.29                     | 0.66              |
| 43:IX:116:LEU:HG   | 43:IX:117:TYR:CD1  | 2.29                     | 0.66              |
| 61:lp:42:CYS:SG    | 61:lp:59:SER:OG    | 2.51                     | 0.66              |
| 64:sR:60:ARG:O     | 64:sR:64:GLY:N     | 2.28                     | 0.66              |
| 64:sR:115:SER:OG   | 64:sR:116:ASN:N    | 2.29                     | 0.66              |
| 79:s2:464:A:H5'    | 79:s2:465:A:C8     | 2.30                     | 0.66              |
| 79:s2:1461:G:N2    | 79:s2:1465:A:H62   | 1.93                     | 0.66              |
| 80:cB:215:GLY:HA3  | 80:cB:222:ALA:HA   | 1.76                     | 0.66              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 85:l5:493:G:C6     | 85:l5:660:A:N1     | 2.64                     | 0.66              |
| 85:l5:495:C:H2'    | 85:l5:496:G:C8     | 2.30                     | 0.66              |
| 85:l5:1332:C:H2'   | 85:l5:1333:A:H8    | 1.60                     | 0.66              |
| 80:CB:225:LEU:HD11 | 80:CB:256:MET:HE1  | 1.78                     | 0.66              |
| 80:CB:340:MET:HA   | 80:CB:343:TRP:HE3  | 1.60                     | 0.66              |
| 85:L5:518:G:H1     | 85:L5:643:C:H2'    | 1.59                     | 0.66              |
| 85:L5:1270:A:OP1   | 47:Lb:107:ARG:NH2  | 2.28                     | 0.66              |
| 85:L5:4582:C:OP2   | 23:LB:28:LYS:NZ    | 2.28                     | 0.66              |
| 25:LD:208:MET:HE1  | 25:LD:233:PRO:HG3  | 1.77                     | 0.66              |
| 43:LX:112:ALA:O    | 43:LX:116:LEU:HG   | 1.94                     | 0.66              |
| 44:LY:41:LYS:HG2   | 44:LY:42:TYR:CD1   | 2.30                     | 0.66              |
| 66:SF:51:HIS:HB3   | 69:SQ:50:LYS:HE3   | 1.77                     | 0.66              |
| 69:SQ:18:THR:HB    | 69:SQ:75:GLY:HA2   | 1.76                     | 0.66              |
| 72:SU:18:HIS:CE1   | 72:SU:94:PRO:HA    | 2.30                     | 0.66              |
| 77:SZ:43:LYS:HG3   | 77:SZ:45:ASN:HB3   | 1.75                     | 0.66              |
| 1:CH:64:GLU:OE2    | 1:CH:67:GLU:N      | 2.28                     | 0.66              |
| 6:sG:193:ALA:O     | 6:sG:197:GLN:HG3   | 1.96                     | 0.66              |
| 6:sG:215:LYS:O     | 6:sG:215:LYS:NZ    | 2.27                     | 0.66              |
| 10:sA:77:ILE:HG22  | 10:sA:99:ILE:HB    | 1.76                     | 0.66              |
| 11:sB:76:ASN:ND2   | 11:sB:77:ASP:OD1   | 2.28                     | 0.66              |
| 13:sV:11:LEU:HD22  | 15:sC:167:ARG:HH22 | 1.61                     | 0.66              |
| 23:IB:302:ASN:HD22 | 23:IB:313:SER:HB2  | 1.61                     | 0.66              |
| 26:lE:191:GLN:N    | 26:lE:191:GLN:OE1  | 2.28                     | 0.66              |
| 79:s2:1215:C:O2    | 79:s2:1219:C:N4    | 2.25                     | 0.66              |
| 80:cB:590:LEU:HD21 | 80:cB:603:TYR:HB3  | 1.78                     | 0.66              |
| 85:l5:266:C:HO2'   | 85:l5:267:G:H8     | 1.44                     | 0.66              |
| 85:l5:3599:A:H2'   | 85:l5:3600:G:H8    | 1.61                     | 0.66              |
| 85:l5:4274:A:H2'   | 85:l5:4275:G:C8    | 2.30                     | 0.66              |
| 15:SC:272:HIS:CD2  | 15:SC:275:LYS:NZ   | 2.64                     | 0.66              |
| 85:L5:513:U:N3     | 85:L5:516:C:OP2    | 2.27                     | 0.66              |
| 85:L5:1577:G:O2'   | 85:L5:1612:G:H4'   | 1.96                     | 0.66              |
| 85:L5:1927:U:OP1   | 85:L5:1949:U:O2'   | 2.06                     | 0.66              |
| 85:L5:1972:G:H2'   | 85:L5:1973:G:C8    | 2.29                     | 0.66              |
| 85:L5:3653:A:H4'   | 22:LA:179:ILE:HB   | 1.75                     | 0.66              |
| 85:L5:3916:G:H2'   | 85:L5:3917:A:H8    | 1.60                     | 0.66              |
| 85:L5:4239:A:H2'   | 85:L5:4240:G:H8    | 1.59                     | 0.66              |
| 20:L7:57:C:H2'     | 20:L7:58:A:H8      | 1.60                     | 0.66              |
| 31:LJ:32:ARG:O     | 31:LJ:126:TYR:OH   | 2.13                     | 0.66              |
| 37:LQ:186:TYR:CE2  | 37:LQ:188:ASN:ND2  | 2.63                     | 0.66              |
| 48:Lc:30:GLY:O     | 48:Lc:34:THR:OG1   | 2.14                     | 0.66              |
| 77:SZ:112:ASN:OD1  | 77:SZ:113:THR:N    | 2.28                     | 0.66              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 79:S2:145:G:H2'   | 79:S2:146:G:C8     | 2.29                     | 0.66              |
| 79:S2:525:A:H2'   | 79:S2:526:A:C8     | 2.30                     | 0.66              |
| 79:S2:694:G:H2'   | 79:S2:695:C:O4'    | 1.95                     | 0.66              |
| 5:sX:128:VAL:HG13 | 5:sX:133:LEU:HD11  | 1.78                     | 0.66              |
| 10:sA:157:VAL:O   | 13:sV:65:SER:OG    | 2.13                     | 0.66              |
| 11:sB:78:GLU:CD   | 11:sB:78:GLU:N     | 2.54                     | 0.66              |
| 22:lA:2:GLY:N     | 85:l5:3919:C:OP1   | 2.29                     | 0.66              |
| 24:lC:358:ALA:HA  | 24:lC:361:LEU:HD12 | 1.77                     | 0.66              |
| 79:s2:836:G:N2    | 85:L5:4090:G:O2'   | 2.28                     | 0.66              |
| 79:s2:1402:A:N6   | 79:s2:1441:U:O2'   | 2.28                     | 0.66              |
| 80:cB:160:MET:HE1 | 80:cB:215:GLY:N    | 2.10                     | 0.66              |
| 85:l5:181:C:H3'   | 85:l5:182:G:H8     | 1.59                     | 0.66              |
| 85:l5:1333:A:H2'  | 85:l5:1334:A:H8    | 1.61                     | 0.66              |
| 85:l5:2361:G:N2   | 85:l5:3860:A:OP2   | 2.25                     | 0.66              |
| 85:l5:4274:A:H2'  | 85:l5:4275:G:H8    | 1.60                     | 0.66              |
| 80:CB:396:MET:SD  | 80:CB:416:VAL:HG13 | 2.36                     | 0.66              |
| 15:SC:167:ARG:HB3 | 15:SC:177:PRO:HB2  | 1.77                     | 0.66              |
| 85:L5:1317:U:OP1  | 46:La:21:ARG:NH1   | 2.29                     | 0.66              |
| 41:LU:61:VAL:HG23 | 41:LU:74:SER:HB2   | 1.77                     | 0.66              |
| 68:SP:31:GLU:O    | 68:SP:34:MET:HG2   | 1.95                     | 0.66              |
| 71:ST:10:ASN:HD21 | 71:ST:13:GLU:HG2   | 1.60                     | 0.66              |
| 79:S2:857:U:H2'   | 79:S2:858:A:C8     | 2.30                     | 0.66              |
| 7:sJ:79:ARG:NH2   | 79:s2:820:U:OP2    | 2.29                     | 0.66              |
| 17:sO:14:VAL:H    | 17:sO:15:ILE:HA    | 1.61                     | 0.66              |
| 22:lA:204:MET:HE1 | 22:lA:208:GLU:CD   | 2.21                     | 0.66              |
| 23:lB:113:GLU:HB2 | 23:lB:178:ALA:HB2  | 1.78                     | 0.66              |
| 24:lC:10:VAL:HA   | 24:lC:153:VAL:HG23 | 1.78                     | 0.66              |
| 35:lO:74:ARG:NH1  | 85:l5:4586:G:OP2   | 2.29                     | 0.66              |
| 64:sR:31:ASN:N    | 79:s2:1455:A:OP1   | 2.29                     | 0.66              |
| 64:sR:102:THR:O   | 64:sR:106:LEU:HG   | 1.95                     | 0.66              |
| 65:sD:150:MET:HE2 | 65:sD:152:PHE:CZ   | 2.31                     | 0.66              |
| 77:sZ:66:LYS:HB3  | 77:sZ:111:ARG:HE   | 1.61                     | 0.66              |
| 80:cB:209:LEU:HA  | 80:cB:257:MET:CE   | 2.24                     | 0.66              |
| 82:pE:16:C:H5''   | 82:pE:60:U:H3      | 1.61                     | 0.66              |
| 85:l5:989:U:O2    | 85:l5:1064:G:O6    | 2.13                     | 0.66              |
| 85:l5:4532:U:OP2  | 85:l5:4554:G:N1    | 2.28                     | 0.66              |
| 85:L5:439:G:O2'   | 51:Lf:91:ASN:ND2   | 2.27                     | 0.66              |
| 85:L5:1339:U:H2'  | 85:L5:1340:C:C6    | 2.31                     | 0.66              |
| 85:L5:1654:G:N2   | 85:L5:1678:C:OP1   | 2.28                     | 0.66              |
| 85:L5:2341:A:OP2  | 46:La:4:ARG:NH2    | 2.28                     | 0.66              |
| 85:L5:3732:A:H2'  | 85:L5:3733:A:C8    | 2.31                     | 0.66              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 85:L5:4741:C:H4'  | 85:L5:4742:G:H5'   | 1.77                     | 0.66              |
| 24:LC:284:MET:HG3 | 24:LC:287:THR:HB   | 1.78                     | 0.66              |
| 34:LN:161:MET:SD  | 34:LN:161:MET:N    | 2.60                     | 0.66              |
| 44:LY:23:SER:OG   | 44:LY:75:ARG:NH1   | 2.27                     | 0.66              |
| 56:Lk:54:GLU:O    | 56:Lk:57:LYS:N     | 2.29                     | 0.66              |
| 68:SP:18:ARG:HH21 | 70:SS:88:LYS:HG3   | 1.61                     | 0.66              |
| 74:Sd:12:ARG:NH2  | 79:S2:1513:C:OP1   | 2.29                     | 0.66              |
| 11:sB:144:LYS:HD2 | 11:sB:208:HIS:HB3  | 1.78                     | 0.66              |
| 23:lB:234:ARG:NH1 | 85:l5:4566:U:O2'   | 2.25                     | 0.66              |
| 26:lE:101:ASN:OD1 | 26:lE:105:ARG:NH2  | 2.28                     | 0.66              |
| 32:lL:59:VAL:HG21 | 32:lL:73:GLY:HA3   | 1.77                     | 0.66              |
| 51:lf:19:ARG:NH1  | 85:l5:1886:G:OP1   | 2.29                     | 0.66              |
| 64:sR:29:HIS:HB2  | 79:s2:1455:A:N9    | 2.11                     | 0.66              |
| 79:s2:543:C:H3'   | 79:s2:544:G:H8     | 1.61                     | 0.66              |
| 80:CB:394:LEU:CD1 | 80:CB:396:MET:HE1  | 2.25                     | 0.66              |
| 80:CB:401:MET:HG3 | 80:CB:529:LYS:HD2  | 1.78                     | 0.66              |
| 7:SJ:17:ARG:HH12  | 7:SJ:18:ARG:HE     | 1.42                     | 0.66              |
| 12:SH:125:VAL:O   | 12:SH:129:ILE:HG23 | 1.96                     | 0.66              |
| 85:L5:1812:C:H2'  | 85:L5:1813:U:C6    | 2.31                     | 0.66              |
| 85:L5:2017:A:HO2' | 85:L5:2018:C:H6    | 1.41                     | 0.66              |
| 85:L5:2338:C:O2'  | 62:Lr:13:CYS:SG    | 2.54                     | 0.66              |
| 85:L5:2348:G:OP1  | 85:L5:2351:C:N4    | 2.29                     | 0.66              |
| 85:L5:2749:C:H2'  | 85:L5:2750:G:C8    | 2.31                     | 0.66              |
| 25:LD:42:ASN:HD21 | 40:LT:68:THR:HA    | 1.60                     | 0.66              |
| 32:LL:25:TRP:NE1  | 34:LN:199:GLN:OE1  | 2.24                     | 0.66              |
| 35:LO:174:LEU:HA  | 35:LO:177:LEU:HD12 | 1.77                     | 0.66              |
| 45:LZ:123:LYS:O   | 45:LZ:126:LYS:NZ   | 2.29                     | 0.66              |
| 52:Lg:46:CYS:N    | 52:Lg:82:MET:HE1   | 2.11                     | 0.66              |
| 70:SS:1:MET:SD    | 70:SS:2:SER:N      | 2.69                     | 0.66              |
| 79:S2:1232:U:H3   | 79:S2:1526:G:H1    | 1.43                     | 0.66              |
| 79:S2:1639:G:N2   | 82:PE:42:G:O4'     | 2.27                     | 0.66              |
| 79:S2:1805:G:H2'  | 79:S2:1806:A:H8    | 1.61                     | 0.66              |
| 1:CH:49:ASN:HB3   | 1:CH:51:GLN:HE22   | 1.60                     | 0.66              |
| 15:sC:121:ARG:HE  | 15:sC:123:ARG:NH2  | 1.94                     | 0.66              |
| 29:IH:93:ARG:HD2  | 29:IH:143:GLU:HG3  | 1.78                     | 0.66              |
| 41:lU:41:GLN:O    | 41:lU:44:GLN:NE2   | 2.29                     | 0.66              |
| 79:s2:141:A:H4'   | 79:s2:142:C:H3'    | 1.77                     | 0.66              |
| 79:s2:1755:C:H2'  | 79:s2:1756:C:C6    | 2.30                     | 0.66              |
| 85:l5:1321:G:H22  | 85:l5:4445:U:H5'   | 1.61                     | 0.66              |
| 85:l5:1992:U:H4'  | 85:l5:1993:C:H5''  | 1.78                     | 0.66              |
| 80:CB:769:HIS:HB3 | 85:L5:1981:G:N3    | 2.11                     | 0.66              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:SL:22:ARG:NH2    | 4:SL:27:GLU:O      | 2.28                     | 0.66              |
| 12:SH:143:ARG:NE   | 18:SW:53:ILE:HD13  | 2.11                     | 0.66              |
| 15:SC:168:GLY:N    | 15:SC:179:THR:O    | 2.21                     | 0.66              |
| 85:L5:493:G:C6     | 85:L5:660:A:N1     | 2.64                     | 0.66              |
| 85:L5:1468:C:OP1   | 46:La:132:ARG:NH1  | 2.29                     | 0.66              |
| 37:LQ:121:LEU:CD1  | 37:LQ:125:GLN:HG3  | 2.26                     | 0.66              |
| 44:LY:57:VAL:HA    | 44:LY:104:VAL:HG12 | 1.76                     | 0.66              |
| 66:SF:124:ASP:OD2  | 73:Sc:47:LYS:HD3   | 1.95                     | 0.66              |
| 67:SK:95:ARG:HD3   | 67:SK:95:ARG:H     | 1.60                     | 0.66              |
| 77:SZ:47:LEU:HD22  | 77:SZ:80:ARG:H     | 1.61                     | 0.66              |
| 79:S2:388:U:H2'    | 79:S2:389:A:H8     | 1.60                     | 0.66              |
| 83:Ls:58:ASN:ND2   | 83:Ls:84:GLY:O     | 2.26                     | 0.66              |
| 87:IW:96:GLN:OE1   | 87:IW:96:GLN:N     | 2.27                     | 0.66              |
| 7:sJ:61:LEU:HD21   | 7:sJ:94:LEU:HB2    | 1.77                     | 0.65              |
| 20:l7:83:A:H4'     | 27:lF:224:THR:HB   | 1.79                     | 0.65              |
| 22:lA:245:ARG:HH22 | 85:l5:3656:A:H4'   | 1.60                     | 0.65              |
| 27:lF:34:ARG:NH1   | 85:l5:1271:G:O3'   | 2.29                     | 0.65              |
| 60:lo:33:LEU:HA    | 60:lo:38:LYS:HG2   | 1.78                     | 0.65              |
| 61:lp:38:THR:HA    | 61:lp:45:THR:HA    | 1.77                     | 0.65              |
| 62:lr:46:ARG:NH2   | 85:l5:667:A:OP1    | 2.28                     | 0.65              |
| 70:sS:46:ARG:HH21  | 71:sT:48:TYR:HA    | 1.59                     | 0.65              |
| 79:s2:691:G:OP2    | 79:s2:691:G:N2     | 2.21                     | 0.65              |
| 79:s2:694:G:H5''   | 79:s2:730:C:H5     | 1.61                     | 0.65              |
| 80:cB:506:ARG:HG3  | 80:cB:575:PRO:HG2  | 1.77                     | 0.65              |
| 85:l5:2413:U:H2'   | 85:l5:2414:G:H8    | 1.61                     | 0.65              |
| 85:l5:4888:U:O2    | 85:l5:4931:G:N1    | 2.15                     | 0.65              |
| 80:CB:427:VAL:CB   | 80:CB:485:ILE:HD11 | 2.20                     | 0.65              |
| 11:SB:33:VAL:HG12  | 11:SB:96:CYS:HB3   | 1.78                     | 0.65              |
| 85:L5:161:G:H2'    | 85:L5:162:A:H8     | 1.61                     | 0.65              |
| 85:L5:4100:C:C3'   | 85:L5:4107:G:H5''  | 2.27                     | 0.65              |
| 85:L5:4101:C:OP1   | 85:L5:4107:G:H3'   | 1.96                     | 0.65              |
| 22:LA:103:PRO:HA   | 22:LA:163:ARG:HA   | 1.78                     | 0.65              |
| 25:LD:196:ARG:HA   | 25:LD:199:ILE:HG12 | 1.78                     | 0.65              |
| 26:LE:150:LEU:CD1  | 26:LE:194:VAL:HB   | 2.26                     | 0.65              |
| 46:La:113:GLY:O    | 46:La:136:LYS:NZ   | 2.28                     | 0.65              |
| 64:SR:102:THR:O    | 64:SR:106:LEU:HG   | 1.96                     | 0.65              |
| 70:SS:8:LYS:HE2    | 70:SS:10:GLN:HE22  | 1.61                     | 0.65              |
| 79:S2:683:G:N1     | 79:S2:1022:U:OP2   | 2.28                     | 0.65              |
| 1:cH:82:GLN:NE2    | 79:s2:1278:A:O2'   | 2.28                     | 0.65              |
| 36:IP:75:GLN:OE1   | 36:IP:75:GLN:N     | 2.21                     | 0.65              |
| 70:sS:145:THR:OG1  | 79:s2:1523:C:OP1   | 2.15                     | 0.65              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 80:cB:820:LEU:HG   | 80:cB:830:ARG:NH2  | 2.11                     | 0.65              |
| 85:l5:4591:U:H2'   | 85:l5:4592:C:C6    | 2.31                     | 0.65              |
| 80:CB:306:ASN:HB2  | 80:CB:308:LYS:HE3  | 1.77                     | 0.65              |
| 80:CB:659:PRO:O    | 80:CB:699:GLY:N    | 2.28                     | 0.65              |
| 3:SI:184:ARG:NH2   | 79:S2:303:C:O2     | 2.30                     | 0.65              |
| 15:SC:84:PHE:HB3   | 15:SC:86:LEU:HD23  | 1.78                     | 0.65              |
| 85:L5:2306:G:N2    | 85:L5:2331:G:O2'   | 2.28                     | 0.65              |
| 85:L5:3589:G:N2    | 85:L5:3590:G:N7    | 2.44                     | 0.65              |
| 85:L5:3607:U:H2'   | 85:L5:3608:A:H8    | 1.62                     | 0.65              |
| 24:LC:323:ARG:HA   | 24:LC:326:LEU:HD12 | 1.78                     | 0.65              |
| 25:LD:200:MET:CE   | 25:LD:237:GLU:HA   | 2.26                     | 0.65              |
| 53:Lh:15:GLU:OE1   | 53:Lh:15:GLU:N     | 2.19                     | 0.65              |
| 64:SR:59:LYS:HE2   | 64:SR:63:ARG:HH22  | 1.62                     | 0.65              |
| 70:SS:7:GLU:CD     | 70:SS:7:GLU:H      | 2.04                     | 0.65              |
| 75:Sg:40:ILE:HB    | 75:Sg:59:LEU:HB3   | 1.78                     | 0.65              |
| 79:S2:1518:C:H5''  | 79:S2:1519:U:H5''  | 1.78                     | 0.65              |
| 1:cH:54:ILE:N      | 9:se:59:SER:O      | 2.30                     | 0.65              |
| 10:sA:63:ARG:CZ    | 13:sV:36:VAL:HA    | 2.25                     | 0.65              |
| 31:IJ:108:GLY:HA2  | 31:IJ:129:ASP:HA   | 1.78                     | 0.65              |
| 32:IL:204:GLU:OE1  | 32:IL:205:GLN:NE2  | 2.28                     | 0.65              |
| 35:IO:126:VAL:HG13 | 35:IO:127:VAL:HG13 | 1.78                     | 0.65              |
| 53:lh:32:ARG:O     | 53:lh:32:ARG:HD3   | 1.96                     | 0.65              |
| 67:sK:55:ARG:NH1   | 79:s2:1277:C:O3'   | 2.28                     | 0.65              |
| 71:sT:97:LYS:NZ    | 79:s2:1570:G:N7    | 2.45                     | 0.65              |
| 79:s2:327:G:H5''   | 79:s2:328:U:C2     | 2.31                     | 0.65              |
| 80:cB:395:MET:HE3  | 80:cB:486:THR:HG22 | 1.77                     | 0.65              |
| 80:cB:488:PHE:HE1  | 80:cB:490:HIS:HB2  | 1.61                     | 0.65              |
| 85:l5:1480:C:O2'   | 85:l5:1482:G:OP2   | 2.14                     | 0.65              |
| 85:l5:2600:A:N6    | 85:l5:2745:A:OP2   | 2.28                     | 0.65              |
| 85:l5:4586:G:O6    | 85:l5:4717:A:N6    | 2.29                     | 0.65              |
| 5:SX:84:PHE:HD1    | 5:SX:105:PHE:HZ    | 1.43                     | 0.65              |
| 17:SO:57:THR:H     | 17:SO:60:MET:CG    | 2.10                     | 0.65              |
| 85:L5:1762:C:N3    | 85:L5:1770:A:N1    | 2.44                     | 0.65              |
| 85:L5:2716:C:O3'   | 41:LU:107:LYS:NZ   | 2.27                     | 0.65              |
| 85:L5:3641:U:OP2   | 85:L5:3646:A:N6    | 2.29                     | 0.65              |
| 24:LC:331:TYR:CE1  | 27:LF:55:LYS:HA    | 2.29                     | 0.65              |
| 65:SD:194:PRO:HB3  | 65:SD:197:LYS:HB2  | 1.78                     | 0.65              |
| 73:Sc:17:VAL:HG22  | 73:Sc:30:VAL:HG23  | 1.77                     | 0.65              |
| 81:AP:9:A:H1'      | 81:AP:45:G:H2'     | 1.78                     | 0.65              |
| 84:Lt:22:VAL:HA    | 84:Lt:48:LYS:HG2   | 1.77                     | 0.65              |
| 2:sE:69:PHE:HE2    | 8:sY:17:LEU:CD2    | 2.09                     | 0.65              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 16:sN:91:LEU:HG    | 16:sN:122:ILE:CD1  | 2.27                     | 0.65              |
| 27:IF:147:LEU:HD21 | 85:l5:943:A:C8     | 2.31                     | 0.65              |
| 39:IS:127:MET:HE1  | 40:IT:155:PRO:CA   | 2.26                     | 0.65              |
| 43:IX:74:TYR:CE1   | 43:IX:116:LEU:HD13 | 2.32                     | 0.65              |
| 45:lZ:112:ARG:NH2  | 85:l5:2573:A:H1'   | 2.12                     | 0.65              |
| 48:lc:17:ARG:HD2   | 48:lc:103:ASP:HB2  | 1.79                     | 0.65              |
| 54:li:42:ASP:OD1   | 54:li:43:MET:N     | 2.30                     | 0.65              |
| 57:ll:28:ARG:O     | 57:ll:33:ASN:ND2   | 2.30                     | 0.65              |
| 58:lm:94:MET:HG2   | 58:lm:105:PRO:HA   | 1.79                     | 0.65              |
| 63:lz:199:GLN:NE2  | 63:lz:201:VAL:O    | 2.29                     | 0.65              |
| 65:sD:179:GLN:N    | 65:sD:179:GLN:OE1  | 2.29                     | 0.65              |
| 65:sD:224:SER:HG   | 75:sg:188:HIS:CD2  | 2.15                     | 0.65              |
| 66:sF:145:ARG:NH1  | 79:s2:1220:A:O2'   | 2.27                     | 0.65              |
| 79:s2:558:G:H1'    | 79:s2:559:G:C8     | 2.32                     | 0.65              |
| 80:cB:140:GLU:HG3  | 80:cB:188:ILE:HD12 | 1.79                     | 0.65              |
| 80:cB:764:ASN:OD1  | 85:l5:1982:G:N2    | 2.29                     | 0.65              |
| 85:l5:216:C:OP2    | 85:l5:219:G:O2'    | 2.15                     | 0.65              |
| 85:l5:4742:G:OP1   | 85:l5:4900:C:N4    | 2.30                     | 0.65              |
| 80:CB:27:HIS:O     | 80:CB:32:LYS:NZ    | 2.29                     | 0.65              |
| 2:SE:126:VAL:HG22  | 2:SE:158:ASP:H     | 1.61                     | 0.65              |
| 11:SB:33:VAL:HG23  | 11:SB:44:ILE:HB    | 1.77                     | 0.65              |
| 17:SO:57:THR:H     | 17:SO:60:MET:HG2   | 1.62                     | 0.65              |
| 85:L5:2287:G:N7    | 46:La:10:LYS:NZ    | 2.45                     | 0.65              |
| 85:L5:2373:C:H2'   | 85:L5:2374:A:H8    | 1.62                     | 0.65              |
| 85:L5:4178:A:H2'   | 85:L5:4179:G:H8    | 1.61                     | 0.65              |
| 85:L5:4966:A:OP1   | 23:LB:126:LYS:NZ   | 2.27                     | 0.65              |
| 23:LB:385:LYS:O    | 23:LB:389:MET:HB3  | 1.96                     | 0.65              |
| 64:SR:49:LYS:NZ    | 79:S2:1454:A:OP1   | 2.25                     | 0.65              |
| 71:ST:102:ARG:NH1  | 71:ST:105:GLN:OE1  | 2.29                     | 0.65              |
| 79:S2:1004:U:H2'   | 79:S2:1005:G:H8    | 1.60                     | 0.65              |
| 79:S2:1275:G:N2    | 79:S2:1506:A:OP2   | 2.29                     | 0.65              |
| 29:lH:85:THR:HG23  | 29:lH:86:LEU:HG    | 1.77                     | 0.65              |
| 34:lN:14:LYS:HZ3   | 85:l5:280:G:H5''   | 1.61                     | 0.65              |
| 34:lN:43:THR:OG1   | 34:lN:131:GLU:OE2  | 2.15                     | 0.65              |
| 38:IR:74:ARG:NH1   | 85:l5:2891:U:OP2   | 2.30                     | 0.65              |
| 41:lU:105:ASN:HD22 | 41:lU:111:GLU:HB3  | 1.60                     | 0.65              |
| 58:lm:79:GLU:OE1   | 58:lm:82:LEU:N     | 2.21                     | 0.65              |
| 64:sR:26:ASN:OD1   | 64:sR:58:MET:HE2   | 1.95                     | 0.65              |
| 79:s2:752:G:OP2    | 79:s2:752:G:N2     | 2.29                     | 0.65              |
| 79:s2:1099:G:N2    | 79:s2:1133:A:N1    | 2.44                     | 0.65              |
| 85:l5:2458:C:H1'   | 85:l5:3671:G:H21   | 1.62                     | 0.65              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 85:l5:2744:A:H2'   | 85:l5:2745:A:C8    | 2.32                     | 0.65              |
| 85:l5:4967:A:H2'   | 85:l5:4968:A:H8    | 1.60                     | 0.65              |
| 2:SE:123:LEU:HD22  | 2:SE:124:CYS:H     | 1.62                     | 0.65              |
| 7:SJ:12:THR:HG23   | 79:S2:520:A:H5''   | 1.79                     | 0.65              |
| 8:SY:13:MET:HE2    | 8:SY:13:MET:HA     | 1.77                     | 0.65              |
| 10:SA:222:VAL:HG13 | 10:SA:223:THR:HG23 | 1.77                     | 0.65              |
| 85:L5:332:C:H5'    | 34:LN:150:TRP:CZ3  | 2.31                     | 0.65              |
| 85:L5:1396:G:O2'   | 85:L5:1468:C:O2'   | 2.11                     | 0.65              |
| 85:L5:2386:U:H2'   | 85:L5:2387:G:C8    | 2.29                     | 0.65              |
| 85:L5:4860:G:O3'   | 35:LO:169:ARG:NH2  | 2.30                     | 0.65              |
| 26:LE:127:SER:O    | 26:LE:128:HIS:ND1  | 2.30                     | 0.65              |
| 26:LE:153:LEU:HD13 | 51:Lf:105:LEU:HD13 | 1.79                     | 0.65              |
| 59:Ln:16:LYS:HA    | 59:Ln:19:LYS:HD3   | 1.79                     | 0.65              |
| 71:ST:38:LYS:NZ    | 79:S2:1628:C:OP1   | 2.29                     | 0.65              |
| 84:Lt:43:GLY:O     | 84:Lt:70:GLN:NE2   | 2.30                     | 0.65              |
| 1:cH:85:ARG:NE     | 1:cH:90:LEU:O      | 2.29                     | 0.65              |
| 14:sa:45:VAL:HG21  | 14:sa:64:LEU:HD12  | 1.77                     | 0.65              |
| 26:lE:253:VAL:HA   | 26:lE:256:GLN:HE21 | 1.62                     | 0.65              |
| 34:lN:97:SER:O     | 34:lN:100:SER:OG   | 2.13                     | 0.65              |
| 47:lb:116:LEU:HD12 | 47:lb:117:ARG:HG3  | 1.77                     | 0.65              |
| 52:lg:43:LYS:HZ3   | 85:l5:2597:G:H5''  | 1.61                     | 0.65              |
| 69:sQ:131:LYS:NZ   | 79:s2:1479:G:O2'   | 2.29                     | 0.65              |
| 79:s2:150:A:N6     | 79:s2:168:C:O2     | 2.29                     | 0.65              |
| 79:s2:1217:A:H2'   | 79:s2:1218:C:H6    | 1.62                     | 0.65              |
| 79:s2:1388:A:C6    | 79:s2:1389:C:H1'   | 2.32                     | 0.65              |
| 80:cB:229:ALA:HB1  | 80:cB:256:MET:HE1  | 1.79                     | 0.65              |
| 80:cB:630:GLN:N    | 80:cB:630:GLN:OE1  | 2.28                     | 0.65              |
| 80:CB:654:PRO:HD2  | 80:CB:658:GLY:HA3  | 1.79                     | 0.65              |
| 5:SX:68:LYS:NZ     | 79:S2:617:G:OP2    | 2.28                     | 0.65              |
| 19:Sb:40:CYS:SG    | 19:Sb:41:TYR:N     | 2.67                     | 0.65              |
| 85:L5:325:U:H2'    | 85:L5:326:C:C6     | 2.32                     | 0.65              |
| 85:L5:3726:A:H2'   | 85:L5:3727:A:C8    | 2.31                     | 0.65              |
| 85:L5:3973:G:H21   | 85:L5:4051:C:H4'   | 1.61                     | 0.65              |
| 21:L8:60:G:O6      | 53:Lh:62:ASN:ND2   | 2.25                     | 0.65              |
| 25:LD:239:MET:HE1  | 25:LD:240:TYR:CD1  | 2.31                     | 0.65              |
| 36:LP:138:PRO:CB   | 36:LP:140:MET:HE3  | 2.27                     | 0.65              |
| 69:SQ:146:ARG:HH22 | 82:PE:33:U:H2'     | 1.62                     | 0.65              |
| 78:Sf:113:LYS:HD3  | 78:Sf:114:ILE:H    | 1.61                     | 0.65              |
| 79:S2:1468:C:H2'   | 79:S2:1469:A:H8    | 1.60                     | 0.65              |
| 84:Lt:114:ARG:HG2  | 84:Lt:119:ARG:HH22 | 1.61                     | 0.65              |
| 11:sB:107:ARG:HH22 | 17:sO:133:THR:N    | 1.95                     | 0.65              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 12:sH:60:ILE:HB   | 12:sH:92:VAL:HG12  | 1.79                     | 0.65              |
| 15:sC:60:TRP:CD1  | 15:sC:61:MET:N     | 2.65                     | 0.65              |
| 29:lH:175:PHE:HE2 | 85:l5:4603:C:H4'   | 1.61                     | 0.65              |
| 36:lP:140:MET:HE3 | 36:lP:140:MET:HA   | 1.78                     | 0.65              |
| 62:lr:71:ARG:HH22 | 85:l5:668:C:H5'    | 1.61                     | 0.65              |
| 71:sT:134:ILE:HA  | 71:sT:137:GLN:HE22 | 1.61                     | 0.65              |
| 72:sU:61:LEU:HB2  | 72:sU:82:MET:HB2   | 1.79                     | 0.65              |
| 79:s2:388:U:H2'   | 79:s2:389:A:H8     | 1.60                     | 0.65              |
| 85:l5:926:G:H2'   | 85:l5:927:G:H8     | 1.61                     | 0.65              |
| 85:l5:1092:G:H2'  | 85:l5:1093:C:C6    | 2.32                     | 0.65              |
| 85:l5:2638:G:H22  | 85:l5:2719:C:P     | 2.18                     | 0.65              |
| 85:l5:3595:U:H5'' | 85:l5:3597:G:OP2   | 1.97                     | 0.65              |
| 80:CB:748:GLU:N   | 80:CB:811:GLN:O    | 2.18                     | 0.65              |
| 2:SE:212:ASP:OD1  | 2:SE:216:ASN:N     | 2.30                     | 0.65              |
| 6:SG:57:ASP:OD1   | 6:SG:61:PHE:N      | 2.29                     | 0.65              |
| 7:SJ:63:LEU:O     | 7:SJ:70:ARG:NH1    | 2.29                     | 0.65              |
| 18:SW:23:ARG:CZ   | 19:Sb:4:ALA:HA     | 2.26                     | 0.65              |
| 85:L5:1281:G:OP1  | 24:LC:316:LYS:NZ   | 2.22                     | 0.65              |
| 85:L5:2318:G:N2   | 85:L5:2321:G:OP2   | 2.21                     | 0.65              |
| 30:LI:52:MET:SD   | 30:LI:152:LEU:HB3  | 2.37                     | 0.65              |
| 34:LN:113:LEU:HB2 | 34:LN:134:LEU:HD12 | 1.79                     | 0.65              |
| 66:SF:29:GLN:NE2  | 66:SF:31:ASN:OD1   | 2.29                     | 0.65              |
| 66:SF:40:ALA:HA   | 66:SF:45:TYR:CZ    | 2.32                     | 0.65              |
| 81:AP:23:C:H2'    | 81:AP:24:A:C8      | 2.31                     | 0.65              |
| 82:PE:23:A:H2'    | 82:PE:24:G:C8      | 2.32                     | 0.65              |
| 11:sB:75:GLN:HB3  | 11:sB:78:GLU:OE1   | 1.96                     | 0.65              |
| 23:lB:325:GLU:HG3 | 23:lB:327:THR:HG23 | 1.78                     | 0.65              |
| 28:lG:120:LYS:HZ3 | 28:lG:125:LYS:HG3  | 1.62                     | 0.65              |
| 45:lZ:4:PHE:O     | 45:lZ:9:LYS:NZ     | 2.30                     | 0.65              |
| 51:lf:23:GLU:N    | 51:lf:23:GLU:OE2   | 2.30                     | 0.65              |
| 63:lz:208:SER:H   | 63:lz:211:GLY:HA3  | 1.62                     | 0.65              |
| 64:sR:5:ARG:HD3   | 64:sR:9:VAL:HG23   | 1.79                     | 0.65              |
| 80:cB:21:ASN:HD22 | 80:cB:101:ASN:HB2  | 1.62                     | 0.65              |
| 80:cB:526:ARG:NH1 | 80:cB:565:HIS:O    | 2.30                     | 0.65              |
| 85:l5:1818:G:N2   | 85:l5:1818:G:OP2   | 2.29                     | 0.65              |
| 5:SX:68:LYS:HB3   | 5:SX:91:LEU:HD22   | 1.77                     | 0.65              |
| 6:SG:188:LYS:O    | 6:SG:192:ILE:HG12  | 1.97                     | 0.65              |
| 8:SY:42:GLU:HA    | 8:SY:52:PRO:HB3    | 1.79                     | 0.65              |
| 10:SA:143:PRO:HB3 | 13:SV:32:ILE:HG12  | 1.77                     | 0.65              |
| 14:Sa:13:LYS:HE2  | 79:S2:1133:A:C4'   | 2.25                     | 0.65              |
| 15:SC:142:LYS:NZ  | 15:SC:143:CYS:O    | 2.30                     | 0.65              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 19:Sb:54:VAL:HG23  | 19:Sb:63:LEU:HD13 | 1.79                     | 0.65              |
| 85:L5:2373:C:O4'   | 49:Ld:69:ASN:ND2  | 2.29                     | 0.65              |
| 85:L5:4507:A:H2'   | 85:L5:4508:C:C6   | 2.31                     | 0.65              |
| 21:L8:83:C:N4      | 44:LY:50:ARG:HH22 | 1.94                     | 0.65              |
| 22:LA:245:ARG:O    | 22:LA:245:ARG:NH1 | 2.30                     | 0.65              |
| 28:LG:194:VAL:HG13 | 28:LG:196:ARG:HB2 | 1.79                     | 0.65              |
| 36:LP:18:ARG:C     | 36:LP:94:MET:HE1  | 2.22                     | 0.65              |
| 41:LU:66:SER:O     | 41:LU:69:LYS:NZ   | 2.29                     | 0.65              |
| 74:Sd:13:LYS:HG3   | 74:Sd:14:PHE:HD1  | 1.62                     | 0.65              |
| 87:IW:46:PRO:HB2   | 87:IW:54:LEU:HD11 | 1.77                     | 0.65              |
| 9:se:45:VAL:O      | 79:s2:548:C:O2'   | 2.13                     | 0.65              |
| 15:sC:187:ARG:NH1  | 79:s2:1142:G:OP1  | 2.30                     | 0.65              |
| 17:sO:50:LYS:HD2   | 79:s2:976:G:H1'   | 1.79                     | 0.65              |
| 19:sb:55:LEU:HD11  | 19:sb:60:SER:HA   | 1.78                     | 0.65              |
| 39:lS:161:ARG:HE   | 39:lS:164:LYS:HB2 | 1.62                     | 0.65              |
| 74:sd:13:LYS:HG3   | 74:sd:14:PHE:H    | 1.61                     | 0.65              |
| 79:s2:138:C:OP2    | 79:s2:1774:C:O2'  | 2.15                     | 0.65              |
| 79:s2:1711:U:H2'   | 79:s2:1712:A:C8   | 2.31                     | 0.65              |
| 79:s2:1726:G:N1    | 79:s2:1809:A:N7   | 2.45                     | 0.65              |
| 83:ls:145:THR:HG22 | 83:ls:154:ILE:HA  | 1.79                     | 0.65              |
| 85:l5:444:G:H2'    | 85:l5:445:U:C6    | 2.32                     | 0.65              |
| 85:l5:468:U:O2     | 85:l5:686:A:N6    | 2.29                     | 0.65              |
| 85:l5:2638:G:H2'   | 85:l5:2639:U:C6   | 2.32                     | 0.65              |
| 80:CB:7:ASP:HB2    | 8:SY:131:PRO:HA   | 1.79                     | 0.65              |
| 80:CB:219:HIS:HB3  | 80:CB:340:MET:HE3 | 1.78                     | 0.65              |
| 3:SI:44:HIS:ND1    | 79:S2:1740:C:OP1  | 2.29                     | 0.65              |
| 4:SL:94:HIS:HB3    | 4:SL:103:GLU:HB3  | 1.77                     | 0.65              |
| 6:SG:131:ARG:HD2   | 79:S2:168:C:H4'   | 1.78                     | 0.65              |
| 12:SH:18:GLU:OE2   | 12:SH:49:LYS:NZ   | 2.30                     | 0.65              |
| 85:L5:1397:A:H8    | 46:La:114:LYS:HB2 | 1.61                     | 0.65              |
| 85:L5:1645:C:H2'   | 85:L5:1646:A:H8   | 1.61                     | 0.65              |
| 85:L5:3599:A:H2'   | 85:L5:3600:G:C8   | 2.32                     | 0.65              |
| 85:L5:4102:C:N3    | 85:L5:4105:A:O2'  | 2.29                     | 0.65              |
| 50:Le:26:ASP:OD1   | 50:Le:26:ASP:N    | 2.30                     | 0.65              |
| 71:ST:105:GLN:HA   | 71:ST:108:GLU:OE2 | 1.96                     | 0.65              |
| 75:Sg:78:ALA:HB3   | 75:Sg:92:LEU:HD21 | 1.78                     | 0.65              |
| 79:S2:1289:U:H2'   | 79:S2:1290:G:C8   | 2.32                     | 0.65              |
| 79:S2:1702:G:O6    | 79:S2:1836:G:N2   | 2.30                     | 0.65              |
| 15:sC:92:GLU:OE1   | 15:sC:92:GLU:N    | 2.21                     | 0.65              |
| 26:lE:262:LYS:HG2  | 26:lE:268:GLN:NE2 | 2.11                     | 0.65              |
| 33:lM:70:GLN:HG3   | 85:l5:735:G:H5''  | 1.78                     | 0.65              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 41:lU:23:LEU:HD22 | 41:lU:83:LEU:HD11  | 1.79                     | 0.65              |
| 46:la:27:LYS:NZ   | 85:l5:1518:A:OP1   | 2.23                     | 0.65              |
| 50:le:45:VAL:HG12 | 50:le:52:GLN:HB3   | 1.79                     | 0.65              |
| 64:sR:60:ARG:NE   | 79:s2:1464:C:OP1   | 2.30                     | 0.65              |
| 67:sK:49:MET:HE1  | 67:sK:69:TRP:CG    | 2.32                     | 0.65              |
| 85:l5:452:A:H62   | 85:l5:1293:G:H3'   | 1.62                     | 0.65              |
| 80:CB:8:GLN:CB    | 8:SY:130:LYS:HD2   | 2.27                     | 0.65              |
| 80:CB:370:GLU:N   | 80:CB:370:GLU:OE1  | 2.31                     | 0.65              |
| 6:SG:67:VAL:HB    | 6:SG:100:CYS:H     | 1.62                     | 0.65              |
| 8:SY:57:VAL:HG13  | 8:SY:60:PHE:HZ     | 1.62                     | 0.65              |
| 85:L5:676:C:H2'   | 85:L5:677:G:H8     | 1.62                     | 0.65              |
| 85:L5:1186:U:H2'  | 85:L5:1187:G:C4    | 2.32                     | 0.65              |
| 85:L5:1492:G:H4'  | 47:Lb:41:ARG:HH21  | 1.62                     | 0.65              |
| 85:L5:1700:G:OP2  | 85:L5:1704:C:N4    | 2.29                     | 0.65              |
| 85:L5:2406:G:N7   | 57:Ll:2:SER:N      | 2.44                     | 0.65              |
| 85:L5:4691:A:H4'  | 29:LH:71:ARG:HG2   | 1.77                     | 0.65              |
| 33:LM:25:VAL:HG13 | 33:LM:38:VAL:HG11  | 1.79                     | 0.65              |
| 62:Lr:38:PHE:O    | 62:Lr:45:HIS:NE2   | 2.29                     | 0.65              |
| 66:SF:20:PHE:O    | 66:SF:22:LYS:NZ    | 2.23                     | 0.65              |
| 75:Sg:79:LEU:HD22 | 75:Sg:87:LEU:HD21  | 1.78                     | 0.65              |
| 79:S2:430:C:H2'   | 79:S2:431:G:H8     | 1.62                     | 0.65              |
| 79:S2:920:A:H62   | 79:S2:1021:U:H3    | 1.43                     | 0.65              |
| 82:PE:23:A:H2'    | 82:PE:24:G:H8      | 1.62                     | 0.65              |
| 38:lR:117:ARG:HD3 | 85:l5:2663:G:O3'   | 1.95                     | 0.64              |
| 43:IX:93:ASN:HB3  | 43:IX:139:ARG:HH21 | 1.61                     | 0.64              |
| 54:li:53:TYR:HB2  | 54:li:76:ARG:HG3   | 1.77                     | 0.64              |
| 79:s2:692:G:N1    | 79:s2:738:C:O2     | 2.29                     | 0.64              |
| 79:s2:941:C:H2'   | 79:s2:942:G:H8     | 1.59                     | 0.64              |
| 79:s2:1172:U:H2'  | 79:s2:1173:A:H8    | 1.61                     | 0.64              |
| 79:s2:1473:G:N2   | 79:s2:1476:A:OP2   | 2.29                     | 0.64              |
| 79:s2:1854:U:H2'  | 79:s2:1855:G:H8    | 1.62                     | 0.64              |
| 85:l5:3809:G:OP2  | 85:l5:3809:G:N2    | 2.28                     | 0.64              |
| 85:l5:4741:C:H4'  | 85:l5:4742:G:H5'   | 1.80                     | 0.64              |
| 11:SB:151:ARG:NH1 | 79:S2:1102:G:OP2   | 2.31                     | 0.64              |
| 17:SO:121:ARG:NH1 | 73:Sc:60:GLU:OE2   | 2.30                     | 0.64              |
| 85:L5:299:C:H2'   | 85:L5:300:A:H8     | 1.61                     | 0.64              |
| 85:L5:1552:G:O2'  | 85:L5:1574:G:N2    | 2.30                     | 0.64              |
| 85:L5:2277:C:H2'  | 85:L5:2278:G:C8    | 2.32                     | 0.64              |
| 85:L5:4294:C:O3'  | 60:Lo:13:LYS:NZ    | 2.30                     | 0.64              |
| 48:Lc:38:ILE:HD12 | 48:Lc:39:ARG:N     | 2.12                     | 0.64              |
| 63:Lz:85:MET:SD   | 63:Lz:93:LEU:HD11  | 2.37                     | 0.64              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 75:Sg:62:HIS:ND1   | 75:Sg:82:SER:HB3   | 2.13                     | 0.64              |
| 79:S2:525:A:H2'    | 79:S2:526:A:H8     | 1.62                     | 0.64              |
| 79:S2:1523:C:H2'   | 79:S2:1524:G:H8    | 1.62                     | 0.64              |
| 84:Lt:131:GLU:HB2  | 84:Lt:152:ILE:HG23 | 1.79                     | 0.64              |
| 1:CH:104:GLN:HB2   | 65:SD:178:ARG:NH2  | 2.13                     | 0.64              |
| 7:sJ:30:LYS:HA     | 9:se:38:TYR:HE2    | 1.62                     | 0.64              |
| 10:sA:85:ARG:HD3   | 10:sA:204:TYR:HA   | 1.78                     | 0.64              |
| 16:sN:43:LYS:O     | 16:sN:43:LYS:NZ    | 2.25                     | 0.64              |
| 29:IH:129:ARG:HH22 | 85:l5:4704:C:H4'   | 1.62                     | 0.64              |
| 35:lO:35:VAL:HG21  | 35:lO:80:PHE:HE1   | 1.62                     | 0.64              |
| 39:IS:139:ARG:NE   | 85:l5:1952:G:OP1   | 2.29                     | 0.64              |
| 42:IV:45:ILE:HG21  | 42:IV:53:PRO:HB3   | 1.79                     | 0.64              |
| 43:IX:124:VAL:HG22 | 43:IX:138:VAL:HG12 | 1.78                     | 0.64              |
| 47:lb:61:ASN:O     | 47:lb:65:MET:HG3   | 1.97                     | 0.64              |
| 55:lj:2:THR:HG22   | 55:lj:4:GLY:H      | 1.62                     | 0.64              |
| 67:sK:27:VAL:HG12  | 67:sK:46:MET:HE1   | 1.80                     | 0.64              |
| 71:sT:78:ILE:HD11  | 79:s2:1587:G:C5    | 2.32                     | 0.64              |
| 79:s2:1779:G:H2'   | 79:s2:1780:G:C8    | 2.33                     | 0.64              |
| 2:SE:149:TYR:CE1   | 6:SG:205:GLU:HG2   | 2.32                     | 0.64              |
| 10:SA:29:ASN:OD1   | 10:SA:30:LEU:N     | 2.30                     | 0.64              |
| 85:L5:730:G:N3     | 27:LF:73:ARG:NH2   | 2.43                     | 0.64              |
| 85:L5:1304:C:H2'   | 85:L5:1305:C:H6    | 1.63                     | 0.64              |
| 85:L5:1563:A:H2'   | 85:L5:1564:A:C8    | 2.32                     | 0.64              |
| 85:L5:1687:U:H2'   | 85:L5:1688:G:C8    | 2.32                     | 0.64              |
| 85:L5:2289:C:N4    | 62:Lr:23:GLN:O     | 2.27                     | 0.64              |
| 85:L5:4054:C:OP1   | 63:Lz:1:MET:N      | 2.29                     | 0.64              |
| 23:LB:84:MET:HE2   | 23:LB:84:MET:HA    | 1.79                     | 0.64              |
| 29:LH:7:ASN:HD22   | 29:LH:56:ARG:HH12  | 1.45                     | 0.64              |
| 30:LI:62:SER:HA    | 30:LI:65:LEU:CD1   | 2.28                     | 0.64              |
| 42:LV:82:ILE:HG23  | 42:LV:121:VAL:HG23 | 1.77                     | 0.64              |
| 43:LX:69:ASN:OD1   | 43:LX:71:LEU:HD23  | 1.96                     | 0.64              |
| 75:Sg:256:ILE:HB   | 75:Sg:270:LEU:HB3  | 1.79                     | 0.64              |
| 79:S2:1101:U:H2'   | 79:S2:1102:G:C8    | 2.32                     | 0.64              |
| 87:LW:101:ARG:HG3  | 87:LW:105:ARG:HD3  | 1.79                     | 0.64              |
| 2:sE:16:LYS:NZ     | 79:s2:848:U:OP2    | 2.29                     | 0.64              |
| 2:sE:18:TRP:HH2    | 2:sE:39:ARG:HA     | 1.62                     | 0.64              |
| 14:sa:13:LYS:HE2   | 79:s2:1133:A:H4'   | 1.78                     | 0.64              |
| 20:l7:28:C:OP2     | 25:lD:57:ASN:ND2   | 2.31                     | 0.64              |
| 24:lC:173:LYS:O    | 24:lC:175:LYS:NZ   | 2.28                     | 0.64              |
| 32:lL:190:ARG:HB3  | 32:lL:191:LEU:HD12 | 1.79                     | 0.64              |
| 38:lR:157:ASP:OD1  | 38:lR:158:GLN:N    | 2.31                     | 0.64              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 47:lb:5:LYS:NZ     | 85:l5:1873:A:OP2   | 2.25                     | 0.64              |
| 47:lb:25:ARG:HH22  | 85:l5:1844:G:H5''  | 1.62                     | 0.64              |
| 50:le:63:ASN:OD1   | 50:le:64:LYS:N     | 2.30                     | 0.64              |
| 64:sR:93:GLN:N     | 64:sR:93:GLN:OE1   | 2.30                     | 0.64              |
| 69:sQ:74:GLY:O     | 69:sQ:80:GLN:NE2   | 2.29                     | 0.64              |
| 79:s2:464:A:H61    | 80:cB:49:ALA:H     | 1.46                     | 0.64              |
| 79:s2:1216:C:N4    | 79:s2:1342:U:OP1   | 2.30                     | 0.64              |
| 79:s2:1595:U:H2'   | 79:s2:1596:U:C6    | 2.32                     | 0.64              |
| 85:l5:4419:U:OP1   | 85:l5:4475:G:N2    | 2.30                     | 0.64              |
| 85:l5:4563:U:H2'   | 85:l5:4564:A:H8    | 1.62                     | 0.64              |
| 80:CB:284:LYS:NZ   | 80:CB:286:PRO:HA   | 2.13                     | 0.64              |
| 85:L5:1332:C:H2'   | 85:L5:1333:A:H8    | 1.63                     | 0.64              |
| 85:L5:1762:C:C4    | 85:L5:1770:A:C2    | 2.85                     | 0.64              |
| 85:L5:2484:A:H62   | 85:L5:2494:U:H3    | 1.45                     | 0.64              |
| 85:L5:3727:A:H2'   | 85:L5:3728:A:C8    | 2.33                     | 0.64              |
| 85:L5:3809:G:OP2   | 85:L5:3809:G:N2    | 2.18                     | 0.64              |
| 85:L5:4094:G:N2    | 85:L5:4109:G:H4'   | 2.13                     | 0.64              |
| 85:L5:4101:C:C2    | 85:L5:4104:G:C4'   | 2.71                     | 0.64              |
| 85:L5:4883:C:N4    | 26:LE:181:LEU:O    | 2.30                     | 0.64              |
| 26:LE:222:LEU:H    | 26:LE:237:LYS:HZ2  | 1.44                     | 0.64              |
| 27:LF:219:GLY:O    | 27:LF:246:ARG:NH2  | 2.29                     | 0.64              |
| 32:LL:178:ALA:N    | 46:La:134:GLU:OE2  | 2.31                     | 0.64              |
| 34:LN:119:TYR:HE2  | 34:LN:133:ILE:HD11 | 1.61                     | 0.64              |
| 66:SF:146:ARG:HA   | 66:SF:149:GLN:HE21 | 1.63                     | 0.64              |
| 70:SS:139:THR:HG21 | 79:S2:1231:C:OP2   | 1.97                     | 0.64              |
| 79:S2:1199:A:H2'   | 79:S2:1200:A:C8    | 2.32                     | 0.64              |
| 87:LW:96:GLN:OE1   | 87:LW:101:ARG:NH2  | 2.26                     | 0.64              |
| 1:CH:108:ASP:OD2   | 65:SD:178:ARG:NH1  | 2.30                     | 0.64              |
| 25:ID:56:THR:HG22  | 25:ID:58:ARG:H     | 1.63                     | 0.64              |
| 25:ID:265:ARG:HE   | 25:ID:267:ASN:HB2  | 1.62                     | 0.64              |
| 39:IS:95:ARG:HH12  | 39:IS:112:ASP:HB3  | 1.61                     | 0.64              |
| 56:lk:18:LYS:NZ    | 85:l5:2773:G:O2'   | 2.31                     | 0.64              |
| 56:lk:40:ARG:HD3   | 56:lk:41:TYR:CZ    | 2.31                     | 0.64              |
| 70:sS:64:VAL:O     | 70:sS:68:ILE:HG12  | 1.97                     | 0.64              |
| 79:s2:325:C:N3     | 79:s2:326:C:O2'    | 2.31                     | 0.64              |
| 80:cB:9:ILE:O      | 80:cB:13:MET:CB    | 2.45                     | 0.64              |
| 80:cB:141:THR:O    | 80:cB:145:GLN:NE2  | 2.30                     | 0.64              |
| 85:l5:139:G:H2'    | 85:l5:140:G:C8     | 2.32                     | 0.64              |
| 8:SY:102:THR:OG1   | 8:SY:106:GLN:OE1   | 2.14                     | 0.64              |
| 85:L5:4936:G:C5    | 26:LE:183:ARG:HD2  | 2.33                     | 0.64              |
| 32:LL:121:ARG:HA   | 32:LL:124:LEU:HD23 | 1.78                     | 0.64              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 43:LX:96:LEU:HG    | 43:LX:140:LEU:HD11 | 1.78                     | 0.64              |
| 46:La:73:VAL:HB    | 46:La:108:TYR:HD1  | 1.61                     | 0.64              |
| 69:SQ:123:ASP:O    | 69:SQ:126:ARG:NH1  | 2.31                     | 0.64              |
| 74:Sd:54:LYS:NZ    | 79:S2:1481:G:O3'   | 2.31                     | 0.64              |
| 75:Sg:18:VAL:O     | 75:Sg:287:THR:OG1  | 2.15                     | 0.64              |
| 79:S2:639:C:H2'    | 79:S2:640:A:C8     | 2.32                     | 0.64              |
| 84:Lt:126:SER:O    | 84:Lt:130:LYS:HG2  | 1.97                     | 0.64              |
| 8:sY:104:ARG:NH2   | 79:s2:507:G:OP2    | 2.31                     | 0.64              |
| 10:sA:18:PHE:HA    | 10:sA:173:LEU:HD21 | 1.79                     | 0.64              |
| 15:sC:169:TYR:OH   | 15:sC:175:GLY:O    | 2.11                     | 0.64              |
| 18:sW:51:GLU:N     | 18:sW:62:VAL:O     | 2.29                     | 0.64              |
| 19:sb:51:GLN:O     | 19:sb:51:GLN:NE2   | 2.31                     | 0.64              |
| 24:lC:180:ILE:HD13 | 24:lC:224:ILE:HG21 | 1.78                     | 0.64              |
| 36:lP:32:THR:HA    | 36:lP:58:VAL:HG21  | 1.80                     | 0.64              |
| 47:lb:3:LYS:HD3    | 85:l5:4194:U:H5'   | 1.80                     | 0.64              |
| 64:sR:51:ALA:HA    | 64:sR:54:VAL:CG2   | 2.28                     | 0.64              |
| 69:sQ:104:SER:HA   | 69:sQ:107:GLU:OE2  | 1.96                     | 0.64              |
| 76:sM:38:ALA:O     | 76:sM:41:ALA:HB3   | 1.97                     | 0.64              |
| 79:s2:1004:U:H2'   | 79:s2:1005:G:H8    | 1.62                     | 0.64              |
| 79:s2:1351:G:H1    | 79:s2:1360:U:H3    | 1.45                     | 0.64              |
| 80:cB:649:ILE:HA   | 80:cB:663:THR:HG22 | 1.79                     | 0.64              |
| 80:cB:655:ASP:H    | 80:cB:684:GLN:NE2  | 1.95                     | 0.64              |
| 83:ls:58:ASN:ND2   | 85:l5:2022:C:OP1   | 2.29                     | 0.64              |
| 85:l5:261:G:H2'    | 85:l5:262:G:C8     | 2.32                     | 0.64              |
| 85:l5:909:A:N1     | 85:l5:910:G:O6     | 2.30                     | 0.64              |
| 85:l5:2491:C:O2'   | 85:l5:2492:C:O4'   | 2.13                     | 0.64              |
| 85:l5:2759:G:O2'   | 85:l5:2762:G:N2    | 2.30                     | 0.64              |
| 2:SE:166:THR:HB    | 2:SE:168:LYS:HG2   | 1.77                     | 0.64              |
| 10:SA:157:VAL:O    | 13:SV:65:SER:OG    | 2.16                     | 0.64              |
| 85:L5:959:G:O2'    | 85:L5:2263:A:N6    | 2.30                     | 0.64              |
| 85:L5:1502:G:OP1   | 37:LQ:65:ARG:NH1   | 2.30                     | 0.64              |
| 85:L5:4083:U:O2'   | 85:L5:4086:G:OP2   | 2.16                     | 0.64              |
| 22:LA:242:ARG:NH2  | 22:LA:243:THR:O    | 2.31                     | 0.64              |
| 36:LP:5:SER:OG     | 36:LP:118:GLN:NE2  | 2.29                     | 0.64              |
| 69:SQ:19:ALA:HB2   | 69:SQ:75:GLY:HA3   | 1.79                     | 0.64              |
| 71:ST:58:ALA:O     | 71:ST:62:ARG:HG3   | 1.97                     | 0.64              |
| 79:S2:928:G:H1     | 79:S2:1013:U:H3    | 1.45                     | 0.64              |
| 81:AP:9:A:N6       | 81:AP:22:U:OP2     | 2.31                     | 0.64              |
| 81:AP:18:G:O2'     | 81:AP:57:G:N2      | 2.23                     | 0.64              |
| 84:Lt:50:THR:OG1   | 84:Lt:72:GLU:OE2   | 2.14                     | 0.64              |
| 3:sI:144:LYS:NZ    | 79:s2:204:G:O6     | 2.30                     | 0.64              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 5:sX:58:GLU:OE2    | 79:s2:1823:A:O2'   | 2.14                     | 0.64              |
| 6:sG:132:ARG:NH1   | 79:s2:151:C:O2     | 2.30                     | 0.64              |
| 22:lA:71:LYS:NZ    | 85:l5:2594:C:O2'   | 2.24                     | 0.64              |
| 25:ID:258:LYS:C    | 25:ID:259:LYS:HD3  | 2.23                     | 0.64              |
| 26:lE:94:LYS:HE2   | 85:l5:688:U:H5'    | 1.79                     | 0.64              |
| 32:lL:47:ALA:O     | 32:lL:149:GLN:NE2  | 2.28                     | 0.64              |
| 39:lS:127:MET:HE1  | 40:lT:155:PRO:HA   | 1.79                     | 0.64              |
| 43:lX:47:ARG:NH1   | 85:l5:2473:A:OP1   | 2.26                     | 0.64              |
| 43:lX:116:LEU:HG   | 43:lX:117:TYR:HD1  | 1.63                     | 0.64              |
| 52:lg:103:VAL:O    | 52:lg:107:LEU:HD22 | 1.98                     | 0.64              |
| 79:s2:1361:G:OP2   | 79:s2:1362:U:O2'   | 2.15                     | 0.64              |
| 80:cB:429:ILE:N    | 80:cB:443:TYR:O    | 2.31                     | 0.64              |
| 85:l5:1759:G:H1    | 85:l5:1773:U:H3    | 1.45                     | 0.64              |
| 85:l5:3717:A:H2'   | 85:l5:3718:A:C8    | 2.32                     | 0.64              |
| 6:SG:32:MET:SD     | 6:SG:100:CYS:HB2   | 2.38                     | 0.64              |
| 85:L5:1266:G:H5'   | 47:Lb:99:ILE:HD11  | 1.80                     | 0.64              |
| 85:L5:1677:U:H4'   | 85:L5:1680:G:C2    | 2.33                     | 0.64              |
| 85:L5:3607:U:H2'   | 85:L5:3608:A:C8    | 2.33                     | 0.64              |
| 21:L8:153:C:H4'    | 28:LG:185:LYS:HG3  | 1.79                     | 0.64              |
| 22:LA:117:GLU:HG3  | 22:LA:163:ARG:H    | 1.61                     | 0.64              |
| 23:LB:353:VAL:C    | 23:LB:354:GLN:HE21 | 2.06                     | 0.64              |
| 26:LE:119:GLU:OE1  | 50:Le:7:LEU:HD13   | 1.98                     | 0.64              |
| 38:LR:126:LYS:HE3  | 38:LR:131:VAL:HG21 | 1.79                     | 0.64              |
| 45:LZ:111:ARG:HH12 | 45:LZ:115:LYS:HB2  | 1.61                     | 0.64              |
| 75:Sg:72:SER:OG    | 75:Sg:74:ASP:OD1   | 2.15                     | 0.64              |
| 75:Sg:244:ASN:ND2  | 75:Sg:294:ASP:O    | 2.30                     | 0.64              |
| 77:SZ:41:ARG:NH2   | 79:S2:1600:G:OP1   | 2.30                     | 0.64              |
| 79:S2:793:G:H2'    | 79:S2:794:A:H8     | 1.63                     | 0.64              |
| 81:AP:50:U:O4      | 81:AP:64:G:O6      | 2.14                     | 0.64              |
| 87:LW:101:ARG:HG3  | 87:LW:105:ARG:CD   | 2.27                     | 0.64              |
| 2:sE:49:ARG:NH2    | 79:s2:496:C:OP1    | 2.31                     | 0.64              |
| 6:sG:69:THR:N      | 6:sG:100:CYS:SG    | 2.71                     | 0.64              |
| 10:sA:120:ARG:O    | 10:sA:143:PRO:HD2  | 1.97                     | 0.64              |
| 11:sB:149:GLN:NE2  | 79:s2:1123:C:H4'   | 2.13                     | 0.64              |
| 12:sH:38:ALA:O     | 12:sH:41:ARG:NH2   | 2.30                     | 0.64              |
| 25:ID:217:ASP:HA   | 25:ID:220:LYS:HD2  | 1.79                     | 0.64              |
| 28:lG:50:ASP:HA    | 43:lX:40:ILE:HD11  | 1.78                     | 0.64              |
| 64:sR:30:THR:N     | 79:s2:1455:A:H5'   | 2.10                     | 0.64              |
| 65:sD:106:ARG:NE   | 65:sD:173:ARG:HD3  | 2.12                     | 0.64              |
| 66:sF:60:ARG:HH21  | 73:sc:49:PRO:HB3   | 1.62                     | 0.64              |
| 67:sK:65:ARG:NH1   | 74:sd:25:SER:OG    | 2.30                     | 0.64              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 69:sQ:10:VAL:HG12  | 69:sQ:95:TYR:HD2   | 1.62                     | 0.64              |
| 71:sT:18:LEU:HD22  | 71:sT:58:ALA:HA    | 1.78                     | 0.64              |
| 80:cB:200:MET:HE2  | 80:cB:200:MET:HA   | 1.79                     | 0.64              |
| 80:cB:692:LEU:O    | 80:cB:839:ARG:NH2  | 2.28                     | 0.64              |
| 85:l5:2079:G:H2'   | 85:l5:2080:U:C6    | 2.33                     | 0.64              |
| 80:CB:120:ARG:NH2  | 80:CB:495:ARG:O    | 2.30                     | 0.64              |
| 10:SA:120:ARG:HH11 | 15:SC:266:TYR:HB3  | 1.62                     | 0.64              |
| 12:SH:127:ASP:OD1  | 12:SH:127:ASP:N    | 2.29                     | 0.64              |
| 85:L5:454:U:H1'    | 50:Le:5:ARG:HH12   | 1.62                     | 0.64              |
| 85:L5:4239:A:H2'   | 85:L5:4240:G:C8    | 2.33                     | 0.64              |
| 85:L5:4405:G:O2'   | 30:LI:4:ARG:NH2    | 2.30                     | 0.64              |
| 21:L8:141:C:H2'    | 21:L8:142:U:C6     | 2.32                     | 0.64              |
| 21:L8:153:C:H2'    | 21:L8:154:G:C8     | 2.33                     | 0.64              |
| 39:LS:94:TYR:HE2   | 39:LS:138:ARG:HD3  | 1.63                     | 0.64              |
| 53:Lh:54:ILE:O     | 53:Lh:58:LEU:HG    | 1.98                     | 0.64              |
| 54:Li:90:LEU:HA    | 54:Li:93:VAL:HG12  | 1.79                     | 0.64              |
| 66:SF:167:LYS:HB2  | 66:SF:171:GLU:HG3  | 1.79                     | 0.64              |
| 75:Sg:159:ASN:ND2  | 75:Sg:162:ASN:HD22 | 1.95                     | 0.64              |
| 79:S2:1410:C:H2'   | 79:S2:1411:G:C8    | 2.33                     | 0.64              |
| 79:S2:1792:G:H2'   | 79:S2:1793:A:H8    | 1.62                     | 0.64              |
| 16:sN:34:LYS:NZ    | 16:sN:38:TYR:HE2   | 1.96                     | 0.64              |
| 18:sW:2:VAL:HA     | 79:s2:1092:G:H4'   | 1.79                     | 0.64              |
| 24:lC:303:ARG:O    | 37:lQ:38:ARG:NH2   | 2.26                     | 0.64              |
| 26:lE:110:ARG:NH1  | 85:l5:967:C:H2'    | 2.13                     | 0.64              |
| 26:lE:199:THR:HG21 | 33:lM:107:PHE:HB2  | 1.79                     | 0.64              |
| 28:lG:34:LYS:HE3   | 85:l5:4129:G:O4'   | 1.98                     | 0.64              |
| 31:lJ:111:GLU:OE2  | 31:lJ:114:ASP:N    | 2.30                     | 0.64              |
| 44:lY:121:ARG:NH1  | 85:l5:194:C:O2     | 2.31                     | 0.64              |
| 64:sR:26:ASN:HB3   | 64:sR:59:LYS:HD3   | 1.79                     | 0.64              |
| 68:sP:32:GLN:N     | 68:sP:32:GLN:OE1   | 2.30                     | 0.64              |
| 70:sS:21:ASP:OD1   | 70:sS:23:ARG:NH1   | 2.31                     | 0.64              |
| 79:s2:837:A:H4'    | 79:s2:838:G:H4'    | 1.78                     | 0.64              |
| 79:s2:1221:G:H2'   | 79:s2:1222:G:C8    | 2.33                     | 0.64              |
| 80:cB:176:GLN:HB3  | 80:cB:180:ARG:NH1  | 2.13                     | 0.64              |
| 80:cB:512:LYS:NZ   | 80:cB:570:ILE:O    | 2.27                     | 0.64              |
| 80:cB:713:ALA:HA   | 80:cB:716:ARG:NH2  | 2.13                     | 0.64              |
| 80:cB:767:ARG:NH1  | 80:cB:792:GLU:OE2  | 2.30                     | 0.64              |
| 82:pE:34:U:O2'     | 82:pE:35:U:OP1     | 2.15                     | 0.64              |
| 83:ls:39:GLN:O     | 83:ls:43:ILE:HG12  | 1.98                     | 0.64              |
| 85:l5:1993:C:H2'   | 85:l5:1994:C:C6    | 2.33                     | 0.64              |
| 85:l5:2348:G:OP1   | 85:l5:2351:C:N4    | 2.31                     | 0.64              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 80:CB:653:GLY:N    | 80:CB:660:ASN:O   | 2.31                     | 0.64              |
| 4:SL:79:LYS:HG2    | 4:SL:81:LYS:HG2   | 1.78                     | 0.64              |
| 6:SG:1:MET:CE      | 6:SG:106:LEU:HB3  | 2.23                     | 0.64              |
| 16:SN:56:ASP:OD2   | 19:Sb:52:THR:N    | 2.24                     | 0.64              |
| 85:L5:194:C:O2     | 44:LY:121:ARG:NH1 | 2.31                     | 0.64              |
| 85:L5:364:G:H2'    | 55:Lj:56:ARG:NE   | 2.12                     | 0.64              |
| 85:L5:1258:G:H2'   | 85:L5:1259:G:C8   | 2.32                     | 0.64              |
| 85:L5:1708:G:H2'   | 85:L5:1709:C:H3'  | 1.78                     | 0.64              |
| 85:L5:3893:C:H2'   | 85:L5:3894:A:H8   | 1.63                     | 0.64              |
| 85:L5:4096:C:C4'   | 85:L5:4110:C:H5'' | 2.28                     | 0.64              |
| 20:L7:95:C:OP1     | 39:LS:43:ARG:NH1  | 2.31                     | 0.64              |
| 25:LD:44:TYR:OH    | 40:LT:67:VAL:HG11 | 1.97                     | 0.64              |
| 62:Lr:28:GLU:HG2   | 62:Lr:31:ASN:HB2  | 1.79                     | 0.64              |
| 63:Lz:198:TRP:CD1  | 63:Lz:199:GLN:H   | 2.15                     | 0.64              |
| 66:SF:164:ARG:NH1  | 79:S2:1636:G:O2'  | 2.31                     | 0.64              |
| 70:SS:8:LYS:NZ     | 70:SS:59:LEU:O    | 2.21                     | 0.64              |
| 3:sI:98:LYS:HB3    | 79:s2:377:G:H5'   | 1.80                     | 0.64              |
| 15:sC:168:GLY:N    | 15:sC:179:THR:O   | 2.25                     | 0.64              |
| 18:sW:28:ARG:HD2   | 18:sW:60:LYS:HE3  | 1.80                     | 0.64              |
| 25:ID:39:GLN:NE2   | 25:ID:46:THR:OG1  | 2.31                     | 0.64              |
| 25:ID:289:ARG:NH2  | 85:l5:1178:G:O2'  | 2.31                     | 0.64              |
| 38:IR:84:THR:HG23  | 38:IR:87:ALA:H    | 1.63                     | 0.64              |
| 44:IY:111:LEU:HD12 | 44:IY:116:LYS:HG3 | 1.80                     | 0.64              |
| 70:sS:142:ARG:NH1  | 79:s2:1228:A:O3'  | 2.31                     | 0.64              |
| 71:sT:110:LEU:HG   | 71:sT:112:MET:SD  | 2.37                     | 0.64              |
| 79:s2:300:U:H2'    | 79:s2:301:A:C8    | 2.33                     | 0.64              |
| 79:s2:588:G:H4'    | 79:s2:589:G:H5'   | 1.79                     | 0.64              |
| 79:s2:1203:G:H2'   | 79:s2:1204:A:C8   | 2.33                     | 0.64              |
| 85:l5:1942:A:H2'   | 85:l5:1943:A:H8   | 1.62                     | 0.64              |
| 85:l5:2520:C:H2'   | 85:l5:2521:G:H8   | 1.63                     | 0.64              |
| 80:CB:410:PHE:HZ   | 80:CB:526:ARG:HG2 | 1.63                     | 0.64              |
| 80:CB:579:TYR:O    | 80:CB:580:ARG:NH1 | 2.31                     | 0.64              |
| 15:SC:272:HIS:CD2  | 15:SC:275:LYS:HZ2 | 2.15                     | 0.64              |
| 85:L5:1460:C:H5''  | 37:LQ:144:LYS:HG3 | 1.79                     | 0.64              |
| 85:L5:1538:U:H2'   | 85:L5:1539:G:H8   | 1.63                     | 0.64              |
| 85:L5:2062:C:O2'   | 39:LS:111:ARG:NH2 | 2.31                     | 0.64              |
| 85:L5:2274:C:H2'   | 85:L5:2275:G:C8   | 2.33                     | 0.64              |
| 85:L5:2275:G:H2'   | 85:L5:2276:A:H8   | 1.62                     | 0.64              |
| 85:L5:2693:G:OP2   | 56:Lk:33:LYS:NZ   | 2.30                     | 0.64              |
| 85:L5:4101:C:C2    | 85:L5:4106:G:O3'  | 2.51                     | 0.64              |
| 85:L5:4151:G:H2'   | 85:L5:4152:G:H8   | 1.63                     | 0.64              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 38:LR:141:HIS:HA   | 38:LR:144:LYS:HE2  | 1.80                     | 0.64              |
| 64:SR:6:THR:HA     | 79:S2:1373:C:H5'   | 1.80                     | 0.64              |
| 70:SS:40:TYR:HE1   | 70:SS:71:MET:HE2   | 1.61                     | 0.64              |
| 79:S2:1228:A:H2'   | 79:S2:1229:G:C8    | 2.33                     | 0.64              |
| 6:sG:100:CYS:SG    | 6:sG:101:ILE:N     | 2.70                     | 0.64              |
| 11:sB:180:ASP:OD1  | 11:sB:182:LYS:NZ   | 2.30                     | 0.64              |
| 20:l7:54:A:OP1     | 31:lJ:8:LYS:NZ     | 2.31                     | 0.64              |
| 24:lC:204:ARG:NH1  | 85:l5:2298:U:OP1   | 2.31                     | 0.64              |
| 25:lD:90:VAL:HG11  | 25:lD:231:VAL:HG21 | 1.79                     | 0.64              |
| 65:sD:136:VAL:HG23 | 65:sD:186:VAL:HG12 | 1.80                     | 0.64              |
| 66:sF:17:ILE:HD12  | 66:sF:48:TYR:CE2   | 2.33                     | 0.64              |
| 75:sg:18:VAL:O     | 75:sg:287:THR:OG1  | 2.16                     | 0.64              |
| 76:sM:35:ILE:HG23  | 79:s2:1285:G:H5'   | 1.80                     | 0.64              |
| 79:s2:5:U:H2'      | 79:s2:6:G:H8       | 1.63                     | 0.64              |
| 79:s2:528:A:H2'    | 79:s2:529:A:C8     | 2.33                     | 0.64              |
| 79:s2:836:G:O3'    | 28:LG:251:ALA:HB1  | 1.98                     | 0.64              |
| 79:s2:996:A:H2'    | 79:s2:997:A:C8     | 2.32                     | 0.64              |
| 79:s2:1133:A:H2'   | 79:s2:1134:G:H8    | 1.63                     | 0.64              |
| 85:l5:2368:A:H3'   | 85:l5:2827:G:H22   | 1.62                     | 0.64              |
| 85:l5:2848:G:O2'   | 85:l5:3838:U:O4    | 2.14                     | 0.64              |
| 80:CB:21:ASN:HD22  | 80:CB:101:ASN:HB2  | 1.62                     | 0.64              |
| 80:CB:180:ARG:HA   | 80:CB:183:GLU:OE2  | 1.97                     | 0.64              |
| 8:SY:23:MET:SD     | 8:SY:23:MET:N      | 2.71                     | 0.64              |
| 85:L5:651:C:H2'    | 85:L5:652:G:C8     | 2.33                     | 0.64              |
| 85:L5:679:C:H2'    | 85:L5:680:G:C8     | 2.32                     | 0.64              |
| 85:L5:4671:C:O2    | 42:LV:86:LYS:NZ    | 2.31                     | 0.64              |
| 21:L8:39:G:H1'     | 21:L8:103:A:H61    | 1.62                     | 0.64              |
| 54:Li:61:LEU:CD1   | 54:Li:94:LEU:HD23  | 2.27                     | 0.64              |
| 76:SM:67:ALA:O     | 76:SM:71:GLU:HB3   | 1.98                     | 0.64              |
| 2:sE:116:PRO:O     | 2:sE:120:LYS:NZ    | 2.31                     | 0.63              |
| 3:sI:116:HIS:O     | 3:sI:152:ARG:NH2   | 2.31                     | 0.63              |
| 7:sJ:3:VAL:HG13    | 7:sJ:5:ARG:HH11    | 1.62                     | 0.63              |
| 7:sJ:18:ARG:NH2    | 79:s2:3:C:O2       | 2.31                     | 0.63              |
| 17:sO:134:PRO:HB3  | 79:s2:944:A:H5''   | 1.80                     | 0.63              |
| 24:lC:311:ARG:HH12 | 85:l5:958:G:H5'    | 1.63                     | 0.63              |
| 35:lO:65:ASN:ND2   | 85:l5:4565:C:OP1   | 2.30                     | 0.63              |
| 42:IV:95:PHE:O     | 87:IW:20:ARG:N     | 2.27                     | 0.63              |
| 51:lf:83:MET:HE1   | 85:l5:1917:A:OP1   | 1.98                     | 0.63              |
| 66:sF:77:MET:HE1   | 66:sF:84:GLY:C     | 2.22                     | 0.63              |
| 66:sF:87:LEU:HA    | 66:sF:90:VAL:HG12  | 1.80                     | 0.63              |
| 66:sF:123:GLU:HG3  | 66:sF:200:ALA:HB1  | 1.79                     | 0.63              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 79:s2:51:U:H2'     | 79:s2:52:G:C8      | 2.34                     | 0.63              |
| 79:s2:145:G:H2'    | 79:s2:146:G:C8     | 2.33                     | 0.63              |
| 79:s2:1401:A:H2'   | 79:s2:1402:A:C8    | 2.32                     | 0.63              |
| 79:s2:1588:A:H2'   | 79:s2:1589:A:C8    | 2.33                     | 0.63              |
| 83:ls:83:ARG:NH1   | 85:l5:2022:C:OP1   | 2.30                     | 0.63              |
| 85:l5:1207:C:H2'   | 85:l5:1208:G:H8    | 1.62                     | 0.63              |
| 4:SL:57:ASP:OD1    | 4:SL:60:CYS:N      | 2.30                     | 0.63              |
| 11:SB:214:LYS:HD2  | 11:SB:216:LYS:HB3  | 1.80                     | 0.63              |
| 13:SV:39:VAL:HB    | 13:SV:44:GLY:HA2   | 1.79                     | 0.63              |
| 85:L5:109:G:OP2    | 32:LL:74:ARG:NH2   | 2.31                     | 0.63              |
| 85:L5:185:C:O2     | 85:L5:187:U:O2'    | 2.14                     | 0.63              |
| 85:L5:280:G:H5''   | 34:LN:14:LYS:HE2   | 1.79                     | 0.63              |
| 85:L5:691:C:H2'    | 85:L5:692:A:C8     | 2.33                     | 0.63              |
| 85:L5:2098:G:H2'   | 85:L5:2099:G:C8    | 2.33                     | 0.63              |
| 85:L5:2784:C:H2'   | 85:L5:2785:C:H6    | 1.63                     | 0.63              |
| 21:L8:5:U:H2'      | 21:L8:6:C:H6       | 1.63                     | 0.63              |
| 24:LC:302:LEU:CD1  | 37:LQ:38:ARG:HB3   | 2.28                     | 0.63              |
| 35:LO:163:LYS:O    | 35:LO:166:ILE:HG13 | 1.98                     | 0.63              |
| 65:SD:32:ASP:OD2   | 65:SD:65:ARG:NH1   | 2.32                     | 0.63              |
| 65:SD:217:ILE:HG13 | 65:SD:218:LEU:N    | 2.13                     | 0.63              |
| 67:SK:65:ARG:HH11  | 74:Sd:22:ARG:HA    | 1.63                     | 0.63              |
| 72:SU:31:SER:O     | 72:SU:35:VAL:HG13  | 1.98                     | 0.63              |
| 72:SU:56:MET:SD    | 72:SU:57:PRO:HD2   | 2.38                     | 0.63              |
| 79:S2:1275:G:H22   | 79:S2:1506:A:P     | 2.20                     | 0.63              |
| 79:S2:1726:G:O6    | 79:S2:1809:A:N6    | 2.31                     | 0.63              |
| 87:IW:90:ILE:HA    | 87:IW:93:LYS:HZ2   | 1.61                     | 0.63              |
| 1:cH:77:VAL:O      | 1:cH:81:ILE:HG13   | 1.99                     | 0.63              |
| 2:sE:104:ASP:OD1   | 2:sE:108:ARG:N     | 2.24                     | 0.63              |
| 12:sH:169:LYS:O    | 12:sH:172:THR:OG1  | 2.15                     | 0.63              |
| 16:sN:2:GLY:N      | 79:s2:1092:G:OP1   | 2.31                     | 0.63              |
| 23:IB:302:ASN:O    | 23:IB:304:SER:N    | 2.32                     | 0.63              |
| 25:ID:73:MET:HE3   | 25:ID:73:MET:HA    | 1.80                     | 0.63              |
| 28:IG:71:TYR:HE1   | 34:IN:25:VAL:HG21  | 1.63                     | 0.63              |
| 64:sR:3:ARG:HH12   | 79:s2:1467:C:H1'   | 1.62                     | 0.63              |
| 69:sQ:44:PRO:HB2   | 69:sQ:46:THR:HG23  | 1.81                     | 0.63              |
| 72:sU:18:HIS:HB3   | 72:sU:117:ALA:HB2  | 1.79                     | 0.63              |
| 79:s2:1228:A:H2'   | 79:s2:1229:G:C8    | 2.33                     | 0.63              |
| 85:l5:4098:A:H2'   | 85:l5:4099:G:H4'   | 1.79                     | 0.63              |
| 80:CB:55:ARG:HG3   | 80:CB:56:PHE:H     | 1.62                     | 0.63              |
| 80:CB:396:MET:HE2  | 80:CB:396:MET:N    | 2.12                     | 0.63              |
| 2:SE:125:LYS:HB2   | 2:SE:226:PHE:CE1   | 2.33                     | 0.63              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:SJ:140:GLN:HE22  | 8:SY:64:PHE:HB3    | 1.62                     | 0.63              |
| 8:SY:111:LYS:NZ    | 79:S2:54:A:OP1     | 2.28                     | 0.63              |
| 11:SB:150:ILE:HG23 | 64:SR:131:PRO:HA   | 1.79                     | 0.63              |
| 17:SO:141:ARG:NH2  | 79:S2:1856:C:OP1   | 2.31                     | 0.63              |
| 85:L5:1728:U:H5'   | 27:LF:127:LYS:HZ2  | 1.59                     | 0.63              |
| 27:LF:29:LYS:HE2   | 27:LF:32:ARG:HH21  | 1.62                     | 0.63              |
| 27:LF:126:ASN:H    | 27:LF:129:SER:HB2  | 1.62                     | 0.63              |
| 29:LH:123:ILE:HD13 | 29:LH:125:ARG:HH21 | 1.63                     | 0.63              |
| 42:LV:13:LYS:NZ    | 42:LV:59:ASP:OD1   | 2.30                     | 0.63              |
| 73:Sc:20:ARG:HD3   | 73:Sc:28:THR:HG22  | 1.80                     | 0.63              |
| 79:S2:1203:G:H2'   | 79:S2:1204:A:C8    | 2.33                     | 0.63              |
| 10:sA:155:ARG:NH2  | 79:s2:1137:U:O2'   | 2.31                     | 0.63              |
| 12:sH:119:SER:OG   | 12:sH:120:ARG:NH1  | 2.30                     | 0.63              |
| 56:lk:49:ASP:OD1   | 56:lk:50:LYS:N     | 2.30                     | 0.63              |
| 60:lo:61:LYS:HG2   | 85:l5:4372:U:OP2   | 1.98                     | 0.63              |
| 64:sR:14:ARG:NE    | 79:s2:1373:C:O2'   | 2.30                     | 0.63              |
| 64:sR:43:SER:HB2   | 79:s2:1387:G:H5''  | 1.81                     | 0.63              |
| 64:sR:126:MET:SD   | 64:sR:129:LYS:HD2  | 2.38                     | 0.63              |
| 65:sD:158:ILE:HG23 | 65:sD:164:VAL:HG12 | 1.80                     | 0.63              |
| 69:sQ:41:MET:HE1   | 71:sT:9:VAL:C      | 2.22                     | 0.63              |
| 79:s2:388:U:H2'    | 79:s2:389:A:C8     | 2.34                     | 0.63              |
| 79:s2:1010:G:H2'   | 79:s2:1011:A:C8    | 2.33                     | 0.63              |
| 80:cB:62:ASP:HA    | 80:cB:65:GLU:HG2   | 1.79                     | 0.63              |
| 80:cB:710:HIS:CD2  | 80:cB:715:HIS:HB2  | 2.34                     | 0.63              |
| 2:SE:122:LYS:NZ    | 2:SE:143:ASP:OD2   | 2.26                     | 0.63              |
| 2:SE:134:LYS:NZ    | 79:S2:127:C:O2     | 2.31                     | 0.63              |
| 3:SI:184:ARG:NH1   | 79:S2:218:U:O2     | 2.29                     | 0.63              |
| 5:SX:112:VAL:HG23  | 79:S2:621:C:P      | 2.38                     | 0.63              |
| 17:SO:75:MET:HB2   | 17:SO:118:ALA:HB2  | 1.80                     | 0.63              |
| 17:SO:146:ARG:NH1  | 79:S2:1858:G:N7    | 2.46                     | 0.63              |
| 85:L5:1405:C:N4    | 85:L5:1408:G:N3    | 2.41                     | 0.63              |
| 85:L5:1440:U:H3    | 85:L5:2105:A:H2    | 1.46                     | 0.63              |
| 85:L5:1497:A:N7    | 37:LQ:180:ARG:NH2  | 2.45                     | 0.63              |
| 28:LG:30:PRO:HG2   | 45:LZ:124:THR:HA   | 1.79                     | 0.63              |
| 29:LH:85:THR:HG23  | 29:LH:86:LEU:HD13  | 1.80                     | 0.63              |
| 31:LJ:56:THR:HG23  | 31:LJ:63:ARG:HA    | 1.78                     | 0.63              |
| 34:LN:200:LEU:HD22 | 34:LN:204:ARG:HH11 | 1.63                     | 0.63              |
| 37:LQ:122:THR:OG1  | 37:LQ:124:ASP:OD1  | 2.15                     | 0.63              |
| 54:Li:63:VAL:HG13  | 54:Li:65:LYS:HG3   | 1.81                     | 0.63              |
| 56:Lk:55:LYS:O     | 56:Lk:59:SER:OG    | 2.14                     | 0.63              |
| 64:SR:97:GLU:OE1   | 64:SR:118:GLN:NE2  | 2.28                     | 0.63              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 71:ST:32:GLU:H     | 71:ST:32:GLU:CD    | 2.06                     | 0.63              |
| 79:S2:498:C:H2'    | 79:S2:499:G:C8     | 2.34                     | 0.63              |
| 79:S2:1808:U:H2'   | 79:S2:1809:A:C8    | 2.33                     | 0.63              |
| 2:sE:206:ASP:O     | 2:sE:222:LEU:N     | 2.24                     | 0.63              |
| 6:sG:98:ARG:NH2    | 6:sG:105:ASN:OD1   | 2.29                     | 0.63              |
| 14:sa:66:LYS:O     | 14:sa:67:LEU:HD23  | 1.99                     | 0.63              |
| 18:sW:101:PHE:HD1  | 18:sW:112:ASP:CG   | 2.07                     | 0.63              |
| 20:l7:106:G:OP2    | 30:lI:203:HIS:NE2  | 2.32                     | 0.63              |
| 23:lB:34:LYS:NZ    | 23:lB:35:ASP:O     | 2.30                     | 0.63              |
| 28:lG:105:GLU:OE2  | 28:lG:105:GLU:N    | 2.31                     | 0.63              |
| 29:lH:150:ASP:OD2  | 29:lH:153:LEU:HG   | 1.98                     | 0.63              |
| 44:lY:59:ARG:HG3   | 44:lY:103:LYS:HD2  | 1.80                     | 0.63              |
| 63:lz:24:LYS:HD2   | 63:lz:29:LEU:HD12  | 1.78                     | 0.63              |
| 79:s2:640:A:H2'    | 79:s2:641:A:C8     | 2.34                     | 0.63              |
| 80:cB:663:THR:OG1  | 80:cB:703:ASP:OD1  | 2.16                     | 0.63              |
| 80:CB:449:ARG:NH2  | 79:S2:51:U:O2'     | 2.30                     | 0.63              |
| 10:SA:185:MET:O    | 13:SV:45:ARG:NH2   | 2.31                     | 0.63              |
| 18:SW:23:ARG:HH22  | 19:Sb:5:LYS:C      | 2.06                     | 0.63              |
| 85:L5:509:A:N7     | 46:La:105:ARG:NH1  | 2.47                     | 0.63              |
| 85:L5:2275:G:H2'   | 85:L5:2276:A:C8    | 2.34                     | 0.63              |
| 85:L5:4954:G:H2'   | 85:L5:4955:A:H8    | 1.61                     | 0.63              |
| 27:LF:211:PHE:HB3  | 27:LF:213:LEU:HD21 | 1.80                     | 0.63              |
| 33:LM:12:VAL:HB    | 33:LM:60:PHE:HB2   | 1.79                     | 0.63              |
| 57:Ll:9:ILE:H      | 57:Ll:9:ILE:HD12   | 1.62                     | 0.63              |
| 64:SR:1:MET:CE     | 79:S2:1467:C:H3'   | 2.29                     | 0.63              |
| 66:SF:63:LYS:HD3   | 66:SF:71:ARG:HH22  | 1.61                     | 0.63              |
| 67:SK:30:PRO:HA    | 67:SK:41:PRO:HB3   | 1.79                     | 0.63              |
| 79:S2:921:G:N2     | 79:S2:1094:C:OP1   | 2.31                     | 0.63              |
| 79:S2:1201:U:H2'   | 79:S2:1202:U:C6    | 2.33                     | 0.63              |
| 84:Lt:109:ILE:H    | 84:Lt:109:ILE:HD12 | 1.63                     | 0.63              |
| 3:sI:36:THR:O      | 3:sI:95:THR:OG1    | 2.14                     | 0.63              |
| 3:sI:134:GLU:OE2   | 3:sI:138:ASN:ND2   | 2.32                     | 0.63              |
| 21:l8:124:U:OP1    | 85:l5:2544:G:N1    | 2.30                     | 0.63              |
| 27:lF:64:MET:H     | 27:lF:64:MET:HE3   | 1.63                     | 0.63              |
| 27:lF:184:ILE:HG23 | 27:lF:189:ASP:HB3  | 1.80                     | 0.63              |
| 39:lS:160:ARG:HD2  | 85:l5:1922:G:P     | 2.38                     | 0.63              |
| 60:lo:99:ARG:HD3   | 60:lo:99:ARG:N     | 2.13                     | 0.63              |
| 65:sD:75:LYS:NZ    | 67:sK:20:VAL:HG23  | 2.12                     | 0.63              |
| 79:s2:694:G:H2'    | 79:s2:695:C:O4'    | 1.98                     | 0.63              |
| 79:s2:1657:G:H2'   | 79:s2:1658:G:C8    | 2.34                     | 0.63              |
| 80:cB:176:GLN:HB3  | 80:cB:180:ARG:NH2  | 2.12                     | 0.63              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 85:l5:1916:G:N3    | 85:l5:2067:C:O2'   | 2.29                     | 0.63              |
| 2:SE:211:LYS:HE3   | 2:SE:217:SER:HB2   | 1.80                     | 0.63              |
| 7:SJ:132:GLN:HE22  | 79:S2:562:U:H1'    | 1.62                     | 0.63              |
| 14:Sa:10:ARG:NH2   | 79:S2:1860:A:OP2   | 2.28                     | 0.63              |
| 15:SC:91:SER:O     | 15:SC:94:ILE:HG12  | 1.98                     | 0.63              |
| 85:L5:4188:U:H2'   | 85:L5:4189:U:C6    | 2.33                     | 0.63              |
| 85:L5:4291:G:H5'   | 85:L5:4293:U:C6    | 2.34                     | 0.63              |
| 85:L5:4485:C:O3'   | 58:Lm:114:LYS:NZ   | 2.27                     | 0.63              |
| 21:L8:138:C:H2'    | 21:L8:139:G:H8     | 1.64                     | 0.63              |
| 26:LE:119:GLU:OE2  | 26:LE:120:ASP:N    | 2.31                     | 0.63              |
| 35:LO:175:MET:CE   | 35:LO:178:ARG:HD2  | 2.17                     | 0.63              |
| 40:LT:114:GLN:HA   | 40:LT:117:LYS:HD3  | 1.81                     | 0.63              |
| 52:Lg:44:SER:OG    | 52:Lg:46:CYS:SG    | 2.54                     | 0.63              |
| 64:SR:104:GLU:O    | 64:SR:108:LEU:HD22 | 1.98                     | 0.63              |
| 67:SK:60:GLU:HA    | 67:SK:69:TRP:HA    | 1.81                     | 0.63              |
| 68:SP:133:ILE:HD11 | 81:AP:40:C:H4'     | 1.81                     | 0.63              |
| 75:Sg:11:LEU:N     | 75:Sg:307:VAL:O    | 2.30                     | 0.63              |
| 79:S2:1130:G:OP2   | 79:S2:1130:G:N2    | 2.31                     | 0.63              |
| 79:S2:1372:U:P     | 79:S2:1385:G:H22   | 2.20                     | 0.63              |
| 5:sX:76:LYS:HG2    | 79:s2:482:G:H5'    | 1.81                     | 0.63              |
| 10:sA:50:ASN:HD21  | 10:sA:52:LYS:HE3   | 1.63                     | 0.63              |
| 11:sB:197:ILE:HG21 | 11:sB:210:VAL:HG21 | 1.80                     | 0.63              |
| 15:sC:253:PRO:HA   | 15:sC:256:TRP:CE3  | 2.33                     | 0.63              |
| 19:sb:33:MET:CE    | 19:sb:79:PHE:HB2   | 2.29                     | 0.63              |
| 25:lD:202:GLN:NE2  | 25:lD:237:GLU:OE1  | 2.31                     | 0.63              |
| 31:lJ:32:ARG:HE    | 31:lJ:35:ARG:CZ    | 2.10                     | 0.63              |
| 46:la:116:LYS:HE3  | 85:l5:1419:G:C6    | 2.33                     | 0.63              |
| 64:sR:27:ASP:CG    | 79:s2:1455:A:H5''  | 2.24                     | 0.63              |
| 69:sQ:89:SER:OG    | 69:sQ:119:LEU:O    | 2.17                     | 0.63              |
| 76:sM:12:MET:O     | 76:sM:16:THR:OG1   | 2.17                     | 0.63              |
| 79:s2:1392:U:H2'   | 79:s2:1393:G:H8    | 1.62                     | 0.63              |
| 80:cB:401:MET:HE3  | 80:cB:410:PHE:CD2  | 2.34                     | 0.63              |
| 85:l5:161:G:H2'    | 85:l5:162:A:H8     | 1.63                     | 0.63              |
| 85:l5:3585:G:H2'   | 85:l5:3586:G:H8    | 1.63                     | 0.63              |
| 85:l5:3654:G:O2'   | 85:l5:3693:U:OP1   | 2.17                     | 0.63              |
| 85:l5:4101:C:N4    | 85:l5:4107:G:O6    | 2.32                     | 0.63              |
| 85:l5:5025:C:N4    | 85:l5:5027:C:N3    | 2.46                     | 0.63              |
| 80:CB:365:GLN:HA   | 80:CB:368:ARG:HB2  | 1.81                     | 0.63              |
| 5:SX:46:HIS:HE1    | 79:S2:648:A:H1'    | 1.64                     | 0.63              |
| 11:SB:167:LYS:O    | 11:SB:171:ILE:HG23 | 1.99                     | 0.63              |
| 16:SN:128:TYR:O    | 16:SN:131:THR:OG1  | 2.16                     | 0.63              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 18:SW:57:ARG:HG2   | 79:S2:920:A:H4'    | 1.81                     | 0.63              |
| 85:L5:151:G:N7     | 28:LG:141:ASN:ND2  | 2.47                     | 0.63              |
| 85:L5:188:G:N2     | 85:L5:189:G:O6     | 2.31                     | 0.63              |
| 85:L5:499:G:H2'    | 85:L5:504:G:H22    | 1.63                     | 0.63              |
| 85:L5:1332:C:H2'   | 85:L5:1333:A:C8    | 2.33                     | 0.63              |
| 85:L5:1646:A:H2'   | 85:L5:1647:U:C6    | 2.33                     | 0.63              |
| 85:L5:2260:C:O2    | 85:L5:2261:G:N1    | 2.32                     | 0.63              |
| 85:L5:2808:G:O3'   | 38:LR:60:ARG:NH1   | 2.32                     | 0.63              |
| 85:L5:2897:G:H2'   | 85:L5:2898:G:H8    | 1.64                     | 0.63              |
| 85:L5:3916:G:H2'   | 85:L5:3917:A:C8    | 2.33                     | 0.63              |
| 85:L5:4716:C:H2'   | 85:L5:4717:A:H8    | 1.61                     | 0.63              |
| 22:LA:23:ARG:HH22  | 22:LA:54:ARG:HB2   | 1.64                     | 0.63              |
| 24:LC:303:ARG:O    | 37:LQ:38:ARG:NH2   | 2.25                     | 0.63              |
| 25:LD:236:MET:HA   | 25:LD:239:MET:SD   | 2.38                     | 0.63              |
| 28:LG:103:ARG:NH2  | 28:LG:192:ARG:O    | 2.32                     | 0.63              |
| 37:LQ:121:LEU:HD12 | 37:LQ:125:GLN:HG3  | 1.80                     | 0.63              |
| 37:LQ:123:PHE:HA   | 37:LQ:126:LEU:HB3  | 1.81                     | 0.63              |
| 75:Sg:40:ILE:N     | 75:Sg:59:LEU:O     | 2.31                     | 0.63              |
| 79:S2:291:G:H2'    | 79:S2:292:A:C8     | 2.33                     | 0.63              |
| 79:S2:808:A:H2     | 79:S2:855:G:H22    | 1.46                     | 0.63              |
| 2:sE:79:ASP:HB3    | 2:sE:82:TYR:HB2    | 1.79                     | 0.63              |
| 10:sA:120:ARG:NH2  | 15:sC:266:TYR:HB3  | 2.13                     | 0.63              |
| 11:sB:159:GLN:NE2  | 79:s2:931:C:O5'    | 2.32                     | 0.63              |
| 25:ID:117:LYS:O    | 25:ID:117:LYS:NZ   | 2.31                     | 0.63              |
| 34:IN:75:VAL:HG23  | 34:IN:78:GLY:HA2   | 1.80                     | 0.63              |
| 39:IS:54:MET:SD    | 39:IS:54:MET:N     | 2.72                     | 0.63              |
| 53:lh:22:ASP:O     | 53:lh:26:VAL:HG12  | 1.99                     | 0.63              |
| 62:lr:32:LEU:HA    | 62:lr:113:ARG:HH21 | 1.63                     | 0.63              |
| 69:sQ:139:ALA:HB2  | 79:s2:1650:A:H5''  | 1.81                     | 0.63              |
| 75:sg:31:ILE:O     | 75:sg:43:TRP:N     | 2.29                     | 0.63              |
| 82:pE:15:G:N2      | 82:pE:21:A:H1'     | 2.14                     | 0.63              |
| 85:l5:268:G:H2'    | 85:l5:269:G:H8     | 1.63                     | 0.63              |
| 85:l5:4940:C:H5'   | 85:l5:4941:G:H5''  | 1.79                     | 0.63              |
| 15:SC:132:ASP:OD1  | 15:SC:136:HIS:N    | 2.31                     | 0.63              |
| 18:SW:105:THR:OG1  | 79:S2:862:A:N3     | 2.32                     | 0.63              |
| 85:L5:1541:C:H5''  | 22:LA:21:LYS:HG2   | 1.81                     | 0.63              |
| 85:L5:1939:A:H5'   | 85:L5:1940:G:H4'   | 1.81                     | 0.63              |
| 85:L5:2730:U:H2'   | 85:L5:2731:C:C6    | 2.33                     | 0.63              |
| 85:L5:4630:G:H2'   | 85:L5:4631:G:H8    | 1.64                     | 0.63              |
| 24:LC:331:TYR:CZ   | 27:LF:55:LYS:HD2   | 2.34                     | 0.63              |
| 35:LO:28:LEU:HD21  | 35:LO:94:ARG:HH21  | 1.64                     | 0.63              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 36:LP:14:SER:O     | 36:LP:105:LYS:NZ   | 2.26                     | 0.63              |
| 57:Ll:20:ASN:ND2   | 57:Ll:42:ARG:O     | 2.29                     | 0.63              |
| 64:SR:34:VAL:HG12  | 75:Sg:150:TRP:CZ2  | 2.33                     | 0.63              |
| 72:SU:82:MET:HE1   | 74:Sd:52:PHE:HA    | 1.81                     | 0.63              |
| 79:S2:1797:U:H2'   | 79:S2:1798:C:C6    | 2.34                     | 0.63              |
| 79:S2:1805:G:H2'   | 79:S2:1806:A:C8    | 2.34                     | 0.63              |
| 84:Lt:19:GLY:HA2   | 84:Lt:48:LYS:HE2   | 1.80                     | 0.63              |
| 3:sI:2:GLY:N       | 79:s2:1798:C:O2'   | 2.31                     | 0.63              |
| 10:sA:11:LYS:O     | 10:sA:14:ASP:N     | 2.31                     | 0.63              |
| 12:sH:125:VAL:O    | 12:sH:129:ILE:HG23 | 1.99                     | 0.63              |
| 15:sC:108:LYS:HD3  | 15:sC:233:LEU:HD12 | 1.80                     | 0.63              |
| 18:sW:86:LEU:HD11  | 18:sW:113:HIS:HB2  | 1.81                     | 0.63              |
| 29:lH:106:GLN:HB3  | 29:lH:111:LEU:HB3  | 1.81                     | 0.63              |
| 42:IV:86:LYS:NZ    | 85:l5:4671:C:O2    | 2.32                     | 0.63              |
| 43:lX:77:ILE:HA    | 43:lX:100:VAL:HG12 | 1.80                     | 0.63              |
| 48:lc:34:THR:O     | 48:lc:38:ILE:HG23  | 1.98                     | 0.63              |
| 54:li:89:GLU:HA    | 54:li:92:ASN:HD21  | 1.63                     | 0.63              |
| 62:lr:93:ILE:O     | 62:lr:96:MET:HG2   | 1.99                     | 0.63              |
| 71:sT:33:TRP:CZ3   | 79:s2:1567:G:H5'   | 2.33                     | 0.63              |
| 75:sg:199:THR:HG21 | 75:sg:240:CYS:HA   | 1.81                     | 0.63              |
| 78:sf:138:ARG:CZ   | 79:s2:1293:A:H1'   | 2.28                     | 0.63              |
| 79:s2:291:G:H2'    | 79:s2:292:A:C8     | 2.33                     | 0.63              |
| 79:s2:1808:U:H2'   | 79:s2:1809:A:C8    | 2.34                     | 0.63              |
| 80:cB:197:SER:HA   | 80:cB:201:GLY:HA2  | 1.81                     | 0.63              |
| 83:ls:118:PRO:HA   | 83:ls:164:GLY:H    | 1.62                     | 0.63              |
| 85:l5:259:C:H2'    | 85:l5:260:C:C6     | 2.33                     | 0.63              |
| 85:l5:1503:A:H4'   | 85:l5:1504:G:H5'   | 1.80                     | 0.63              |
| 85:l5:4527:G:OP2   | 85:l5:4527:G:N2    | 2.32                     | 0.63              |
| 80:CB:481:LYS:HD2  | 80:CB:532:PRO:HA   | 1.81                     | 0.63              |
| 13:SV:38:GLU:HB2   | 13:SV:47:ASN:HD21  | 1.64                     | 0.63              |
| 18:SW:12:LYS:NZ    | 79:S2:1153:C:OP1   | 2.31                     | 0.63              |
| 85:L5:387:G:HO2'   | 85:L5:412:G:H1     | 1.45                     | 0.63              |
| 85:L5:920:C:H2'    | 85:L5:921:C:H6     | 1.63                     | 0.63              |
| 85:L5:3967:G:O6    | 85:L5:4055:U:O4    | 2.17                     | 0.63              |
| 85:L5:4586:G:O6    | 85:L5:4717:A:N6    | 2.32                     | 0.63              |
| 21:L8:70:G:O2'     | 21:L8:87:G:N2      | 2.31                     | 0.63              |
| 23:LB:116:ARG:O    | 23:LB:177:LYS:NZ   | 2.32                     | 0.63              |
| 38:LR:133:LYS:NZ   | 38:LR:134:ASN:OD1  | 2.31                     | 0.63              |
| 56:Lk:7:GLU:OE2    | 56:Lk:7:GLU:N      | 2.28                     | 0.63              |
| 63:Lz:109:ALA:HB1  | 63:Lz:139:THR:HB   | 1.80                     | 0.63              |
| 79:S2:21:U:H2'     | 79:S2:22:A:H8      | 1.63                     | 0.63              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 79:S2:321:C:OP2    | 87:LW:123:LYS:NZ   | 2.30                     | 0.63              |
| 79:S2:1263:U:H5'   | 79:S2:1264:C:H2'   | 1.81                     | 0.63              |
| 79:S2:1657:G:H2'   | 79:S2:1658:G:H8    | 1.63                     | 0.63              |
| 10:sA:120:ARG:HE   | 15:sC:65:LYS:NZ    | 1.97                     | 0.63              |
| 11:sB:134:LEU:HD13 | 61:lp:92:GLN:HG3   | 1.81                     | 0.63              |
| 13:sV:30:ALA:O     | 13:sV:60:ARG:NH2   | 2.32                     | 0.63              |
| 22:lA:234:LYS:NZ   | 85:l5:3666:C:OP1   | 2.31                     | 0.63              |
| 38:lR:128:LYS:NZ   | 85:l5:2666:U:O4    | 2.31                     | 0.63              |
| 41:lU:21:PHE:HB3   | 41:lU:72:VAL:HG22  | 1.81                     | 0.63              |
| 56:lk:27:LYS:O     | 56:lk:70:LYS:NZ    | 2.31                     | 0.63              |
| 66:sF:76:MET:HE2   | 66:sF:89:THR:HG22  | 1.81                     | 0.63              |
| 71:sT:129:ARG:HA   | 71:sT:129:ARG:CZ   | 2.28                     | 0.63              |
| 76:sM:18:LEU:HD22  | 76:sM:123:VAL:HG12 | 1.81                     | 0.63              |
| 79:s2:440:G:OP1    | 79:s2:1798:C:O2'   | 2.16                     | 0.63              |
| 4:SL:109:MET:HE3   | 4:SL:140:PHE:CD2   | 2.25                     | 0.63              |
| 85:L5:300:A:H2'    | 85:L5:301:G:H8     | 1.64                     | 0.63              |
| 85:L5:1289:C:OP1   | 26:LE:218:LYS:NZ   | 2.31                     | 0.63              |
| 85:L5:1390:G:N2    | 85:L5:1393:G:OP2   | 2.25                     | 0.63              |
| 85:L5:1739:G:H2'   | 85:L5:1740:C:C6    | 2.33                     | 0.63              |
| 85:L5:1872:G:O2'   | 85:L5:4219:A:N3    | 2.27                     | 0.63              |
| 85:L5:2022:C:OP1   | 83:Ls:83:ARG:NH2   | 2.31                     | 0.63              |
| 85:L5:5058:A:H2'   | 85:L5:5059:C:C6    | 2.34                     | 0.63              |
| 21:L8:102:G:OP2    | 21:L8:104:A:O2'    | 2.15                     | 0.63              |
| 29:LH:92:MET:HE2   | 29:LH:179:ILE:HG13 | 1.80                     | 0.63              |
| 36:LP:125:MET:HA   | 36:LP:125:MET:HE3  | 1.81                     | 0.63              |
| 58:Lm:80:PRO:HA    | 58:Lm:83:ARG:HE    | 1.64                     | 0.63              |
| 64:SR:132:ARG:NH1  | 79:S2:1101:U:OP1   | 2.32                     | 0.63              |
| 79:S2:21:U:H2'     | 79:S2:22:A:C8      | 2.33                     | 0.63              |
| 79:S2:563:G:N7     | 79:S2:586:G:N2     | 2.46                     | 0.63              |
| 79:S2:1248:U:H2'   | 79:S2:1249:C:C6    | 2.34                     | 0.63              |
| 81:AP:49:C:H2'     | 81:AP:50:U:H6      | 1.64                     | 0.63              |
| 1:CH:26:ILE:HG22   | 1:CH:30:ARG:HE     | 1.64                     | 0.62              |
| 3:sI:104:ILE:O     | 3:sI:171:LEU:N     | 2.31                     | 0.62              |
| 3:sI:110:ARG:HB2   | 3:sI:166:PHE:CZ    | 2.34                     | 0.62              |
| 6:sG:110:ASN:ND2   | 79:s2:165:G:O4'    | 2.32                     | 0.62              |
| 10:sA:62:ALA:O     | 10:sA:66:VAL:HG12  | 1.99                     | 0.62              |
| 11:sB:87:ILE:H     | 11:sB:101:HIS:HB2  | 1.64                     | 0.62              |
| 15:sC:60:TRP:HE1   | 15:sC:62:PRO:HA    | 1.64                     | 0.62              |
| 18:sW:94:LEU:HD21  | 18:sW:102:ILE:HG12 | 1.79                     | 0.62              |
| 30:II:39:LYS:NZ    | 85:l5:1750:G:OP1   | 2.24                     | 0.62              |
| 41:lU:65:ARG:O     | 41:lU:67:LYS:NZ    | 2.32                     | 0.62              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 59:ln:10:MET:HE2   | 79:s2:1172:U:H4'   | 1.80                     | 0.62              |
| 68:sP:31:GLU:HG2   | 68:sP:32:GLN:OE1   | 1.99                     | 0.62              |
| 79:s2:146:G:N2     | 79:s2:173:A:N1     | 2.43                     | 0.62              |
| 79:s2:1588:A:H2'   | 79:s2:1589:A:H8    | 1.64                     | 0.62              |
| 79:s2:1862:G:O2'   | 79:s2:1864:U:OP2   | 2.17                     | 0.62              |
| 85:l5:4348:A:N6    | 85:l5:4364:G:H1    | 1.96                     | 0.62              |
| 85:l5:4537:C:H2'   | 85:l5:4538:G:H8    | 1.63                     | 0.62              |
| 80:CB:412:ALA:O    | 80:CB:472:LEU:N    | 2.31                     | 0.62              |
| 80:CB:613:LEU:HD21 | 80:CB:641:TRP:HE1  | 1.62                     | 0.62              |
| 2:SE:57:THR:OG1    | 2:SE:59:ASP:OD1    | 2.16                     | 0.62              |
| 3:SI:31:ARG:NE     | 79:S2:380:G:OP1    | 2.32                     | 0.62              |
| 3:SI:141:ARG:NE    | 79:S2:191:A:OP1    | 2.32                     | 0.62              |
| 12:SH:173:PHE:HB2  | 12:SH:187:PHE:HE1  | 1.64                     | 0.62              |
| 85:L5:3606:U:H2'   | 85:L5:3607:U:C6    | 2.34                     | 0.62              |
| 30:LI:11:TYR:O     | 30:LI:59:GLN:NE2   | 2.32                     | 0.62              |
| 33:LM:96:GLU:OE2   | 33:LM:100:ARG:NH1  | 2.32                     | 0.62              |
| 49:Ld:54:MET:O     | 49:Ld:54:MET:HE3   | 1.98                     | 0.62              |
| 50:Le:85:LEU:HD21  | 50:Le:111:ILE:HD12 | 1.81                     | 0.62              |
| 63:Lz:145:VAL:HG23 | 63:Lz:146:ALA:H    | 1.63                     | 0.62              |
| 66:SF:63:LYS:O     | 66:SF:71:ARG:NH1   | 2.30                     | 0.62              |
| 76:SM:83:LYS:HA    | 76:SM:105:GLY:HA3  | 1.80                     | 0.62              |
| 84:Lt:126:SER:HB3  | 84:Lt:130:LYS:HE2  | 1.80                     | 0.62              |
| 37:lQ:68:ARG:HH12  | 85:l5:1420:A:H3'   | 1.62                     | 0.62              |
| 39:lS:118:ARG:NH2  | 85:l5:2059:C:O2    | 2.32                     | 0.62              |
| 79:s2:1420:G:O2'   | 79:s2:1421:A:O4'   | 2.13                     | 0.62              |
| 80:cB:176:GLN:O    | 80:cB:180:ARG:HG2  | 1.98                     | 0.62              |
| 85:l5:4503:A:H2'   | 85:l5:4504:C:C6    | 2.34                     | 0.62              |
| 2:SE:202:PRO:HB2   | 4:SL:42:LEU:HD13   | 1.81                     | 0.62              |
| 4:SL:82:MET:SD     | 4:SL:82:MET:N      | 2.72                     | 0.62              |
| 10:SA:186:ARG:HG3  | 13:SV:46:PHE:HZ    | 1.64                     | 0.62              |
| 15:SC:194:ARG:NH1  | 79:S2:1156:U:O4    | 2.32                     | 0.62              |
| 15:SC:230:THR:HG21 | 79:S2:4:C:H5'      | 1.79                     | 0.62              |
| 85:L5:1732:C:H2'   | 85:L5:1733:G:C8    | 2.33                     | 0.62              |
| 85:L5:1762:C:C4    | 85:L5:1770:A:N1    | 2.66                     | 0.62              |
| 85:L5:2811:G:N1    | 85:L5:2814:C:OP2   | 2.28                     | 0.62              |
| 85:L5:3805:U:H2'   | 85:L5:3806:G:H8    | 1.63                     | 0.62              |
| 41:LU:100:LEU:HD13 | 41:LU:112:LEU:HD21 | 1.81                     | 0.62              |
| 49:Ld:64:ILE:HG22  | 49:Ld:106:VAL:HG12 | 1.81                     | 0.62              |
| 64:SR:99:ASP:O     | 64:SR:102:THR:OG1  | 2.14                     | 0.62              |
| 79:S2:432:G:H2'    | 79:S2:433:A:C8     | 2.34                     | 0.62              |
| 84:Lt:105:THR:HG22 | 84:Lt:107:ASP:H    | 1.63                     | 0.62              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 84:Lt:114:ARG:CZ   | 84:Lt:130:LYS:HA   | 2.29                     | 0.62              |
| 87:LW:7:SER:N      | 87:LW:30:GLN:O     | 2.29                     | 0.62              |
| 1:CH:49:ASN:ND2    | 79:S2:638:C:H1'    | 2.14                     | 0.62              |
| 4:sL:81:LYS:HG2    | 4:sL:82:MET:H      | 1.64                     | 0.62              |
| 8:sY:34:THR:OG1    | 79:s2:570:C:O2     | 2.16                     | 0.62              |
| 11:sB:107:ARG:HH22 | 17:sO:132:VAL:C    | 2.06                     | 0.62              |
| 12:sH:177:TYR:HA   | 12:sH:180:LEU:CD2  | 2.30                     | 0.62              |
| 32:IL:74:ARG:NH2   | 85:l5:109:G:OP2    | 2.33                     | 0.62              |
| 35:IO:96:GLN:NE2   | 85:l5:3888:G:O6    | 2.25                     | 0.62              |
| 37:IQ:155:ALA:O    | 37:IQ:158:THR:OG1  | 2.17                     | 0.62              |
| 40:IT:116:LYS:O    | 40:IT:120:LYS:HG3  | 2.00                     | 0.62              |
| 58:lm:94:MET:HE3   | 58:lm:95:ILE:H     | 1.63                     | 0.62              |
| 61:lp:17:ARG:NH2   | 85:l5:1577:G:OP1   | 2.33                     | 0.62              |
| 64:sR:45:LYS:HB3   | 79:s2:1369:A:H62   | 1.63                     | 0.62              |
| 67:sK:80:ARG:CZ    | 67:sK:89:ILE:O     | 2.47                     | 0.62              |
| 79:s2:832:G:H2'    | 79:s2:833:C:C6     | 2.33                     | 0.62              |
| 79:s2:1757:G:C8    | 79:s2:1758:G:H1'   | 2.34                     | 0.62              |
| 80:cB:143:LEU:HD21 | 80:cB:188:ILE:HD11 | 1.81                     | 0.62              |
| 85:l5:4605:A:H2'   | 85:l5:4606:G:C8    | 2.34                     | 0.62              |
| 8:SY:74:MET:HG3    | 8:SY:76:TYR:HE1    | 1.63                     | 0.62              |
| 11:SB:138:PHE:N    | 11:SB:214:LYS:O    | 2.27                     | 0.62              |
| 12:SH:160:LYS:HE3  | 12:SH:192:PHE:HA   | 1.80                     | 0.62              |
| 12:SH:170:VAL:HG13 | 12:SH:187:PHE:CD1  | 2.34                     | 0.62              |
| 18:SW:105:THR:HG22 | 18:SW:126:LEU:HD11 | 1.80                     | 0.62              |
| 85:L5:88:A:H5''    | 46:La:59:LYS:HD2   | 1.80                     | 0.62              |
| 85:L5:491:G:H5'    | 24:LC:2:ALA:HB3    | 1.81                     | 0.62              |
| 85:L5:3664:G:H2'   | 85:L5:3665:G:H8    | 1.63                     | 0.62              |
| 20:L7:60:G:O2'     | 25:LD:268:ARG:NH1  | 2.32                     | 0.62              |
| 56:Lk:26:LYS:HB3   | 56:Lk:33:LYS:HB2   | 1.81                     | 0.62              |
| 60:Lo:31:ASP:OD2   | 60:Lo:32:SER:N     | 2.32                     | 0.62              |
| 65:SD:217:ILE:HG13 | 65:SD:219:PRO:HD3  | 1.80                     | 0.62              |
| 72:SU:65:THR:HG22  | 72:SU:78:ASP:HB3   | 1.80                     | 0.62              |
| 74:Sd:14:PHE:HB2   | 79:S2:1661:A:C8    | 2.34                     | 0.62              |
| 79:S2:924:G:N2     | 79:S2:1018:U:O2    | 2.26                     | 0.62              |
| 83:Ls:41:GLN:O     | 83:Ls:44:ARG:N     | 2.32                     | 0.62              |
| 87:IW:13:ILE:HD12  | 87:IW:32:LEU:HD13  | 1.81                     | 0.62              |
| 8:sY:19:GLN:HG3    | 8:sY:81:TYR:HB3    | 1.81                     | 0.62              |
| 10:sA:38:ILE:HD13  | 10:sA:47:TYR:HB3   | 1.82                     | 0.62              |
| 15:sC:81:ILE:HG12  | 15:sC:88:ILE:HD11  | 1.80                     | 0.62              |
| 22:IA:159:SER:O    | 22:IA:162:ASN:ND2  | 2.27                     | 0.62              |
| 23:IB:222:VAL:O    | 23:IB:343:ARG:NH1  | 2.33                     | 0.62              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 30:II:49:GLY:O     | 30:II:168:SER:OG   | 2.17                     | 0.62              |
| 40:IT:11:THR:HA    | 40:IT:14:MET:HB3   | 1.82                     | 0.62              |
| 54:II:58:MET:SD    | 54:II:58:MET:N     | 2.67                     | 0.62              |
| 63:Iz:200:ASN:OD1  | 63:Iz:201:VAL:N    | 2.32                     | 0.62              |
| 66:sF:77:MET:HB2   | 66:sF:89:THR:HG21  | 1.80                     | 0.62              |
| 67:sK:1:MET:HE1    | 79:s2:1274:G:OP2   | 1.99                     | 0.62              |
| 75:sg:100:ARG:NH1  | 79:s2:1399:C:H5''  | 2.13                     | 0.62              |
| 79:s2:150:A:N6     | 79:s2:168:C:C2     | 2.67                     | 0.62              |
| 79:s2:1324:G:N2    | 79:s2:1504:U:O2    | 2.26                     | 0.62              |
| 80:cB:16:LYS:NZ    | 80:cB:387:SER:O    | 2.26                     | 0.62              |
| 80:cB:448:GLN:HB2  | 80:cB:473:VAL:HG13 | 1.81                     | 0.62              |
| 85:I5:497:G:N2     | 85:I5:498:C:H41    | 1.98                     | 0.62              |
| 85:I5:512:U:O4     | 85:I5:647:G:O6     | 2.17                     | 0.62              |
| 85:I5:1471:U:H2'   | 85:I5:1472:C:H6    | 1.63                     | 0.62              |
| 85:I5:2008:U:N3    | 85:I5:2011:C:OP2   | 2.22                     | 0.62              |
| 85:I5:3611:A:H2    | 85:I5:5016:A:H8    | 1.47                     | 0.62              |
| 85:I5:3948:C:O2'   | 85:I5:4065:G:N1    | 2.27                     | 0.62              |
| 85:I5:4364:G:H2'   | 85:I5:4365:C:H6    | 1.64                     | 0.62              |
| 2:SE:73:ASP:O      | 2:SE:75:LYS:NZ     | 2.32                     | 0.62              |
| 85:L5:226:G:OP2    | 44:LY:1:MET:N      | 2.22                     | 0.62              |
| 85:L5:1534:A:H1'   | 55:Lj:11:ARG:NE    | 2.15                     | 0.62              |
| 85:L5:1942:A:N3    | 85:L5:4432:C:O2'   | 2.29                     | 0.62              |
| 85:L5:2580:U:HO2'  | 45:LZ:79:HIS:HD1   | 1.47                     | 0.62              |
| 25:LD:205:ALA:HA   | 25:LD:208:MET:SD   | 2.40                     | 0.62              |
| 27:LF:190:LEU:HD12 | 27:LF:191:ILE:N    | 2.14                     | 0.62              |
| 30:LI:82:ARG:O     | 30:LI:82:ARG:NH1   | 2.27                     | 0.62              |
| 32:LL:63:THR:HG22  | 32:LL:65:ARG:H     | 1.64                     | 0.62              |
| 50:Le:82:VAL:CA    | 50:Le:85:LEU:HD23  | 2.24                     | 0.62              |
| 66:SF:127:ARG:HG3  | 66:SF:128:ILE:H    | 1.63                     | 0.62              |
| 71:ST:83:GLN:N     | 71:ST:91:HIS:O     | 2.31                     | 0.62              |
| 79:S2:695:C:N4     | 79:S2:736:C:O2'    | 2.33                     | 0.62              |
| 79:S2:1705:C:H2'   | 79:S2:1706:G:C8    | 2.34                     | 0.62              |
| 3:sI:32:PRO:O      | 3:sI:56:ARG:NH1    | 2.32                     | 0.62              |
| 18:sW:91:ASN:OD1   | 18:sW:92:ASN:ND2   | 2.33                     | 0.62              |
| 19:sb:22:LYS:HG2   | 79:s2:921:G:C2     | 2.35                     | 0.62              |
| 20:I7:23:A:N3      | 20:I7:118:C:O2'    | 2.28                     | 0.62              |
| 21:I8:137:A:H2'    | 21:I8:138:C:C6     | 2.35                     | 0.62              |
| 25:ID:34:LYS:HB2   | 40:IT:27:LEU:HD11  | 1.80                     | 0.62              |
| 38:IR:117:ARG:HD2  | 85:I5:2663:G:H5''  | 1.80                     | 0.62              |
| 41:IU:79:SER:H     | 41:IU:82:TYR:HD2   | 1.47                     | 0.62              |
| 42:IV:82:ILE:HB    | 42:IV:121:VAL:HG23 | 1.82                     | 0.62              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 55:lj:46:LYS:NZ    | 85:l5:23:C:OP2     | 2.32                     | 0.62              |
| 61:lp:30:GLU:OE2   | 61:lp:34:HIS:ND1   | 2.32                     | 0.62              |
| 64:sR:41:ILE:CG2   | 79:s2:1387:G:H2'   | 2.30                     | 0.62              |
| 66:sF:128:ILE:HD11 | 73:sc:23:SER:HB3   | 1.80                     | 0.62              |
| 66:sF:144:LEU:HD12 | 73:sc:51:ARG:HD2   | 1.81                     | 0.62              |
| 70:sS:86:ARG:NH2   | 79:s2:1611:G:O4'   | 2.33                     | 0.62              |
| 77:sZ:79:ILE:HG21  | 77:sZ:84:ALA:HB2   | 1.80                     | 0.62              |
| 80:cB:302:ASP:HA   | 80:cB:305:MET:HE3  | 1.81                     | 0.62              |
| 85:l5:1076:C:H2'   | 85:l5:1077:C:C6    | 2.34                     | 0.62              |
| 85:l5:1086:C:H2'   | 85:l5:1087:A:H8    | 1.63                     | 0.62              |
| 85:l5:1187:G:OP2   | 85:l5:1187:G:N2    | 2.32                     | 0.62              |
| 85:l5:4967:A:H2'   | 85:l5:4968:A:C8    | 2.34                     | 0.62              |
| 80:CB:595:SER:O    | 80:CB:598:LYS:NZ   | 2.31                     | 0.62              |
| 4:SL:77:VAL:HA     | 4:SL:88:ILE:HG22   | 1.81                     | 0.62              |
| 10:SA:18:PHE:HZ    | 10:SA:51:LEU:HD22  | 1.64                     | 0.62              |
| 85:L5:365:U:H2'    | 85:L5:366:A:H8     | 1.63                     | 0.62              |
| 85:L5:753:C:H5     | 85:L5:910:G:H1     | 1.46                     | 0.62              |
| 85:L5:1304:C:H2'   | 85:L5:1305:C:C6    | 2.35                     | 0.62              |
| 85:L5:2274:C:H2'   | 85:L5:2275:G:H8    | 1.64                     | 0.62              |
| 85:L5:2906:G:N2    | 85:L5:3585:G:N7    | 2.47                     | 0.62              |
| 85:L5:4260:U:H2'   | 85:L5:4261:C:H6    | 1.64                     | 0.62              |
| 85:L5:4716:C:OP1   | 23:LB:276:HIS:ND1  | 2.32                     | 0.62              |
| 21:L8:94:G:OP2     | 55:Lj:72:ARG:NH1   | 2.31                     | 0.62              |
| 24:LC:101:MET:SD   | 24:LC:104:PRO:HA   | 2.39                     | 0.62              |
| 44:LY:23:SER:HA    | 44:LY:26:ARG:HB2   | 1.82                     | 0.62              |
| 67:SK:92:ALA:HA    | 67:SK:95:ARG:NH1   | 2.13                     | 0.62              |
| 72:SU:26:SER:HB3   | 72:SU:110:VAL:HA   | 1.81                     | 0.62              |
| 79:S2:558:G:H1'    | 79:S2:559:G:C8     | 2.34                     | 0.62              |
| 79:S2:1205:C:H2'   | 79:S2:1206:G:H8    | 1.62                     | 0.62              |
| 79:S2:1748:G:H1    | 79:S2:1786:U:H3    | 1.47                     | 0.62              |
| 11:sB:97:LEU:HD12  | 11:sB:232:HIS:CG   | 2.34                     | 0.62              |
| 14:sa:85:ARG:HH12  | 79:s2:1209:A:H4'   | 1.65                     | 0.62              |
| 17:sO:95:ILE:HB    | 17:sO:129:ILE:HD13 | 1.82                     | 0.62              |
| 35:lO:81:TRP:HB2   | 35:lO:104:VAL:HG21 | 1.82                     | 0.62              |
| 41:lU:101:ARG:NH2  | 85:l5:2702:C:OP1   | 2.33                     | 0.62              |
| 47:lb:65:MET:SD    | 47:lb:66:SER:N     | 2.72                     | 0.62              |
| 48:lc:32:LYS:HE2   | 85:l5:2675:G:C5    | 2.35                     | 0.62              |
| 54:li:66:ASP:OD2   | 54:li:87:ARG:NH2   | 2.33                     | 0.62              |
| 64:sR:32:LYS:HD3   | 79:s2:1453:C:N3    | 2.15                     | 0.62              |
| 64:sR:42:PRO:HA    | 79:s2:1388:A:C8    | 2.33                     | 0.62              |
| 75:sg:298:LEU:HB2  | 75:sg:310:TRP:HB2  | 1.81                     | 0.62              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 79:s2:1438:A:H2'   | 79:s2:1439:A:C8    | 2.34                     | 0.62              |
| 85:l5:307:A:N3     | 85:l5:310:G:O2'    | 2.31                     | 0.62              |
| 85:l5:1762:C:C4    | 85:l5:1770:A:C2    | 2.87                     | 0.62              |
| 85:l5:3805:U:H2'   | 85:l5:3806:G:H8    | 1.63                     | 0.62              |
| 7:SJ:127:ARG:HA    | 7:SJ:130:ILE:HD12  | 1.82                     | 0.62              |
| 12:SH:100:ILE:HD11 | 12:SH:125:VAL:HG21 | 1.80                     | 0.62              |
| 85:L5:229:G:H5''   | 44:LY:11:ARG:HG3   | 1.82                     | 0.62              |
| 85:L5:1345:A:H2'   | 85:L5:1346:C:C6    | 2.34                     | 0.62              |
| 85:L5:4272:G:OP2   | 85:L5:4272:G:N2    | 2.22                     | 0.62              |
| 24:LC:61:GLN:OE1   | 24:LC:61:GLN:N     | 2.26                     | 0.62              |
| 27:LF:217:ARG:O    | 27:LF:246:ARG:NH2  | 2.31                     | 0.62              |
| 29:LH:126:VAL:HG11 | 29:LH:161:ILE:HG22 | 1.81                     | 0.62              |
| 32:LL:46:ILE:HB    | 32:LL:49:ARG:HB2   | 1.81                     | 0.62              |
| 35:LO:54:TYR:HE2   | 35:LO:145:VAL:HG11 | 1.63                     | 0.62              |
| 50:Le:103:VAL:O    | 50:Le:108:ARG:NH2  | 2.31                     | 0.62              |
| 69:SQ:71:ARG:NH1   | 79:S2:1407:U:O3'   | 2.28                     | 0.62              |
| 79:S2:472:C:O2     | 79:S2:475:C:N4     | 2.32                     | 0.62              |
| 1:cH:88:LYS:N      | 1:cH:88:LYS:HD3    | 2.14                     | 0.62              |
| 10:sA:73:ASP:OD1   | 10:sA:120:ARG:HG3  | 1.99                     | 0.62              |
| 14:sa:15:ARG:NH2   | 79:s2:993:G:N7     | 2.41                     | 0.62              |
| 16:sN:48:SER:O     | 16:sN:52:VAL:HG23  | 1.99                     | 0.62              |
| 19:sb:11:SER:OG    | 19:sb:13:GLU:OE1   | 2.12                     | 0.62              |
| 20:l7:15:C:H2'     | 20:l7:16:A:H8      | 1.64                     | 0.62              |
| 23:lB:302:ASN:HD21 | 23:lB:314:ILE:H    | 1.47                     | 0.62              |
| 30:lI:171:TRP:HB2  | 30:lI:178:ALA:HA   | 1.82                     | 0.62              |
| 44:lY:34:LEU:HD11  | 44:lY:47:MET:HG2   | 1.81                     | 0.62              |
| 51:lF:78:HIS:NE2   | 85:l5:1916:G:O2'   | 2.29                     | 0.62              |
| 75:sg:79:LEU:HA    | 75:sg:89:LEU:HA    | 1.82                     | 0.62              |
| 76:sM:58:GLU:HG2   | 76:sM:61:TYR:H     | 1.63                     | 0.62              |
| 79:s2:1457:U:H2'   | 79:s2:1458:G:C8    | 2.35                     | 0.62              |
| 80:cB:585:GLU:HA   | 80:cB:608:PRO:HG3  | 1.80                     | 0.62              |
| 85:l5:85:G:O2'     | 85:l5:97:G:O6      | 2.18                     | 0.62              |
| 85:l5:1762:C:C4    | 85:l5:1770:A:N1    | 2.67                     | 0.62              |
| 85:l5:4093:G:N2    | 85:l5:4114:C:N3    | 2.47                     | 0.62              |
| 4:SL:9:ALA:O       | 4:SL:11:GLN:NE2    | 2.32                     | 0.62              |
| 4:SL:94:HIS:N      | 4:SL:103:GLU:O     | 2.29                     | 0.62              |
| 16:SN:62:GLN:HE22  | 79:S2:1017:U:P     | 2.22                     | 0.62              |
| 18:SW:24:GLN:OE1   | 18:SW:64:ASN:ND2   | 2.29                     | 0.62              |
| 18:SW:57:ARG:HD2   | 79:S2:919:A:H4'    | 1.82                     | 0.62              |
| 85:L5:1461:C:H2'   | 85:L5:1462:A:H8    | 1.64                     | 0.62              |
| 85:L5:1779:U:OP2   | 25:LD:5:LYS:NZ     | 2.32                     | 0.62              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 85:L5:4097:G:O6    | 85:L5:4116:C:N3    | 2.33                     | 0.62              |
| 85:L5:4954:G:H2'   | 85:L5:4955:A:C8    | 2.34                     | 0.62              |
| 28:LG:182:CYS:SG   | 28:LG:184:ILE:HD11 | 2.38                     | 0.62              |
| 34:LN:103:GLU:HG3  | 34:LN:160:GLU:HB2  | 1.80                     | 0.62              |
| 35:LO:190:ASP:N    | 35:LO:190:ASP:OD2  | 2.29                     | 0.62              |
| 45:LZ:121:ARG:HD3  | 45:LZ:126:LYS:HE2  | 1.82                     | 0.62              |
| 55:Lj:34:CYS:SG    | 55:Lj:37:CYS:N     | 2.72                     | 0.62              |
| 72:SU:72:GLU:HG2   | 79:S2:1491:G:H1'   | 1.81                     | 0.62              |
| 79:S2:931:C:H2'    | 79:S2:932:G:C8     | 2.35                     | 0.62              |
| 79:S2:1562:C:H2'   | 79:S2:1563:G:H8    | 1.63                     | 0.62              |
| 79:S2:1856:C:H2'   | 79:S2:1857:G:H8    | 1.64                     | 0.62              |
| 21:l8:123:U:O2'    | 21:l8:128:C:N4     | 2.31                     | 0.62              |
| 26:lE:267:LEU:N    | 26:lE:267:LEU:HD22 | 2.13                     | 0.62              |
| 29:lH:150:ASP:OD1  | 29:lH:152:GLU:N    | 2.31                     | 0.62              |
| 31:lJ:32:ARG:HA    | 31:lJ:32:ARG:NE    | 2.15                     | 0.62              |
| 38:lR:114:LYS:O    | 38:lR:146:LYS:NZ   | 2.32                     | 0.62              |
| 40:lT:90:ASN:HD22  | 85:l5:4313:A:H1'   | 1.65                     | 0.62              |
| 41:lU:88:LYS:HA    | 41:lU:97:ARG:HH21  | 1.65                     | 0.62              |
| 47:lb:33:LYS:NZ    | 85:l5:4299:U:OP1   | 2.32                     | 0.62              |
| 64:sR:7:LYS:HB3    | 79:s2:1366:G:O6    | 2.00                     | 0.62              |
| 65:sD:106:ARG:HD3  | 65:sD:175:VAL:HG22 | 1.80                     | 0.62              |
| 66:sF:143:PRO:HA   | 66:sF:146:ARG:HB3  | 1.82                     | 0.62              |
| 75:sg:271:LYS:HZ1  | 75:sg:274:VAL:HB   | 1.65                     | 0.62              |
| 79:s2:16:G:H2'     | 79:s2:17:C:C6      | 2.35                     | 0.62              |
| 79:s2:1416:C:H5''  | 79:s2:1417:C:OP2   | 1.99                     | 0.62              |
| 80:cB:152:LYS:HG3  | 80:cB:359:PRO:CG   | 2.29                     | 0.62              |
| 85:l5:300:A:H2'    | 85:l5:301:G:H8     | 1.63                     | 0.62              |
| 85:l5:4291:G:H5'   | 85:l5:4293:U:C6    | 2.34                     | 0.62              |
| 80:CB:727:ARG:HG2  | 80:CB:854:PHE:HA   | 1.82                     | 0.62              |
| 6:SG:234:LEU:HD11  | 6:SG:237:LEU:HB3   | 1.81                     | 0.62              |
| 8:SY:74:MET:HG3    | 8:SY:76:TYR:CE1    | 2.34                     | 0.62              |
| 10:SA:66:VAL:HG11  | 10:SA:185:MET:HG3  | 1.82                     | 0.62              |
| 11:SB:25:PHE:HA    | 11:SB:28:LYS:HG2   | 1.82                     | 0.62              |
| 15:SC:263:LYS:HD2  | 15:SC:267:GLN:HG2  | 1.82                     | 0.62              |
| 85:L5:4049:U:O4'   | 85:L5:4051:C:N4    | 2.33                     | 0.62              |
| 85:L5:4111:U:H5'   | 85:L5:4116:C:N4    | 2.13                     | 0.62              |
| 85:L5:4139:G:N2    | 85:L5:4140:C:H41   | 1.98                     | 0.62              |
| 85:L5:4353:U:H5''  | 85:L5:4354:U:H5'   | 1.80                     | 0.62              |
| 69:SQ:100:VAL:HG22 | 69:SQ:101:ASP:H    | 1.63                     | 0.62              |
| 70:SS:138:THR:HA   | 70:SS:141:ARG:HH21 | 1.65                     | 0.62              |
| 75:Sg:213:ASP:HB2  | 75:Sg:215:GLN:HE21 | 1.64                     | 0.62              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 79:S2:1528:G:O2'   | 79:S2:1666:C:OP1   | 2.17                     | 0.62              |
| 1:CH:85:ARG:HH22   | 79:S2:1321:G:H5'   | 1.65                     | 0.62              |
| 3:sI:54:LYS:HE3    | 79:s2:381:C:H5''   | 1.82                     | 0.62              |
| 6:sG:57:ASP:HB2    | 6:sG:98:ARG:HG3    | 1.82                     | 0.62              |
| 6:sG:132:ARG:NH2   | 79:s2:167:G:C2     | 2.67                     | 0.62              |
| 6:sG:132:ARG:NE    | 79:s2:168:C:H1'    | 2.14                     | 0.62              |
| 36:IP:72:GLN:HE22  | 85:l5:4971:A:H5'   | 1.64                     | 0.62              |
| 64:sR:28:PHE:O     | 64:sR:29:HIS:ND1   | 2.21                     | 0.62              |
| 69:sQ:54:PRO:HG2   | 69:sQ:88:ILE:HD11  | 1.82                     | 0.62              |
| 71:sT:44:GLU:HG2   | 71:sT:45:LEU:HD13  | 1.81                     | 0.62              |
| 79:s2:1033:G:H1    | 79:s2:1080:A:HO2'  | 1.48                     | 0.62              |
| 83:ls:124:PRO:HA   | 83:ls:157:ASP:HB3  | 1.80                     | 0.62              |
| 85:l5:2017:A:O2'   | 85:l5:2018:C:O5'   | 2.17                     | 0.62              |
| 85:l5:4069:U:H2'   | 85:l5:4070:U:C6    | 2.35                     | 0.62              |
| 80:CB:650:TRP:CZ2  | 80:CB:676:LYS:HG2  | 2.35                     | 0.62              |
| 4:SL:133:PRO:O     | 79:S2:383:G:O2'    | 2.18                     | 0.62              |
| 8:SY:114:MET:HA    | 8:SY:114:MET:HE3   | 1.82                     | 0.62              |
| 12:SH:26:ALA:HA    | 12:SH:29:GLU:OE1   | 1.99                     | 0.62              |
| 85:L5:150:U:O4     | 28:LG:187:LYS:NZ   | 2.28                     | 0.62              |
| 85:L5:1091:C:H2'   | 85:L5:1092:G:C8    | 2.33                     | 0.62              |
| 85:L5:1095:A:H2    | 85:L5:1200:G:C2    | 2.16                     | 0.62              |
| 85:L5:1367:C:O2'   | 85:L5:1369:C:OP2   | 2.17                     | 0.62              |
| 85:L5:2373:C:H2'   | 85:L5:2374:A:C8    | 2.35                     | 0.62              |
| 85:L5:2406:G:O6    | 85:L5:2785:C:N4    | 2.32                     | 0.62              |
| 85:L5:2693:G:OP1   | 56:Lk:35:LYS:NZ    | 2.30                     | 0.62              |
| 85:L5:3607:U:OP2   | 38:LR:76:MET:HE3   | 1.99                     | 0.62              |
| 85:L5:4101:C:H5'   | 85:L5:4107:G:H3'   | 1.82                     | 0.62              |
| 85:L5:4102:C:N3    | 85:L5:4105:A:C4    | 2.67                     | 0.62              |
| 85:L5:4250:G:H5''  | 31:LJ:98:ASN:HD22  | 1.63                     | 0.62              |
| 85:L5:4459:U:H2'   | 85:L5:4460:U:H6    | 1.65                     | 0.62              |
| 85:L5:4635:A:OP1   | 85:L5:4636:U:O2'   | 2.17                     | 0.62              |
| 34:LN:146:PRO:HB2  | 53:Lh:104:THR:HG22 | 1.82                     | 0.62              |
| 72:SU:65:THR:HG23  | 72:SU:67:LYS:H     | 1.65                     | 0.62              |
| 79:S2:300:U:H2'    | 79:S2:301:A:C8     | 2.34                     | 0.62              |
| 79:S2:1205:C:H2'   | 79:S2:1206:G:C8    | 2.34                     | 0.62              |
| 81:AP:22:U:H2'     | 81:AP:23:C:C6      | 2.34                     | 0.62              |
| 4:sL:84:ARG:HD3    | 79:s2:374:G:C4'    | 2.27                     | 0.62              |
| 4:sL:111:VAL:HA    | 4:sL:138:VAL:HG12  | 1.82                     | 0.62              |
| 7:sJ:35:TYR:CE2    | 7:sJ:106:LEU:HB3   | 2.34                     | 0.62              |
| 12:sH:154:ILE:HD13 | 12:sH:185:VAL:HG22 | 1.82                     | 0.62              |
| 16:sN:57:SER:HG    | 16:sN:58:HIS:HD1   | 1.46                     | 0.62              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 16:sN:63:VAL:O     | 16:sN:67:THR:HG22  | 2.00                     | 0.62              |
| 21:l8:148:A:H2'    | 21:l8:149:G:C8     | 2.35                     | 0.62              |
| 23:lB:292:LEU:O    | 23:lB:297:LYS:NZ   | 2.22                     | 0.62              |
| 25:lD:108:ARG:NH2  | 25:lD:253:TYR:HB2  | 2.15                     | 0.62              |
| 36:lP:107:LEU:HD11 | 36:lP:152:GLU:CD   | 2.24                     | 0.62              |
| 38:lR:101:ILE:HD13 | 38:lR:104:ARG:HH21 | 1.65                     | 0.62              |
| 42:lV:117:ILE:HD12 | 42:lV:135:ASN:C    | 2.25                     | 0.62              |
| 46:la:16:SER:OG    | 85:l5:2283:G:OP1   | 2.16                     | 0.62              |
| 47:lb:95:ARG:O     | 47:lb:99:ILE:HG13  | 1.99                     | 0.62              |
| 54:li:30:ARG:NH2   | 85:l5:278:G:OP2    | 2.33                     | 0.62              |
| 64:sR:3:ARG:NH2    | 79:s2:1467:C:H1'   | 2.14                     | 0.62              |
| 75:sg:188:HIS:HB3  | 75:sg:219:TRP:CZ3  | 2.35                     | 0.62              |
| 75:sg:218:LEU:O    | 75:sg:219:TRP:HD1  | 1.82                     | 0.62              |
| 80:cB:22:MET:HE3   | 80:cB:358:LEU:HG   | 1.81                     | 0.62              |
| 85:l5:257:C:H2'    | 85:l5:258:G:C8     | 2.34                     | 0.62              |
| 85:l5:1755:C:H42   | 85:l5:1775:A:H61   | 1.48                     | 0.62              |
| 85:l5:2295:C:H2'   | 85:l5:2296:G:H8    | 1.65                     | 0.62              |
| 85:l5:2705:G:H22   | 85:l5:2710:C:H5    | 1.47                     | 0.62              |
| 4:SL:132:ARG:HG2   | 4:SL:133:PRO:HD2   | 1.81                     | 0.62              |
| 5:SX:32:LEU:HD22   | 5:SX:34:THR:H      | 1.64                     | 0.62              |
| 8:SY:112:ASN:ND2   | 79:S2:53:C:OP1     | 2.29                     | 0.62              |
| 85:L5:161:G:H2'    | 85:L5:162:A:C8     | 2.35                     | 0.62              |
| 85:L5:1414:C:O2'   | 85:L5:1415:G:H5'   | 2.00                     | 0.62              |
| 85:L5:1942:A:H2'   | 85:L5:1943:A:H8    | 1.65                     | 0.62              |
| 85:L5:2908:U:O2'   | 85:L5:3586:G:O6    | 2.14                     | 0.62              |
| 85:L5:4322:G:N2    | 85:L5:4325:A:OP2   | 2.28                     | 0.62              |
| 25:LD:204:VAL:O    | 25:LD:208:MET:HG3  | 2.00                     | 0.62              |
| 35:LO:34:VAL:HG21  | 35:LO:112:TYR:HE1  | 1.64                     | 0.62              |
| 68:SP:44:ARG:NH1   | 68:SP:82:ASP:O     | 2.30                     | 0.62              |
| 69:SQ:21:ALA:O     | 69:SQ:87:SER:OG    | 2.18                     | 0.62              |
| 72:SU:51:LYS:NZ    | 79:S2:1401:A:O2'   | 2.33                     | 0.62              |
| 75:Sg:8:ARG:HE     | 75:Sg:52:TYR:HE2   | 1.47                     | 0.62              |
| 75:Sg:212:LYS:HA   | 75:Sg:235:ILE:CD1  | 2.27                     | 0.62              |
| 76:SM:45:ARG:NH2   | 76:SM:71:GLU:OE2   | 2.33                     | 0.62              |
| 2:sE:234:PRO:O     | 2:sE:234:PRO:HD2   | 2.00                     | 0.61              |
| 5:sX:67:ARG:NH1    | 79:s2:617:G:N7     | 2.47                     | 0.61              |
| 12:sH:111:LYS:NZ   | 79:s2:747:U:O2     | 2.33                     | 0.61              |
| 19:sb:70:LYS:NZ    | 79:s2:1107:G:OP2   | 2.32                     | 0.61              |
| 26:lE:178:PRO:HB2  | 26:lE:181:LEU:HB3  | 1.81                     | 0.61              |
| 42:lV:99:GLU:OE1   | 87:lW:24:THR:N     | 2.25                     | 0.61              |
| 52:lg:24:ARG:NH2   | 85:l5:2639:U:H5'   | 2.14                     | 0.61              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 53:lh:8:ASP:N      | 53:lh:8:ASP:OD1    | 2.33                     | 0.61              |
| 53:lh:87:LYS:HB2   | 55:lj:78:PHE:HB3   | 1.82                     | 0.61              |
| 53:lh:93:ARG:HE    | 85:l5:19:G:P       | 2.23                     | 0.61              |
| 56:lk:33:LYS:NZ    | 85:l5:2693:G:OP2   | 2.32                     | 0.61              |
| 60:lo:99:ARG:HD3   | 60:lo:99:ARG:H     | 1.64                     | 0.61              |
| 63:lz:23:ARG:HA    | 63:lz:212:LYS:HD3  | 1.81                     | 0.61              |
| 63:lz:32:VAL:N     | 63:lz:170:GLY:O    | 2.32                     | 0.61              |
| 66:sF:77:MET:HE1   | 66:sF:85:LYS:N     | 2.15                     | 0.61              |
| 70:sS:100:ALA:O    | 70:sS:103:LEU:N    | 2.32                     | 0.61              |
| 70:sS:142:ARG:HH22 | 79:s2:1228:A:H5''  | 1.65                     | 0.61              |
| 79:s2:1403:C:N4    | 79:s2:1433:C:OP1   | 2.33                     | 0.61              |
| 80:cB:560:ASP:HB3  | 80:cB:565:HIS:CE1  | 2.35                     | 0.61              |
| 81:aP:9:A:N6       | 81:aP:22:U:OP2     | 2.33                     | 0.61              |
| 82:pE:22:G:N7      | 82:pE:46:G:N2      | 2.44                     | 0.61              |
| 82:pE:38:A:H2'     | 82:pE:39:U:H6      | 1.64                     | 0.61              |
| 83:ls:30:VAL:HG11  | 83:ls:187:LEU:HD13 | 1.82                     | 0.61              |
| 85:l5:3717:A:OP2   | 85:l5:3735:G:N2    | 2.31                     | 0.61              |
| 6:SG:170:ARG:NH2   | 79:S2:71:G:O6      | 2.32                     | 0.61              |
| 14:Sa:62:TYR:HH    | 17:SO:129:ILE:H    | 1.45                     | 0.61              |
| 14:Sa:85:ARG:NH2   | 79:S2:1210:G:H5'   | 2.15                     | 0.61              |
| 16:SN:2:GLY:N      | 79:S2:1092:G:OP1   | 2.32                     | 0.61              |
| 85:L5:1788:A:HO2'  | 85:L5:4209:G:HO2'  | 1.43                     | 0.61              |
| 85:L5:4102:C:N3    | 85:L5:4105:A:C2'   | 2.62                     | 0.61              |
| 85:L5:4108:G:O2'   | 85:L5:4109:G:OP1   | 2.17                     | 0.61              |
| 85:L5:4566:U:O2'   | 23:LB:234:ARG:NH1  | 2.31                     | 0.61              |
| 21:L8:39:G:O2'     | 21:L8:104:A:N1     | 2.32                     | 0.61              |
| 27:LF:132:MET:N    | 27:LF:132:MET:HE2  | 2.15                     | 0.61              |
| 33:LM:52:PHE:HA    | 33:LM:55:MET:CE    | 2.29                     | 0.61              |
| 42:LV:112:MET:HE1  | 42:LV:117:ILE:HD11 | 1.81                     | 0.61              |
| 76:SM:63:LYS:HA    | 76:SM:66:GLU:OE2   | 2.00                     | 0.61              |
| 77:SZ:97:ILE:HG23  | 77:SZ:110:THR:O    | 2.00                     | 0.61              |
| 79:S2:866:U:H2'    | 79:S2:867:G:H8     | 1.62                     | 0.61              |
| 79:S2:878:G:H1     | 79:S2:908:A:N6     | 1.98                     | 0.61              |
| 79:S2:1414:A:H3'   | 79:S2:1415:C:H5''  | 1.82                     | 0.61              |
| 2:sE:101:LEU:HD21  | 2:sE:109:PHE:CE1   | 2.35                     | 0.61              |
| 5:sX:107:ARG:NH2   | 79:s2:18:C:O3'     | 2.33                     | 0.61              |
| 18:sW:102:ILE:HD13 | 18:sW:128:PHE:HB3  | 1.80                     | 0.61              |
| 19:sb:51:GLN:NE2   | 79:s2:928:G:O4'    | 2.23                     | 0.61              |
| 22:lA:119:LYS:NZ   | 85:l5:3663:A:OP1   | 2.33                     | 0.61              |
| 25:lD:35:ARG:NH2   | 85:l5:4326:G:N3    | 2.48                     | 0.61              |
| 27:lF:144:TYR:HE2  | 27:lF:237:GLU:HG3  | 1.65                     | 0.61              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:IJ:21:CYS:SG    | 85:I5:4259:C:O2'   | 2.58                     | 0.61              |
| 33:IM:104:MET:HE3  | 33:IM:105:THR:H    | 1.65                     | 0.61              |
| 35:IO:62:MET:HE1   | 85:I5:2045:G:C2    | 2.35                     | 0.61              |
| 37:IQ:146:ARG:HB3  | 37:IQ:148:VAL:HG22 | 1.82                     | 0.61              |
| 38:IR:136:ARG:NH1  | 85:I5:2896:G:OP1   | 2.34                     | 0.61              |
| 40:IT:38:ASP:N     | 40:IT:38:ASP:OD1   | 2.33                     | 0.61              |
| 49:Id:28:ASN:HB3   | 49:Id:31:LYS:HB3   | 1.82                     | 0.61              |
| 54:li:7:MET:SD     | 54:li:7:MET:N      | 2.73                     | 0.61              |
| 62:lr:71:ARG:NH1   | 85:I5:668:C:O3'    | 2.31                     | 0.61              |
| 65:sD:126:ILE:HG13 | 65:sD:127:MET:N    | 2.14                     | 0.61              |
| 66:sF:139:VAL:CA   | 73:sc:63:ARG:HH22  | 2.06                     | 0.61              |
| 72:sU:100:GLN:N    | 72:sU:100:GLN:OE1  | 2.32                     | 0.61              |
| 75:sg:72:SER:HA    | 75:sg:113:PHE:CE1  | 2.35                     | 0.61              |
| 79:s2:1707:U:O2    | 79:s2:1849:G:N2    | 2.31                     | 0.61              |
| 80:cB:383:MET:HA   | 80:cB:383:MET:HE3  | 1.81                     | 0.61              |
| 80:cB:511:ALA:HA   | 80:cB:570:ILE:HD12 | 1.82                     | 0.61              |
| 80:cB:604:MET:HB3  | 80:cB:704:VAL:HA   | 1.82                     | 0.61              |
| 85:I5:690:C:H2'    | 85:I5:691:C:C6     | 2.35                     | 0.61              |
| 85:I5:4572:U:H2'   | 85:I5:4573:G:C8    | 2.35                     | 0.61              |
| 85:I5:4773:C:N4    | 85:I5:4861:G:O6    | 2.27                     | 0.61              |
| 85:I5:5040:U:H4'   | 85:I5:5041:G:H5'   | 1.81                     | 0.61              |
| 2:SE:44:LEU:HD11   | 2:SE:82:TYR:HB3    | 1.82                     | 0.61              |
| 2:SE:149:TYR:HB3   | 6:SG:209:TYR:CD2   | 2.35                     | 0.61              |
| 6:SG:139:SER:OG    | 79:S2:144:U:OP2    | 2.17                     | 0.61              |
| 8:SY:103:SER:HB3   | 8:SY:106:GLN:HE22  | 1.65                     | 0.61              |
| 12:SH:43:LEU:HD21  | 12:SH:71:SER:HB3   | 1.82                     | 0.61              |
| 12:SH:118:ARG:NH2  | 79:S2:686:U:O2     | 2.26                     | 0.61              |
| 85:L5:173:C:H2'    | 85:L5:174:C:C6     | 2.35                     | 0.61              |
| 85:L5:1555:G:N7    | 61:Lp:4:ARG:NH2    | 2.47                     | 0.61              |
| 85:L5:1751:A:H2'   | 85:L5:1752:G:C8    | 2.35                     | 0.61              |
| 85:L5:2737:C:H2'   | 85:L5:2738:C:C6    | 2.35                     | 0.61              |
| 85:L5:4095:G:O2'   | 85:L5:4109:G:O2'   | 2.17                     | 0.61              |
| 36:LP:148:MET:SD   | 36:LP:148:MET:N    | 2.73                     | 0.61              |
| 38:LR:38:ARG:HA    | 38:LR:41:ILE:HG22  | 1.81                     | 0.61              |
| 70:SS:85:ASN:ND2   | 79:S2:1630:A:O2'   | 2.33                     | 0.61              |
| 71:ST:124:THR:HG23 | 71:ST:127:GLY:H    | 1.64                     | 0.61              |
| 75:Sg:125:ARG:HG3  | 75:Sg:150:TRP:CD1  | 2.35                     | 0.61              |
| 79:S2:1757:G:O6    | 79:S2:1758:G:N2    | 2.33                     | 0.61              |
| 83:Ls:91:THR:OG1   | 83:Ls:93:GLU:OE1   | 2.18                     | 0.61              |
| 1:cH:85:ARG:O      | 1:cH:89:GLY:N      | 2.33                     | 0.61              |
| 2:sE:57:THR:HG22   | 2:sE:60:GLU:HG3    | 1.81                     | 0.61              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:sA:33:GLN:OE1   | 10:sA:154:LEU:HB2  | 2.00                     | 0.61              |
| 19:sb:81:ARG:HH11  | 19:sb:82:LYS:H     | 1.46                     | 0.61              |
| 27:IF:206:ASN:HD22 | 85:l5:1840:G:P     | 2.22                     | 0.61              |
| 37:lQ:115:ARG:NH2  | 85:l5:653:U:O5'    | 2.30                     | 0.61              |
| 38:lR:21:LYS:NZ    | 85:l5:2822:G:OP2   | 2.29                     | 0.61              |
| 43:lX:122:ALA:HB3  | 43:lX:139:ARG:HG3  | 1.82                     | 0.61              |
| 43:lX:125:ASN:ND2  | 85:l5:2437:C:O2'   | 2.34                     | 0.61              |
| 46:la:7:LYS:NZ     | 85:l5:1512:G:OP1   | 2.32                     | 0.61              |
| 50:le:28:TYR:HB2   | 50:le:31:ILE:HG12  | 1.81                     | 0.61              |
| 69:sQ:138:ARG:O    | 69:sQ:140:ARG:NH1  | 2.34                     | 0.61              |
| 75:sg:273:GLU:OE2  | 75:sg:273:GLU:N    | 2.20                     | 0.61              |
| 79:s2:479:C:O3'    | 80:cB:407:LYS:NZ   | 2.32                     | 0.61              |
| 79:s2:1228:A:H2'   | 79:s2:1229:G:H8    | 1.65                     | 0.61              |
| 79:s2:1356:G:H2'   | 79:s2:1357:A:C4    | 2.35                     | 0.61              |
| 79:s2:1581:C:H5'   | 79:s2:1582:C:H5    | 1.63                     | 0.61              |
| 80:cB:4:PHE:N      | 80:cB:45:ILE:O     | 2.27                     | 0.61              |
| 84:lt:147:HIS:NE2  | 84:lt:149:HIS:HB2  | 2.16                     | 0.61              |
| 85:l5:4716:C:H2'   | 85:l5:4717:A:H8    | 1.66                     | 0.61              |
| 80:CB:448:GLN:HB2  | 80:CB:473:VAL:HG13 | 1.83                     | 0.61              |
| 2:SE:188:ASN:HD21  | 2:SE:218:PHE:HB2   | 1.64                     | 0.61              |
| 12:SH:145:ARG:O    | 12:SH:153:LEU:N    | 2.33                     | 0.61              |
| 18:SW:50:PHE:HB2   | 18:SW:63:VAL:HG12  | 1.83                     | 0.61              |
| 85:L5:907:C:H2'    | 85:L5:908:G:C8     | 2.34                     | 0.61              |
| 85:L5:4668:U:OP1   | 23:LB:226:LYS:NZ   | 2.33                     | 0.61              |
| 22:LA:104:VAL:O    | 22:LA:139:HIS:NE2  | 2.33                     | 0.61              |
| 33:LM:5:ARG:HH21   | 33:LM:59:ASP:HB3   | 1.65                     | 0.61              |
| 61:Lp:56:HIS:CE1   | 61:Lp:61:MET:HE3   | 2.30                     | 0.61              |
| 68:SP:28:MET:HE1   | 68:SP:33:LEU:HB2   | 1.82                     | 0.61              |
| 68:SP:37:TYR:O     | 70:SS:88:LYS:NZ    | 2.31                     | 0.61              |
| 79:S2:388:U:H2'    | 79:S2:389:A:C8     | 2.35                     | 0.61              |
| 79:S2:851:C:H5''   | 79:S2:852:G:H5'    | 1.83                     | 0.61              |
| 79:S2:1856:C:H2'   | 79:S2:1857:G:C8    | 2.35                     | 0.61              |
| 84:Lt:53:TRP:CD1   | 84:Lt:54:LYS:H     | 2.17                     | 0.61              |
| 7:sJ:32:ILE:HG13   | 7:sJ:37:LEU:HB2    | 1.83                     | 0.61              |
| 11:sB:107:ARG:NH2  | 17:sO:133:THR:N    | 2.48                     | 0.61              |
| 11:sB:145:LYS:HG3  | 64:sR:134:PRO:HA   | 1.82                     | 0.61              |
| 20:l7:54:A:C4      | 31:lJ:12:MET:HE2   | 2.35                     | 0.61              |
| 21:l8:47:C:H1'     | 21:l8:61:A:H2'     | 1.81                     | 0.61              |
| 27:IF:157:ARG:NE   | 27:IF:248:ASN:OD1  | 2.25                     | 0.61              |
| 29:IH:96:TYR:HH    | 29:IH:141:LYS:HZ3  | 1.45                     | 0.61              |
| 44:IY:102:SER:OG   | 44:IY:103:LYS:NZ   | 2.33                     | 0.61              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 47:lb:41:ARG:HH21  | 85:l5:1492:G:H4'  | 1.64                     | 0.61              |
| 62:lr:87:ARG:NH2   | 85:l5:458:C:OP1   | 2.33                     | 0.61              |
| 64:sR:97:GLU:OE2   | 64:sR:120:THR:HB  | 2.00                     | 0.61              |
| 67:sK:82:TYR:CD2   | 67:sK:83:LEU:HD22 | 2.34                     | 0.61              |
| 71:sT:40:ALA:HB1   | 71:sT:42:HIS:CE1  | 2.36                     | 0.61              |
| 73:sc:13:ARG:NE    | 73:sc:55:VAL:HB   | 2.15                     | 0.61              |
| 77:sZ:47:LEU:HB3   | 77:sZ:80:ARG:HD2  | 1.83                     | 0.61              |
| 78:sf:107:LYS:O    | 78:sf:115:SER:OG  | 2.16                     | 0.61              |
| 79:s2:683:G:N1     | 79:s2:1022:U:OP2  | 2.32                     | 0.61              |
| 79:s2:1748:G:N2    | 79:s2:1786:U:O2   | 2.24                     | 0.61              |
| 85:l5:909:A:H2'    | 85:l5:910:G:H8    | 1.65                     | 0.61              |
| 85:L5:323:C:H2'    | 85:L5:324:A:H8    | 1.64                     | 0.61              |
| 85:L5:2318:G:OP2   | 50:Le:14:LYS:NZ   | 2.32                     | 0.61              |
| 85:L5:2600:A:N6    | 85:L5:2745:A:OP2  | 2.31                     | 0.61              |
| 85:L5:3725:G:N2    | 85:L5:3728:A:OP2  | 2.32                     | 0.61              |
| 85:L5:3786:U:OP1   | 85:L5:4550:G:O2'  | 2.18                     | 0.61              |
| 85:L5:4522:G:O2'   | 85:L5:4525:C:OP2  | 2.17                     | 0.61              |
| 20:L7:46:C:H2'     | 20:L7:47:G:H8     | 1.65                     | 0.61              |
| 29:LH:74:CYS:O     | 29:LH:78:GLN:HG2  | 2.00                     | 0.61              |
| 39:LS:9:GLU:HG2    | 39:LS:67:VAL:HB   | 1.83                     | 0.61              |
| 44:LY:56:GLN:NE2   | 44:LY:65:GLN:OE1  | 2.32                     | 0.61              |
| 63:Lz:198:TRP:CG   | 63:Lz:199:GLN:N   | 2.67                     | 0.61              |
| 79:S2:1004:U:H2'   | 79:S2:1005:G:C8   | 2.36                     | 0.61              |
| 83:Ls:145:THR:HG22 | 83:Ls:154:ILE:HA  | 1.83                     | 0.61              |
| 4:sL:113:LEU:HD12  | 4:sL:142:VAL:HG21 | 1.83                     | 0.61              |
| 10:sA:85:ARG:HH22  | 10:sA:202:TYR:CA  | 2.07                     | 0.61              |
| 15:sC:81:ILE:HD11  | 15:sC:86:LEU:HB2  | 1.82                     | 0.61              |
| 24:lC:75:ARG:NH1   | 85:l5:4391:G:OP1  | 2.28                     | 0.61              |
| 38:lR:92:LYS:NZ    | 85:l5:1573:G:OP1  | 2.32                     | 0.61              |
| 44:IY:88:GLU:N     | 44:IY:88:GLU:OE1  | 2.34                     | 0.61              |
| 65:sD:97:CYS:O     | 65:sD:101:GLN:NE2 | 2.34                     | 0.61              |
| 73:sc:18:LEU:HD23  | 73:sc:29:GLN:HG3  | 1.82                     | 0.61              |
| 76:sM:55:ASN:ND2   | 76:sM:82:ASN:OD1  | 2.32                     | 0.61              |
| 79:s2:874:G:H2'    | 79:s2:875:A:C8    | 2.34                     | 0.61              |
| 79:s2:1845:A:H2'   | 79:s2:1846:G:H8   | 1.66                     | 0.61              |
| 80:cB:79:TYR:HE2   | 80:cB:81:LEU:HD13 | 1.65                     | 0.61              |
| 83:ls:36:GLY:HA2   | 85:l5:1969:G:H4'  | 1.82                     | 0.61              |
| 85:l5:1525:A:HO2'  | 85:l5:3916:G:HO2' | 1.47                     | 0.61              |
| 5:SX:126:ALA:O     | 5:SX:128:VAL:N    | 2.33                     | 0.61              |
| 16:SN:64:ARG:NH1   | 79:S2:919:A:OP2   | 2.34                     | 0.61              |
| 85:L5:2045:G:O6    | 85:L5:3870:C:O2'  | 2.19                     | 0.61              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 85:L5:3610:A:H2'   | 85:L5:3611:A:H8    | 1.65                     | 0.61              |
| 85:L5:3873:G:H2'   | 85:L5:3874:G:C8    | 2.35                     | 0.61              |
| 85:L5:4130:C:H2'   | 85:L5:4131:G:H8    | 1.66                     | 0.61              |
| 30:LI:26:VAL:HG23  | 30:LI:122:PRO:HB2  | 1.83                     | 0.61              |
| 54:Li:36:HIS:O     | 54:Li:40:VAL:HG23  | 1.99                     | 0.61              |
| 65:SD:108:LYS:HD3  | 65:SD:118:ALA:HB1  | 1.82                     | 0.61              |
| 71:ST:113:VAL:HG22 | 71:ST:123:LEU:HG   | 1.80                     | 0.61              |
| 72:SU:58:THR:HG23  | 79:S2:1446:A:H5''  | 1.83                     | 0.61              |
| 79:S2:1744:G:O2'   | 79:S2:1789:G:N2    | 2.23                     | 0.61              |
| 82:PE:43:A:H2'     | 82:PE:44:G:C8      | 2.36                     | 0.61              |
| 84:Lt:113:ALA:O    | 84:Lt:117:ARG:NH1  | 2.33                     | 0.61              |
| 1:CH:77:VAL:CG1    | 1:CH:132:LEU:HD11  | 2.30                     | 0.61              |
| 6:sG:116:LYS:NZ    | 6:sG:119:LYS:O     | 2.32                     | 0.61              |
| 11:sB:116:LYS:HE3  | 79:s2:989:C:H5''   | 1.83                     | 0.61              |
| 12:sH:145:ARG:N    | 12:sH:153:LEU:O    | 2.32                     | 0.61              |
| 21:l8:70:G:O2'     | 21:l8:87:G:N2      | 2.32                     | 0.61              |
| 22:lA:104:VAL:HA   | 22:lA:107:MET:SD   | 2.39                     | 0.61              |
| 24:lC:326:LEU:HD21 | 85:l5:976:G:H4'    | 1.81                     | 0.61              |
| 26:lE:262:LYS:HA   | 26:lE:268:GLN:HE22 | 1.66                     | 0.61              |
| 29:lH:111:LEU:HD22 | 29:lH:127:ARG:HH22 | 1.65                     | 0.61              |
| 32:lL:39:ARG:NH1   | 85:l5:106:A:OP1    | 2.33                     | 0.61              |
| 65:sD:28:GLU:OE1   | 67:sK:70:TYR:OH    | 2.10                     | 0.61              |
| 75:sg:88:ARG:HG3   | 75:sg:100:ARG:HG2  | 1.81                     | 0.61              |
| 79:s2:696:G:H21    | 79:s2:737:G:N2     | 1.99                     | 0.61              |
| 85:l5:179:G:H2'    | 85:l5:180:C:H6     | 1.65                     | 0.61              |
| 85:l5:654:C:H2'    | 85:l5:655:C:C6     | 2.35                     | 0.61              |
| 85:l5:1333:A:H2'   | 85:l5:1334:A:C8    | 2.36                     | 0.61              |
| 85:l5:2079:G:H2'   | 85:l5:2080:U:H6    | 1.66                     | 0.61              |
| 85:l5:4093:G:N7    | 85:l5:4095:G:C2    | 2.68                     | 0.61              |
| 2:SE:62:LYS:NZ     | 79:S2:502:C:O3'    | 2.31                     | 0.61              |
| 4:SL:136:LYS:NZ    | 79:S2:372:U:OP1    | 2.30                     | 0.61              |
| 19:Sb:81:ARG:NH1   | 19:Sb:82:LYS:H     | 1.98                     | 0.61              |
| 85:L5:1461:C:H2'   | 85:L5:1462:A:C8    | 2.35                     | 0.61              |
| 85:L5:2303:C:OP1   | 50:Le:107:ASN:ND2  | 2.32                     | 0.61              |
| 32:LL:130:LYS:HD2  | 32:LL:131:PRO:HD2  | 1.82                     | 0.61              |
| 43:LX:86:ALA:O     | 43:LX:90:ILE:HG12  | 2.00                     | 0.61              |
| 62:Lr:16:PHE:HB3   | 62:Lr:27:THR:H     | 1.64                     | 0.61              |
| 62:Lr:114:ALA:O    | 62:Lr:118:LEU:HG   | 2.00                     | 0.61              |
| 74:Sd:6:LEU:HA     | 74:Sd:9:SER:HB3    | 1.80                     | 0.61              |
| 77:SZ:47:LEU:HD21  | 77:SZ:83:LEU:HG    | 1.82                     | 0.61              |
| 2:sE:69:PHE:CE2    | 8:sY:17:LEU:HD22   | 2.35                     | 0.61              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:sE:192:ILE:CD1  | 2:sE:242:LYS:HG2   | 2.30                     | 0.61              |
| 17:sO:33:ILE:HG22 | 17:sO:97:LEU:HA    | 1.82                     | 0.61              |
| 17:sO:137:SER:OG  | 79:s2:942:G:N2     | 2.29                     | 0.61              |
| 21:l8:138:C:H2'   | 21:l8:139:G:C8     | 2.36                     | 0.61              |
| 26:lE:59:ARG:HD2  | 85:l5:1238:A:C8    | 2.36                     | 0.61              |
| 29:lH:60:TRP:HB2  | 85:l5:4764:A:N1    | 2.15                     | 0.61              |
| 54:li:97:MET:HA   | 54:li:97:MET:HE3   | 1.83                     | 0.61              |
| 79:s2:928:G:H2'   | 79:s2:929:G:H8     | 1.65                     | 0.61              |
| 79:s2:1447:G:H2'  | 79:s2:1448:A:C8    | 2.36                     | 0.61              |
| 79:s2:1712:A:H2'  | 79:s2:1713:C:C6    | 2.35                     | 0.61              |
| 80:cB:693:CYS:HB2 | 80:cB:695:GLU:HG2  | 1.82                     | 0.61              |
| 85:l5:3848:U:H2'  | 85:l5:3849:A:H8    | 1.65                     | 0.61              |
| 2:SE:3:ARG:NH1    | 79:S2:450:C:OP1    | 2.34                     | 0.61              |
| 2:SE:19:MET:HE1   | 79:S2:846:G:C6     | 2.36                     | 0.61              |
| 4:SL:20:LYS:NZ    | 79:S2:222:U:O3'    | 2.33                     | 0.61              |
| 7:SJ:54:ARG:HH21  | 15:SC:202:THR:HG22 | 1.66                     | 0.61              |
| 8:SY:111:LYS:NZ   | 79:S2:56:G:OP1     | 2.33                     | 0.61              |
| 10:SA:18:PHE:CE1  | 10:SA:51:LEU:HD13  | 2.35                     | 0.61              |
| 12:SH:69:LEU:HD13 | 12:SH:96:ALA:HB2   | 1.82                     | 0.61              |
| 18:SW:18:GLU:OE2  | 18:SW:65:LEU:HD11  | 2.01                     | 0.61              |
| 85:L5:352:G:C6    | 24:LC:196:MET:CE   | 2.83                     | 0.61              |
| 85:L5:429:A:H2'   | 85:L5:430:G:C8     | 2.36                     | 0.61              |
| 85:L5:1387:A:H62  | 46:La:74:ASN:HD21  | 1.47                     | 0.61              |
| 85:L5:1727:U:OP1  | 27:LF:131:ASN:ND2  | 2.34                     | 0.61              |
| 85:L5:1825:A:H2'  | 85:L5:1826:G:C8    | 2.35                     | 0.61              |
| 85:L5:1985:G:H21  | 85:L5:2003:G:HO2'  | 1.48                     | 0.61              |
| 85:L5:4774:C:O2'  | 85:L5:4775:C:O2    | 2.15                     | 0.61              |
| 85:L5:4946:U:HO2' | 51:Lf:2:SER:N      | 1.98                     | 0.61              |
| 21:L8:90:C:H2'    | 21:L8:91:A:C8      | 2.36                     | 0.61              |
| 71:ST:105:GLN:NE2 | 79:S2:1564:C:OP1   | 2.33                     | 0.61              |
| 79:S2:1430:C:H2'  | 79:S2:1431:G:C8    | 2.36                     | 0.61              |
| 79:S2:1595:U:H2'  | 79:S2:1596:U:C6    | 2.35                     | 0.61              |
| 3:sI:74:ARG:HH12  | 79:s2:302:A:P      | 2.23                     | 0.61              |
| 6:sG:47:GLY:O     | 6:sG:115:LYS:NZ    | 2.34                     | 0.61              |
| 7:sJ:46:VAL:HG23  | 7:sJ:102:ILE:HD11  | 1.82                     | 0.61              |
| 16:sN:70:LYS:HB3  | 16:sN:73:ARG:HB2   | 1.81                     | 0.61              |
| 21:l8:27:U:H2'    | 21:l8:28:C:H6      | 1.66                     | 0.61              |
| 24:lC:5:ARG:HH22  | 24:lC:26:ALA:HA    | 1.64                     | 0.61              |
| 25:lD:67:ALA:HA   | 25:lD:72:ASP:HA    | 1.83                     | 0.61              |
| 26:lE:183:ARG:HD2 | 85:l5:4936:G:C5    | 2.36                     | 0.61              |
| 27:lF:217:ARG:NH1 | 85:l5:718:C:OP1    | 2.34                     | 0.61              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:IJ:53:ALA:O     | 31:IJ:54:ARG:NH1   | 2.34                     | 0.61              |
| 32:IL:8:MET:HE2    | 37:IQ:168:ARG:HB3  | 1.81                     | 0.61              |
| 34:IN:144:ARG:NH1  | 85:l5:124:C:OP1    | 2.34                     | 0.61              |
| 43:IX:149:VAL:O    | 43:IX:153:ILE:HG12 | 2.01                     | 0.61              |
| 47:lb:23:LYS:NZ    | 85:l5:1723:A:OP2   | 2.25                     | 0.61              |
| 65:sD:1:MET:HA     | 65:sD:1:MET:HE3    | 1.83                     | 0.61              |
| 65:sD:29:LEU:H     | 65:sD:29:LEU:HD12  | 1.64                     | 0.61              |
| 71:sT:75:MET:HE2   | 71:sT:75:MET:HA    | 1.82                     | 0.61              |
| 76:sM:52:LEU:HG    | 76:sM:78:LYS:HZ1   | 1.64                     | 0.61              |
| 78:sf:102:VAL:HG12 | 78:sf:103:LEU:H    | 1.66                     | 0.61              |
| 79:s2:529:A:N1     | 79:s2:555:A:N6     | 2.47                     | 0.61              |
| 79:s2:1667:U:H2'   | 79:s2:1668:U:C6    | 2.35                     | 0.61              |
| 83:ls:132:PRO:HB3  | 83:ls:147:ILE:HG12 | 1.83                     | 0.61              |
| 85:l5:4258:C:H2'   | 85:l5:4259:C:H6    | 1.64                     | 0.61              |
| 80:CB:18:ASN:HD21  | 80:CB:94:ASP:N     | 1.94                     | 0.61              |
| 2:SE:118:GLU:HG2   | 2:SE:121:TYR:HE2   | 1.65                     | 0.61              |
| 4:SL:71:ARG:NH2    | 79:S2:855:G:O2'    | 2.33                     | 0.61              |
| 85:L5:189:G:H2'    | 85:L5:190:G:H8     | 1.66                     | 0.61              |
| 85:L5:257:C:H2'    | 85:L5:258:G:C8     | 2.35                     | 0.61              |
| 85:L5:909:A:H2'    | 85:L5:910:G:C8     | 2.34                     | 0.61              |
| 85:L5:1175:A:H4'   | 25:LD:268:ARG:HH21 | 1.66                     | 0.61              |
| 85:L5:1977:C:OP1   | 84:Lt:57:ARG:NH2   | 2.34                     | 0.61              |
| 85:L5:4087:G:P     | 22:LA:37:ARG:HH22  | 2.23                     | 0.61              |
| 20:L7:117:G:OP1    | 25:LD:253:TYR:OH   | 2.16                     | 0.61              |
| 21:L8:92:U:H2'     | 21:L8:93:C:O4'     | 2.00                     | 0.61              |
| 71:ST:77:LYS:NZ    | 79:S2:1584:G:OP1   | 2.28                     | 0.61              |
| 75:Sg:29:ASP:OD1   | 75:Sg:45:LEU:N     | 2.32                     | 0.61              |
| 79:S2:464:A:H5'    | 79:S2:465:A:C8     | 2.36                     | 0.61              |
| 79:S2:1737:G:H1    | 79:S2:1797:U:H3    | 1.48                     | 0.61              |
| 83:Ls:47:LEU:HD12  | 83:Ls:51:ALA:HB3   | 1.82                     | 0.61              |
| 4:sL:129:GLY:N     | 4:sL:140:PHE:CE1   | 2.69                     | 0.61              |
| 6:sG:216:ARG:C     | 6:sG:218:LYS:H     | 2.08                     | 0.61              |
| 21:l8:58:G:O6      | 55:lj:63:ARG:NH2   | 2.34                     | 0.61              |
| 26:lE:65:ARG:NH1   | 85:l5:1070:G:OP2   | 2.32                     | 0.61              |
| 30:II:98:ARG:NH2   | 85:l5:1865:G:OP2   | 2.29                     | 0.61              |
| 36:IP:34:GLN:NE2   | 85:l5:424:U:OP1    | 2.33                     | 0.61              |
| 59:ln:1:MET:HE3    | 59:ln:2:ARG:H      | 1.66                     | 0.61              |
| 67:sK:29:MET:HG3   | 67:sK:42:ASN:HD21  | 1.66                     | 0.61              |
| 79:s2:1217:A:H2'   | 79:s2:1218:C:C6    | 2.35                     | 0.61              |
| 79:s2:1435:C:O2'   | 79:s2:1437:C:N4    | 2.34                     | 0.61              |
| 80:cB:120:ARG:NH2  | 80:cB:495:ARG:O    | 2.33                     | 0.61              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 80:cB:165:LEU:O   | 80:cB:168:GLN:NE2  | 2.34                     | 0.61              |
| 85:l5:1094:G:O6   | 85:l5:1201:U:O4    | 2.19                     | 0.61              |
| 85:l5:2633:U:H2'  | 85:l5:2634:C:H6    | 1.65                     | 0.61              |
| 85:l5:2694:G:H5'  | 85:l5:2695:A:C2    | 2.36                     | 0.61              |
| 2:SE:89:VAL:HG13  | 2:SE:100:ARG:HE    | 1.66                     | 0.61              |
| 2:SE:137:PRO:HG2  | 2:SE:149:TYR:HA    | 1.81                     | 0.61              |
| 10:SA:94:THR:HG22 | 10:SA:183:LEU:HD21 | 1.81                     | 0.61              |
| 10:SA:214:GLU:N   | 10:SA:214:GLU:OE1  | 2.29                     | 0.61              |
| 14:Sa:13:LYS:HZ1  | 79:S2:1133:A:C1'   | 2.13                     | 0.61              |
| 15:SC:131:GLY:HA3 | 15:SC:137:VAL:HA   | 1.83                     | 0.61              |
| 19:Sb:16:LYS:O    | 19:Sb:16:LYS:NZ    | 2.26                     | 0.61              |
| 85:L5:299:C:H2'   | 85:L5:300:A:C8     | 2.36                     | 0.61              |
| 85:L5:2621:A:N7   | 41:LU:81:ARG:NH1   | 2.48                     | 0.61              |
| 85:L5:4088:C:H2'  | 85:L5:4089:G:H8    | 1.65                     | 0.61              |
| 85:L5:4178:A:H2'  | 85:L5:4179:G:C8    | 2.34                     | 0.61              |
| 85:L5:4474:A:OP2  | 58:Lm:124:LYS:NZ   | 2.34                     | 0.61              |
| 21:L8:102:G:H4'   | 55:Lj:21:ARG:HB2   | 1.83                     | 0.61              |
| 25:LD:51:MET:HE3  | 25:LD:147:ASP:H    | 1.65                     | 0.61              |
| 28:LG:81:ASN:O    | 28:LG:84:THR:OG1   | 2.15                     | 0.61              |
| 56:Lk:9:LYS:NZ    | 56:Lk:9:LYS:O      | 2.34                     | 0.61              |
| 61:Lp:36:LYS:HE3  | 61:Lp:48:LYS:HE2   | 1.81                     | 0.61              |
| 68:SP:21:ASP:H    | 68:SP:24:GLN:HE22  | 1.49                     | 0.61              |
| 79:S2:979:C:H2'   | 79:S2:980:A:H8     | 1.65                     | 0.61              |
| 84:Lt:113:ALA:HA  | 84:Lt:116:MET:HE1  | 1.83                     | 0.61              |
| 8:sY:4:THR:OG1    | 8:sY:32:LYS:NZ     | 2.34                     | 0.61              |
| 13:sV:32:ILE:HG22 | 13:sV:55:ILE:HB    | 1.82                     | 0.61              |
| 15:sC:263:LYS:HD2 | 15:sC:267:GLN:HG2  | 1.83                     | 0.61              |
| 25:lD:287:PHE:C   | 25:lD:291:GLN:HE21 | 2.09                     | 0.61              |
| 26:lE:145:THR:C   | 26:lE:164:PHE:HE2  | 2.09                     | 0.61              |
| 34:lN:169:ARG:NH1 | 85:l5:63:G:OP2     | 2.27                     | 0.61              |
| 42:lV:15:ARG:HB2  | 85:l5:4618:G:H5''  | 1.83                     | 0.61              |
| 48:lc:30:GLY:O    | 48:lc:34:THR:OG1   | 2.16                     | 0.61              |
| 64:sR:11:LYS:HD2  | 79:s2:1372:U:H3'   | 1.80                     | 0.61              |
| 64:sR:41:ILE:HG22 | 79:s2:1387:G:H2'   | 1.82                     | 0.61              |
| 64:sR:99:ASP:O    | 64:sR:102:THR:OG1  | 2.13                     | 0.61              |
| 66:sF:61:PHE:CZ   | 73:sc:51:ARG:HG3   | 2.35                     | 0.61              |
| 69:sQ:6:PRO:HB2   | 69:sQ:7:LEU:HD23   | 1.83                     | 0.61              |
| 70:sS:36:VAL:HG13 | 70:sS:40:TYR:HD1   | 1.64                     | 0.61              |
| 75:sg:271:LYS:NZ  | 75:sg:272:GLN:O    | 2.27                     | 0.61              |
| 79:s2:1639:G:N2   | 82:pE:42:G:O4'     | 2.34                     | 0.61              |
| 79:s2:1748:G:O6   | 79:s2:1786:U:O4    | 2.19                     | 0.61              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 85:l5:2375:A:H2'  | 85:l5:2376:A:C8    | 2.36                     | 0.61              |
| 85:l5:3784:A:O2'  | 85:l5:3785:A:H3'   | 2.01                     | 0.61              |
| 80:CB:27:HIS:HB3  | 80:CB:30:HIS:CE1   | 2.35                     | 0.61              |
| 80:CB:652:PHE:O   | 80:CB:658:GLY:N    | 2.33                     | 0.61              |
| 4:SL:135:SER:OG   | 4:SL:138:VAL:HG12  | 2.01                     | 0.61              |
| 7:SJ:84:ILE:HG22  | 7:SJ:108:ARG:HE    | 1.65                     | 0.61              |
| 10:SA:190:SER:OG  | 10:SA:192:GLU:OE2  | 2.19                     | 0.61              |
| 18:SW:26:LEU:HD11 | 18:SW:60:LYS:HB3   | 1.81                     | 0.61              |
| 18:SW:85:ASP:N    | 18:SW:85:ASP:OD1   | 2.31                     | 0.61              |
| 85:L5:691:C:H2'   | 85:L5:692:A:H8     | 1.65                     | 0.61              |
| 85:L5:1420:A:H5'  | 37:LQ:68:ARG:HH21  | 1.66                     | 0.61              |
| 85:L5:3948:C:O2'  | 85:L5:4065:G:N1    | 2.30                     | 0.61              |
| 85:L5:4095:G:N2   | 85:L5:4110:C:OP1   | 2.33                     | 0.61              |
| 20:L7:2:U:O4      | 20:L7:117:G:O6     | 2.19                     | 0.61              |
| 28:LG:44:ASP:N    | 28:LG:44:ASP:OD2   | 2.33                     | 0.61              |
| 30:LI:99:ILE:HB   | 30:LI:123:GLN:CD   | 2.25                     | 0.61              |
| 34:LN:124:ASP:HB3 | 34:LN:127:TYR:N    | 2.14                     | 0.61              |
| 35:LO:187:LYS:HD3 | 35:LO:187:LYS:N    | 2.16                     | 0.61              |
| 36:LP:115:GLU:N   | 36:LP:115:GLU:OE1  | 2.34                     | 0.61              |
| 38:LR:76:MET:HE1  | 38:LR:88:ARG:NH2   | 2.14                     | 0.61              |
| 41:LU:107:LYS:H   | 41:LU:107:LYS:HD2  | 1.66                     | 0.61              |
| 75:Sg:62:HIS:CE1  | 75:Sg:88:ARG:HB2   | 2.36                     | 0.61              |
| 76:SM:121:LYS:O   | 76:SM:125:GLU:HG3  | 2.00                     | 0.61              |
| 79:S2:1179:G:N2   | 79:S2:1182:A:OP2   | 2.32                     | 0.61              |
| 83:Ls:109:ALA:O   | 83:Ls:184:SER:OG   | 2.17                     | 0.61              |
| 2:sE:73:ASP:OD2   | 2:sE:145:ARG:NH2   | 2.33                     | 0.60              |
| 7:sJ:137:VAL:N    | 7:sJ:140:GLN:O     | 2.34                     | 0.60              |
| 10:sA:149:ASN:HB2 | 10:sA:165:ASN:OD1  | 2.00                     | 0.60              |
| 21:l8:87:G:OP2    | 53:lh:5:LYS:NZ     | 2.34                     | 0.60              |
| 27:lF:149:SER:HB3 | 27:lF:245:ARG:HH12 | 1.65                     | 0.60              |
| 41:lU:21:PHE:HZ   | 41:lU:80:LYS:HA    | 1.66                     | 0.60              |
| 49:ld:65:ASP:OD1  | 49:ld:66:THR:N     | 2.34                     | 0.60              |
| 50:le:124:ASN:ND2 | 85:l5:2325:C:O2'   | 2.33                     | 0.60              |
| 66:sF:148:ASN:ND2 | 79:s2:1677:U:OP1   | 2.34                     | 0.60              |
| 70:sS:88:LYS:HZ3  | 79:s2:1613:G:P     | 2.24                     | 0.60              |
| 75:sg:18:VAL:HG21 | 75:sg:307:VAL:HG22 | 1.82                     | 0.60              |
| 79:s2:107:A:H2'   | 79:s2:108:G:C8     | 2.36                     | 0.60              |
| 80:cB:488:PHE:CE1 | 80:cB:490:HIS:HB2  | 2.36                     | 0.60              |
| 80:CB:150:ARG:HG2 | 80:CB:200:MET:HE3  | 1.83                     | 0.60              |
| 80:CB:336:LEU:O   | 80:CB:340:MET:HG2  | 2.01                     | 0.60              |
| 80:CB:502:SER:OG  | 80:CB:811:GLN:HA   | 2.01                     | 0.60              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:SA:186:ARG:HA   | 13:SV:46:PHE:CZ    | 2.36                     | 0.60              |
| 14:Sa:73:TYR:CE1   | 14:Sa:83:VAL:HG21  | 2.36                     | 0.60              |
| 15:SC:263:LYS:HD2  | 15:SC:267:GLN:CG   | 2.31                     | 0.60              |
| 85:L5:3930:U:H3    | 85:L5:4180:G:H1    | 1.49                     | 0.60              |
| 85:L5:4102:C:C4    | 85:L5:4105:A:C2'   | 2.83                     | 0.60              |
| 85:L5:4736:C:H2'   | 85:L5:4737:G:H8    | 1.66                     | 0.60              |
| 85:L5:4765:G:O6    | 33:LM:4:ARG:NH2    | 2.34                     | 0.60              |
| 85:L5:4906:C:H2'   | 85:L5:4907:G:H8    | 1.66                     | 0.60              |
| 24:LC:334:THR:HG22 | 24:LC:337:ARG:HH21 | 1.64                     | 0.60              |
| 26:LE:161:ARG:NH1  | 26:LE:273:SER:OG   | 2.34                     | 0.60              |
| 33:LM:113:MET:SD   | 33:LM:114:LYS:HG2  | 2.42                     | 0.60              |
| 55:Lj:64:MET:SD    | 55:Lj:67:LEU:HD23  | 2.41                     | 0.60              |
| 62:Lr:107:ARG:HG2  | 62:Lr:108:MET:SD   | 2.41                     | 0.60              |
| 63:Lz:53:VAL:HG22  | 63:Lz:157:PHE:HE1  | 1.66                     | 0.60              |
| 66:SF:101:HIS:HD2  | 66:SF:105:GLY:HA2  | 1.66                     | 0.60              |
| 68:SP:18:ARG:NH2   | 70:SS:88:LYS:O     | 2.33                     | 0.60              |
| 79:S2:54:A:H3'     | 79:S2:451:G:H22    | 1.65                     | 0.60              |
| 79:S2:1405:A:H2'   | 79:S2:1406:G:O4'   | 2.01                     | 0.60              |
| 79:S2:1458:G:H2'   | 79:S2:1459:G:H8    | 1.65                     | 0.60              |
| 79:S2:1478:U:H2'   | 79:S2:1479:G:C8    | 2.36                     | 0.60              |
| 79:S2:1845:A:H2'   | 79:S2:1846:G:C8    | 2.36                     | 0.60              |
| 82:PE:42:G:H2'     | 82:PE:43:A:H8      | 1.65                     | 0.60              |
| 3:sI:84:ASN:ND2    | 3:sI:87:ASN:O      | 2.34                     | 0.60              |
| 10:sA:34:MET:HE1   | 10:sA:150:THR:CA   | 2.28                     | 0.60              |
| 13:sV:20:SER:OG    | 13:sV:22:ARG:NH1   | 2.34                     | 0.60              |
| 15:sC:114:LYS:NZ   | 79:s2:11:A:O2'     | 2.33                     | 0.60              |
| 15:sC:194:ARG:NH1  | 79:s2:1156:U:O4    | 2.33                     | 0.60              |
| 26:lE:118:THR:OG1  | 26:lE:119:GLU:OE2  | 2.15                     | 0.60              |
| 29:lH:92:MET:HE3   | 29:lH:161:ILE:HD11 | 1.83                     | 0.60              |
| 32:lL:124:LEU:HD12 | 32:lL:125:ILE:N    | 2.16                     | 0.60              |
| 36:lP:32:THR:O     | 36:lP:36:ILE:HG22  | 2.01                     | 0.60              |
| 48:lc:33:GLN:OE1   | 85:l5:2675:G:N1    | 2.34                     | 0.60              |
| 65:sD:193:ASP:OD1  | 65:sD:193:ASP:N    | 2.34                     | 0.60              |
| 68:sP:43:ARG:NH2   | 79:s2:1616:U:OP2   | 2.28                     | 0.60              |
| 74:sd:3:HIS:CE1    | 74:sd:5:GLN:HB3    | 2.35                     | 0.60              |
| 79:s2:432:G:H2'    | 79:s2:433:A:H8     | 1.66                     | 0.60              |
| 79:s2:1112:U:O2    | 79:s2:1121:G:O6    | 2.19                     | 0.60              |
| 85:l5:680:G:H2'    | 85:l5:681:G:H8     | 1.65                     | 0.60              |
| 85:l5:2498:C:H2'   | 85:l5:2499:C:H6    | 1.67                     | 0.60              |
| 5:SX:87:ASN:OD1    | 5:SX:88:ASP:N      | 2.33                     | 0.60              |
| 11:SB:127:VAL:HG11 | 11:SB:176:VAL:HG11 | 1.84                     | 0.60              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 85:L5:714:G:H2'    | 85:L5:715:G:H8     | 1.66                     | 0.60              |
| 85:L5:1207:C:H2'   | 85:L5:1208:G:C8    | 2.35                     | 0.60              |
| 85:L5:2633:U:H5''  | 38:LR:61:ALA:HB2   | 1.83                     | 0.60              |
| 85:L5:4101:C:O2    | 85:L5:4107:G:P     | 2.59                     | 0.60              |
| 25:LD:146:LEU:C    | 25:LD:146:LEU:HD12 | 2.25                     | 0.60              |
| 28:LG:102:TYR:OH   | 28:LG:208:ASN:N    | 2.32                     | 0.60              |
| 31:LJ:95:ARG:O     | 31:LJ:175:LEU:N    | 2.31                     | 0.60              |
| 36:LP:50:ASP:OD2   | 36:LP:56:GLN:NE2   | 2.33                     | 0.60              |
| 42:LV:85:ARG:HG2   | 42:LV:101:ASN:HD21 | 1.66                     | 0.60              |
| 53:Lh:87:LYS:HB2   | 53:Lh:91:MET:SD    | 2.41                     | 0.60              |
| 53:Lh:107:GLN:HE22 | 53:Lh:111:GLU:CD   | 2.09                     | 0.60              |
| 62:Lr:108:MET:HA   | 62:Lr:111:ILE:HG12 | 1.81                     | 0.60              |
| 63:Lz:18:LEU:O     | 63:Lz:19:HIS:ND1   | 2.33                     | 0.60              |
| 67:SK:16:PHE:CE2   | 67:SK:80:ARG:HA    | 2.36                     | 0.60              |
| 77:SZ:99:LEU:HD21  | 77:SZ:102:LYS:HB2  | 1.82                     | 0.60              |
| 79:S2:375:U:H2'    | 79:S2:376:A:C8     | 2.36                     | 0.60              |
| 79:S2:640:A:H2'    | 79:S2:641:A:C8     | 2.36                     | 0.60              |
| 79:S2:1217:A:H2'   | 79:S2:1218:C:H6    | 1.66                     | 0.60              |
| 79:S2:1293:A:H3'   | 79:S2:1294:G:H8    | 1.65                     | 0.60              |
| 79:S2:1491:G:H2'   | 79:S2:1492:U:C6    | 2.36                     | 0.60              |
| 22:IA:204:MET:CE   | 22:IA:208:GLU:HB2  | 2.31                     | 0.60              |
| 24:IC:327:LYS:O    | 27:IF:47:ARG:NH1   | 2.31                     | 0.60              |
| 24:IC:331:TYR:CE2  | 24:IC:335:MET:HE2  | 2.36                     | 0.60              |
| 26:IE:165:LEU:HD11 | 26:IE:176:THR:HG22 | 1.84                     | 0.60              |
| 34:IN:145:ASN:O    | 34:IN:148:THR:OG1  | 2.18                     | 0.60              |
| 34:IN:149:GLN:OE1  | 34:IN:149:GLN:N    | 2.29                     | 0.60              |
| 64:sR:27:ASP:O     | 79:s2:1454:A:O2'   | 2.19                     | 0.60              |
| 80:cB:131:CYS:HB3  | 80:cB:157:MET:HE1  | 1.82                     | 0.60              |
| 85:l5:114:G:N2     | 85:l5:158:A:H61    | 1.99                     | 0.60              |
| 85:l5:1332:C:H2'   | 85:l5:1333:A:C8    | 2.36                     | 0.60              |
| 85:l5:1511:U:H2'   | 85:l5:1512:G:H8    | 1.65                     | 0.60              |
| 85:l5:2749:C:H2'   | 85:l5:2750:G:C8    | 2.35                     | 0.60              |
| 85:l5:3607:U:H2'   | 85:l5:3608:A:H8    | 1.66                     | 0.60              |
| 85:l5:4088:C:H2'   | 85:l5:4089:G:C8    | 2.36                     | 0.60              |
| 85:l5:4635:A:OP1   | 85:l5:4636:U:O2'   | 2.19                     | 0.60              |
| 2:SE:72:ILE:HD11   | 2:SE:88:ASP:CB     | 2.23                     | 0.60              |
| 6:SG:71:GLY:O      | 6:SG:99:GLY:N      | 2.33                     | 0.60              |
| 17:SO:103:ASN:ND2  | 17:SO:140:THR:O    | 2.34                     | 0.60              |
| 85:L5:64:A:H1'     | 85:L5:76:A:H1'     | 1.82                     | 0.60              |
| 85:L5:750:U:H1'    | 85:L5:917:A:C8     | 2.37                     | 0.60              |
| 85:L5:1444:G:H1    | 85:L5:2104:G:H21   | 1.49                     | 0.60              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 85:L5:4740:G:O6    | 85:L5:4959:U:O2    | 2.18                     | 0.60              |
| 25:LD:135:ILE:HG23 | 25:LD:138:GLN:HB2  | 1.83                     | 0.60              |
| 25:LD:191:ASN:OD1  | 25:LD:194:VAL:N    | 2.31                     | 0.60              |
| 27:LF:50:ILE:HD12  | 27:LF:186:CYS:HB3  | 1.83                     | 0.60              |
| 30:LI:31:ILE:HD11  | 30:LI:93:PRO:HD3   | 1.82                     | 0.60              |
| 31:LJ:107:PHE:O    | 31:LJ:130:PHE:N    | 2.33                     | 0.60              |
| 46:La:81:LEU:H     | 46:La:81:LEU:HD12  | 1.65                     | 0.60              |
| 49:Ld:18:ASN:OD1   | 49:Ld:20:VAL:N     | 2.35                     | 0.60              |
| 62:Lr:31:ASN:HD22  | 62:Lr:41:ASN:HA    | 1.66                     | 0.60              |
| 63:Lz:90:LEU:HA    | 63:Lz:93:LEU:HD12  | 1.83                     | 0.60              |
| 65:SD:42:THR:HG22  | 72:SU:106:ILE:HD11 | 1.83                     | 0.60              |
| 79:S2:116:U:H3     | 79:S2:347:G:H1     | 1.49                     | 0.60              |
| 79:S2:929:G:H2'    | 79:S2:930:C:O4'    | 2.00                     | 0.60              |
| 79:S2:1752:C:O2'   | 79:S2:1782:G:N2    | 2.25                     | 0.60              |
| 2:sE:69:PHE:CE2    | 8:sY:17:LEU:CD2    | 2.85                     | 0.60              |
| 10:sA:140:VAL:O    | 10:sA:141:ASN:ND2  | 2.34                     | 0.60              |
| 15:sC:114:LYS:HE2  | 79:s2:1358:U:P     | 2.40                     | 0.60              |
| 17:sO:54:CYS:HB3   | 17:sO:81:VAL:HG23  | 1.83                     | 0.60              |
| 34:lN:146:PRO:HB2  | 53:lh:104:THR:HG22 | 1.84                     | 0.60              |
| 38:lR:170:ARG:O    | 38:lR:174:GLU:HG2  | 2.01                     | 0.60              |
| 62:lr:31:ASN:O     | 62:lr:113:ARG:NH2  | 2.33                     | 0.60              |
| 62:lr:114:ALA:O    | 62:lr:117:ILE:HG22 | 2.00                     | 0.60              |
| 75:sg:108:VAL:HA   | 75:sg:124:SER:HA   | 1.83                     | 0.60              |
| 79:s2:5:U:H2'      | 79:s2:6:G:C8       | 2.36                     | 0.60              |
| 79:s2:461:U:H2'    | 79:s2:462:C:C6     | 2.37                     | 0.60              |
| 80:cB:219:HIS:HB2  | 80:cB:221:TRP:CD1  | 2.37                     | 0.60              |
| 81:aP:42:A:H2'     | 81:aP:43:A:H8      | 1.66                     | 0.60              |
| 85:l5:2411:C:H2'   | 85:l5:2412:A:H8    | 1.64                     | 0.60              |
| 85:l5:2495:U:H2'   | 85:l5:2496:G:H8    | 1.66                     | 0.60              |
| 85:l5:2634:C:H2'   | 85:l5:2635:U:H6    | 1.66                     | 0.60              |
| 85:l5:4080:C:H2'   | 85:l5:4081:G:H8    | 1.66                     | 0.60              |
| 3:SI:198:TYR:O     | 3:SI:202:ILE:HG12  | 2.00                     | 0.60              |
| 6:SG:47:GLY:O      | 6:SG:115:LYS:NZ    | 2.35                     | 0.60              |
| 8:SY:57:VAL:HG23   | 8:SY:73:GLY:HA2    | 1.81                     | 0.60              |
| 11:SB:119:THR:HG21 | 11:SB:156:ALA:H    | 1.66                     | 0.60              |
| 11:SB:205:TYR:HD1  | 11:SB:206:PRO:HD2  | 1.65                     | 0.60              |
| 16:SN:19:ARG:HH12  | 16:SN:23:PRO:HG3   | 1.66                     | 0.60              |
| 85:L5:72:C:C5      | 32:LL:67:HIS:CD2   | 2.90                     | 0.60              |
| 85:L5:72:C:C5      | 32:LL:67:HIS:HD2   | 2.18                     | 0.60              |
| 85:L5:981:C:C4     | 26:LE:73:TYR:HE2   | 2.18                     | 0.60              |
| 85:L5:1340:C:H2'   | 85:L5:1341:U:C6    | 2.36                     | 0.60              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 85:L5:1876:U:H2'   | 85:L5:1877:G:H8    | 1.66                     | 0.60              |
| 85:L5:4260:U:H2'   | 85:L5:4261:C:C6    | 2.35                     | 0.60              |
| 85:L5:4922:C:H2'   | 85:L5:4923:C:C6    | 2.35                     | 0.60              |
| 22:LA:180:LEU:HD11 | 61:Lp:26:VAL:HG21  | 1.84                     | 0.60              |
| 38:LR:172:ARG:NH2  | 79:S2:909:G:OP2    | 2.27                     | 0.60              |
| 43:LX:128:ILE:HG22 | 43:LX:134:LYS:HG3  | 1.82                     | 0.60              |
| 53:Lh:67:GLU:OE1   | 53:Lh:71:LYS:NZ    | 2.35                     | 0.60              |
| 64:SR:42:PRO:HG2   | 65:SD:205:PRO:HA   | 1.83                     | 0.60              |
| 66:SF:59:LYS:HG2   | 66:SF:62:ARG:HH11  | 1.67                     | 0.60              |
| 75:Sg:236:ILE:HG22 | 75:Sg:252:THR:HG22 | 1.82                     | 0.60              |
| 79:S2:803:C:H2'    | 79:S2:804:U:C6     | 2.37                     | 0.60              |
| 79:S2:885:U:O2     | 79:S2:901:G:O6     | 2.20                     | 0.60              |
| 79:S2:1438:A:H2'   | 79:S2:1439:A:C8    | 2.36                     | 0.60              |
| 79:S2:1752:C:N4    | 79:S2:1754:G:O6    | 2.35                     | 0.60              |
| 79:S2:1845:A:H2'   | 79:S2:1846:G:H8    | 1.64                     | 0.60              |
| 4:sL:35:ARG:NH2    | 4:sL:55:TYR:O      | 2.33                     | 0.60              |
| 12:sH:43:LEU:HB3   | 12:sH:72:PHE:HE1   | 1.67                     | 0.60              |
| 12:sH:176:VAL:O    | 12:sH:180:LEU:HD22 | 2.02                     | 0.60              |
| 33:IM:89:THR:HG23  | 33:IM:92:ALA:H     | 1.67                     | 0.60              |
| 38:IR:95:TRP:NE1   | 38:IR:99:MET:HE1   | 2.16                     | 0.60              |
| 39:IS:81:TRP:HB2   | 39:IS:128:LYS:HB2  | 1.83                     | 0.60              |
| 42:IV:24:ALA:HB3   | 42:IV:39:ILE:HD13  | 1.83                     | 0.60              |
| 58:lm:126:LYS:HG2  | 58:lm:127:VAL:H    | 1.66                     | 0.60              |
| 62:lr:58:LYS:CA    | 62:lr:121:GLN:NE2  | 2.61                     | 0.60              |
| 63:lz:107:TYR:CE1  | 63:lz:133:LYS:HD3  | 2.36                     | 0.60              |
| 64:sR:5:ARG:NE     | 79:s2:1367:U:H2'   | 2.17                     | 0.60              |
| 64:sR:23:ARG:O     | 64:sR:31:ASN:ND2   | 2.33                     | 0.60              |
| 65:sD:119:CYS:SG   | 65:sD:120:TYR:N    | 2.75                     | 0.60              |
| 66:sF:139:VAL:HA   | 73:sc:63:ARG:CZ    | 2.31                     | 0.60              |
| 75:sg:252:THR:N    | 75:sg:255:SER:O    | 2.35                     | 0.60              |
| 79:s2:563:G:C2     | 79:s2:564:A:C8     | 2.89                     | 0.60              |
| 79:s2:578:C:H2'    | 79:s2:579:C:C6     | 2.36                     | 0.60              |
| 79:s2:836:G:H5''   | 28:LG:255:LYS:HB2  | 1.83                     | 0.60              |
| 79:s2:1115:U:O2'   | 79:s2:1117:C:OP2   | 2.20                     | 0.60              |
| 79:s2:1656:G:O6    | 79:s2:1668:U:O4    | 2.20                     | 0.60              |
| 80:cB:116:THR:HB   | 80:cB:497:MET:HE1  | 1.82                     | 0.60              |
| 81:aP:8:U:H5'      | 81:aP:49:C:H5'     | 1.84                     | 0.60              |
| 85:l5:234:G:N2     | 85:l5:2332:A:O2'   | 2.35                     | 0.60              |
| 85:l5:1317:U:H2'   | 85:l5:1318:C:C6    | 2.37                     | 0.60              |
| 85:l5:1339:U:H2'   | 85:l5:1340:C:C6    | 2.36                     | 0.60              |
| 85:l5:2614:C:O2'   | 85:l5:2808:G:OP1   | 2.15                     | 0.60              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 85:l5:2640:G:H2'   | 85:l5:2641:A:C8    | 2.36                     | 0.60              |
| 85:l5:4887:C:N4    | 85:l5:4932:U:H3    | 1.99                     | 0.60              |
| 80:CB:20:ARG:NH2   | 80:CB:91:GLN:OE1   | 2.34                     | 0.60              |
| 80:CB:43:ALA:CB    | 80:CB:77:LEU:HD21  | 2.30                     | 0.60              |
| 80:CB:626:GLN:O    | 80:CB:631:ARG:NH2  | 2.33                     | 0.60              |
| 2:SE:125:LYS:O     | 2:SE:142:HIS:N     | 2.31                     | 0.60              |
| 8:SY:12:PHE:CE2    | 8:SY:23:MET:HE2    | 2.36                     | 0.60              |
| 85:L5:975:C:O2     | 24:LC:323:ARG:NH1  | 2.34                     | 0.60              |
| 85:L5:1802:A:H5''  | 85:L5:1803:G:H5'   | 1.83                     | 0.60              |
| 85:L5:2620:G:H1    | 85:L5:2636:U:H3    | 1.49                     | 0.60              |
| 85:L5:4186:A:H2'   | 85:L5:4187:G:C8    | 2.36                     | 0.60              |
| 20:L7:64:G:H2'     | 20:L7:65:G:H8      | 1.66                     | 0.60              |
| 20:L7:107:G:H5''   | 25:LD:273:LEU:HD11 | 1.82                     | 0.60              |
| 24:LC:209:ILE:HB   | 24:LC:229:LEU:HD13 | 1.83                     | 0.60              |
| 27:LF:85:ALA:HB2   | 40:LT:138:ALA:H    | 1.65                     | 0.60              |
| 31:LJ:166:PHE:CD1  | 31:LJ:170:TYR:HD1  | 2.19                     | 0.60              |
| 36:LP:30:ARG:CZ    | 36:LP:62:ARG:HE    | 2.14                     | 0.60              |
| 79:S2:496:C:H2'    | 79:S2:497:C:H6     | 1.66                     | 0.60              |
| 79:S2:857:U:H2'    | 79:S2:858:A:H8     | 1.66                     | 0.60              |
| 1:cH:72:ARG:NH1    | 1:cH:113:ARG:HB3   | 2.17                     | 0.60              |
| 11:sB:151:ARG:HG2  | 11:sB:152:LYS:N    | 2.17                     | 0.60              |
| 29:IH:17:ASP:OD1   | 29:IH:18:ILE:N     | 2.33                     | 0.60              |
| 30:II:184:MET:CA   | 30:II:187:LYS:HE3  | 2.26                     | 0.60              |
| 32:IL:89:LYS:HB2   | 53:lh:114:TYR:HE2  | 1.66                     | 0.60              |
| 35:IO:117:ARG:NH2  | 85:l5:4758:U:O2'   | 2.32                     | 0.60              |
| 46:la:35:ALA:HB1   | 85:l5:39:A:H5''    | 1.83                     | 0.60              |
| 48:lc:31:TYR:CE2   | 48:lc:56:ARG:HD2   | 2.37                     | 0.60              |
| 50:le:3:ALA:HB1    | 50:le:121:ARG:HE   | 1.65                     | 0.60              |
| 64:sR:17:ILE:HD12  | 64:sR:57:LEU:HD12  | 1.83                     | 0.60              |
| 70:sS:65:GLU:O     | 70:sS:69:THR:HG23  | 2.02                     | 0.60              |
| 71:sT:47:PRO:HB3   | 79:s2:1540:G:H5'   | 1.83                     | 0.60              |
| 79:s2:974:C:H2'    | 79:s2:975:G:C8     | 2.37                     | 0.60              |
| 79:s2:1204:A:H2'   | 79:s2:1205:C:C6    | 2.36                     | 0.60              |
| 79:s2:1374:C:H3'   | 79:s2:1375:G:H8    | 1.66                     | 0.60              |
| 79:s2:1470:C:H2'   | 79:s2:1471:C:H6    | 1.67                     | 0.60              |
| 80:cB:37:ASP:HB3   | 80:cB:55:ARG:HD2   | 1.83                     | 0.60              |
| 80:cB:91:GLN:OE1   | 80:cB:91:GLN:N     | 2.26                     | 0.60              |
| 85:l5:1315:C:N4    | 85:l5:1316:G:O6    | 2.34                     | 0.60              |
| 85:l5:1669:A:H4'   | 85:l5:1685:G:N2    | 2.17                     | 0.60              |
| 85:l5:4894:A:H5''  | 85:l5:4895:C:H2'   | 1.83                     | 0.60              |
| 80:CB:253:VAL:HG12 | 80:CB:257:MET:SD   | 2.42                     | 0.60              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:SI:48:VAL:HG11   | 3:SI:54:LYS:HE3    | 1.83                     | 0.60              |
| 12:SH:31:GLU:HG3   | 12:SH:37:LYS:HD2   | 1.83                     | 0.60              |
| 85:L5:1951:G:H1'   | 39:LS:117:HIS:HE1  | 1.66                     | 0.60              |
| 85:L5:2019:C:H2'   | 85:L5:2020:U:C6    | 2.37                     | 0.60              |
| 85:L5:2693:G:H2'   | 85:L5:2694:G:C2    | 2.36                     | 0.60              |
| 85:L5:4112:C:O2'   | 85:L5:4113:U:H3'   | 2.02                     | 0.60              |
| 85:L5:4195:G:O2'   | 85:L5:4442:U:OP1   | 2.18                     | 0.60              |
| 85:L5:4286:C:H2'   | 85:L5:4287:G:C8    | 2.37                     | 0.60              |
| 85:L5:4922:C:C4    | 85:L5:4923:C:N4    | 2.70                     | 0.60              |
| 22:LA:129:ALA:HB3  | 22:LA:132:ASN:HD21 | 1.67                     | 0.60              |
| 24:LC:25:PRO:HG2   | 24:LC:260:LEU:HD12 | 1.83                     | 0.60              |
| 54:Li:57:ALA:HB2   | 54:Li:73:ILE:HD11  | 1.83                     | 0.60              |
| 64:SR:52:GLY:O     | 64:SR:55:THR:OG1   | 2.17                     | 0.60              |
| 65:SD:42:THR:HG21  | 65:SD:45:ARG:NH2   | 2.12                     | 0.60              |
| 79:S2:656:G:H21    | 79:S2:663:C:H5''   | 1.67                     | 0.60              |
| 79:S2:1093:A:H2'   | 79:S2:1094:C:C6    | 2.37                     | 0.60              |
| 79:S2:1101:U:H2'   | 79:S2:1102:G:H8    | 1.66                     | 0.60              |
| 83:Ls:5:ASP:O      | 83:Ls:9:TRP:N      | 2.33                     | 0.60              |
| 1:cH:64:GLU:OE2    | 1:cH:67:GLU:N      | 2.35                     | 0.60              |
| 5:sX:4:CYS:C       | 5:sX:5:ARG:HG2     | 2.25                     | 0.60              |
| 8:sY:104:ARG:HH22  | 79:s2:492:C:H5     | 1.50                     | 0.60              |
| 12:sH:101:LEU:HD13 | 12:sH:120:ARG:HB3  | 1.83                     | 0.60              |
| 15:sC:189:GLY:H    | 79:s2:1355:C:N4    | 1.85                     | 0.60              |
| 25:ID:215:ASP:OD1  | 25:ID:218:ALA:N    | 2.35                     | 0.60              |
| 29:IH:51:LYS:HE2   | 85:l5:758:G:H5'    | 1.84                     | 0.60              |
| 33:IM:90:ARG:HG2   | 33:IM:93:LYS:HD2   | 1.84                     | 0.60              |
| 35:IO:62:MET:HE2   | 35:IO:62:MET:N     | 2.16                     | 0.60              |
| 37:IQ:122:THR:OG1  | 37:IQ:124:ASP:OD1  | 2.20                     | 0.60              |
| 39:IS:60:GLU:OE1   | 40:IT:136:ARG:NH2  | 2.34                     | 0.60              |
| 40:IT:14:MET:HE1   | 40:IT:58:HIS:CD2   | 2.36                     | 0.60              |
| 41:IU:84:LYS:HE3   | 41:IU:102:VAL:HG13 | 1.83                     | 0.60              |
| 43:IX:54:LEU:HD12  | 43:IX:55:ARG:N     | 2.17                     | 0.60              |
| 64:sR:8:THR:OG1    | 79:s2:1371:U:OP2   | 2.18                     | 0.60              |
| 64:sR:49:LYS:HE2   | 79:s2:1370:A:N6    | 2.14                     | 0.60              |
| 69:sQ:13:PHE:HB3   | 69:sQ:22:VAL:HG23  | 1.84                     | 0.60              |
| 75:sg:286:CYS:HA   | 75:sg:302:TYR:HA   | 1.83                     | 0.60              |
| 79:s2:464:A:N6     | 80:cB:49:ALA:H     | 1.99                     | 0.60              |
| 79:s2:1410:C:H2'   | 79:s2:1411:G:H8    | 1.64                     | 0.60              |
| 85:l5:1578:U:OP1   | 85:l5:3637:U:O2'   | 2.19                     | 0.60              |
| 85:l5:1762:C:N3    | 85:l5:1770:A:N1    | 2.49                     | 0.60              |
| 85:l5:1878:G:H2'   | 85:l5:1879:C:C6    | 2.36                     | 0.60              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 85:l5:2647:A:H3'   | 85:l5:2648:G:H8    | 1.67                     | 0.60              |
| 85:l5:3615:G:H21   | 87:1W:44:ARG:NH2   | 1.97                     | 0.60              |
| 85:l5:4990:C:H5''  | 85:l5:4991:U:H5''  | 1.84                     | 0.60              |
| 80:CB:173:GLU:OE2  | 80:CB:173:GLU:N    | 2.35                     | 0.60              |
| 80:CB:379:ASP:O    | 80:CB:383:MET:HE2  | 2.00                     | 0.60              |
| 6:SG:50:VAL:HB     | 6:SG:113:ILE:HD13  | 1.83                     | 0.60              |
| 16:SN:62:GLN:HB2   | 16:SN:65:PHE:CE2   | 2.36                     | 0.60              |
| 85:L5:457:G:H2'    | 85:L5:458:C:H6     | 1.65                     | 0.60              |
| 85:L5:710:G:H2'    | 85:L5:711:A:H8     | 1.67                     | 0.60              |
| 85:L5:1818:G:OP2   | 85:L5:1818:G:N2    | 2.21                     | 0.60              |
| 85:L5:2640:G:H2'   | 85:L5:2641:A:C8    | 2.36                     | 0.60              |
| 85:L5:4896:G:OP1   | 33:LM:128:LYS:NZ   | 2.22                     | 0.60              |
| 21:L8:131:G:H4'    | 43:LX:111:GLN:HE22 | 1.65                     | 0.60              |
| 28:LG:172:ALA:HA   | 28:LG:230:TYR:HE1  | 1.67                     | 0.60              |
| 28:LG:216:ALA:O    | 28:LG:220:GLU:HG2  | 2.00                     | 0.60              |
| 44:LY:46:SER:O     | 44:LY:122:LYS:NZ   | 2.34                     | 0.60              |
| 54:Li:7:MET:HE1    | 54:Li:9:VAL:CG2    | 2.31                     | 0.60              |
| 60:Lo:98:LYS:C     | 60:Lo:99:ARG:HE    | 2.10                     | 0.60              |
| 65:SD:101:GLN:HE21 | 65:SD:125:PHE:HE1  | 1.48                     | 0.60              |
| 77:SZ:103:HIS:O    | 77:SZ:107:VAL:HG13 | 2.02                     | 0.60              |
| 81:AP:50:U:H3      | 81:AP:64:G:H1      | 0.73                     | 0.60              |
| 10:sA:33:GLN:NE2   | 13:sV:64:GLU:OE1   | 2.35                     | 0.60              |
| 12:sH:31:GLU:HA    | 12:sH:37:LYS:HE3   | 1.84                     | 0.60              |
| 12:sH:122:LEU:HD11 | 79:s2:688:U:H5'    | 1.84                     | 0.60              |
| 16:sN:55:ARG:NH2   | 79:s2:1015:U:O2'   | 2.35                     | 0.60              |
| 20:l7:58:A:H2'     | 20:l7:59:G:H8      | 1.66                     | 0.60              |
| 22:lA:37:ARG:NH1   | 85:l5:4088:C:OP1   | 2.35                     | 0.60              |
| 27:lF:85:ALA:N     | 40:lT:138:ALA:HB2  | 2.16                     | 0.60              |
| 31:lJ:18:ARG:HD3   | 31:lJ:135:GLY:HA3  | 1.81                     | 0.60              |
| 32:lL:42:LYS:NZ    | 85:l5:107:G:OP1    | 2.35                     | 0.60              |
| 34:lN:178:HIS:ND1  | 85:l5:68:U:OP1     | 2.34                     | 0.60              |
| 42:lV:19:GLY:HA3   | 42:lV:86:LYS:HG2   | 1.84                     | 0.60              |
| 64:sR:41:ILE:HG23  | 79:s2:1387:G:C4    | 2.36                     | 0.60              |
| 69:sQ:125:ARG:HD2  | 79:s2:1648:G:H5''  | 1.83                     | 0.60              |
| 71:sT:137:GLN:N    | 71:sT:137:GLN:OE1  | 2.35                     | 0.60              |
| 75:sg:178:ASN:HD21 | 75:sg:181:ASN:H    | 1.48                     | 0.60              |
| 76:sM:69:CYS:SG    | 76:sM:70:ALA:N     | 2.75                     | 0.60              |
| 76:sM:129:LYS:HA   | 76:sM:132:LYS:HD2  | 1.82                     | 0.60              |
| 79:s2:373:G:H2'    | 79:s2:374:G:H8     | 1.66                     | 0.60              |
| 80:cB:27:HIS:CD2   | 80:cB:138:GLN:HB2  | 2.36                     | 0.60              |
| 80:cB:179:GLN:O    | 80:cB:183:GLU:HG2  | 2.02                     | 0.60              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 85:l5:1304:C:H2'  | 85:l5:1305:C:H6    | 1.66                     | 0.60              |
| 85:l5:1345:A:H2'  | 85:l5:1346:C:C6    | 2.36                     | 0.60              |
| 85:l5:2495:U:H2'  | 85:l5:2496:G:C8    | 2.37                     | 0.60              |
| 80:CB:296:PRO:HA  | 80:CB:299:LYS:HD2  | 1.83                     | 0.60              |
| 2:SE:123:LEU:HD21 | 2:SE:159:THR:HB    | 1.82                     | 0.60              |
| 10:SA:10:MET:HG3  | 64:SR:111:PHE:CE2  | 2.36                     | 0.60              |
| 10:SA:158:ASP:HB2 | 10:SA:159:ILE:HD12 | 1.83                     | 0.60              |
| 11:SB:71:LEU:HD21 | 11:SB:189:ILE:HG23 | 1.83                     | 0.60              |
| 85:L5:1503:A:H4'  | 85:L5:1504:G:H5'   | 1.84                     | 0.60              |
| 85:L5:1629:G:OP2  | 22:LA:9:ARG:NH2    | 2.26                     | 0.60              |
| 85:L5:1777:C:H2'  | 85:L5:1778:C:C6    | 2.37                     | 0.60              |
| 85:L5:3706:C:H5'' | 22:LA:226:ARG:N    | 2.17                     | 0.60              |
| 85:L5:4091:G:N1   | 85:L5:4114:C:N4    | 2.49                     | 0.60              |
| 22:LA:130:SER:HB3 | 22:LA:174:ARG:HH21 | 1.67                     | 0.60              |
| 25:LD:42:ASN:OD1  | 40:LT:67:VAL:HG22  | 2.02                     | 0.60              |
| 27:LF:41:MET:SD   | 27:LF:41:MET:N     | 2.74                     | 0.60              |
| 32:LL:140:SER:HA  | 32:LL:143:GLU:HB2  | 1.83                     | 0.60              |
| 38:LR:31:GLU:OE1  | 38:LR:31:GLU:N     | 2.21                     | 0.60              |
| 54:Li:61:LEU:HD11 | 54:Li:94:LEU:CD2   | 2.31                     | 0.60              |
| 64:SR:44:LYS:NZ   | 79:S2:1451:G:O6    | 2.30                     | 0.60              |
| 66:SF:48:TYR:HE2  | 69:SQ:56:LEU:HD13  | 1.66                     | 0.60              |
| 67:SK:32:HIS:HD2  | 67:SK:33:PRO:HD2   | 1.66                     | 0.60              |
| 68:SP:84:ILE:HD12 | 68:SP:114:HIS:O    | 2.02                     | 0.60              |
| 74:Sd:19:ARG:NH2  | 79:S2:1661:A:OP1   | 2.34                     | 0.60              |
| 76:SM:67:ALA:O    | 76:SM:71:GLU:CB    | 2.50                     | 0.60              |
| 79:S2:1426:U:H2'  | 79:S2:1427:C:C6    | 2.37                     | 0.60              |
| 79:S2:1430:C:H2'  | 79:S2:1431:G:H8    | 1.67                     | 0.60              |
| 79:S2:1657:G:H2'  | 79:S2:1658:G:C8    | 2.37                     | 0.60              |
| 7:sJ:33:GLY:HA3   | 9:se:38:TYR:CD2    | 2.36                     | 0.60              |
| 11:sB:168:MET:HA  | 11:sB:171:ILE:HG22 | 1.83                     | 0.60              |
| 25:ID:50:ARG:NH2  | 25:ID:147:ASP:OD2  | 2.29                     | 0.60              |
| 30:II:207:ASP:OD1 | 30:II:208:LYS:N    | 2.35                     | 0.60              |
| 31:IJ:72:CYS:SG   | 31:IJ:73:THR:N     | 2.74                     | 0.60              |
| 33:IM:100:ARG:NH2 | 35:IO:198:THR:O    | 2.35                     | 0.60              |
| 36:IP:10:ASN:O    | 36:IP:14:SER:OG    | 2.19                     | 0.60              |
| 38:IR:136:ARG:HE  | 38:IR:137:ILE:HD12 | 1.67                     | 0.60              |
| 65:sD:139:SER:HB2 | 65:sD:149:SER:OG   | 2.02                     | 0.60              |
| 66:sF:48:TYR:CZ   | 69:sQ:56:LEU:HD11  | 2.37                     | 0.60              |
| 79:s2:201:C:C2    | 79:s2:202:G:H1'    | 2.37                     | 0.60              |
| 79:s2:432:G:H2'   | 79:s2:433:A:C8     | 2.36                     | 0.60              |
| 80:cB:57:THR:OG1  | 80:cB:104:ASP:OD2  | 2.19                     | 0.60              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 80:cB:420:LEU:HA   | 80:cB:465:PRO:HA   | 1.83                     | 0.60              |
| 84:lt:130:LYS:NZ   | 84:lt:162:CYS:SG   | 2.75                     | 0.60              |
| 85:l5:4258:C:H2'   | 85:l5:4259:C:C6    | 2.35                     | 0.60              |
| 3:SI:133:GLU:HG3   | 3:SI:134:GLU:OE1   | 2.02                     | 0.60              |
| 5:SX:77:ASN:O      | 5:SX:79:LYS:NZ     | 2.35                     | 0.60              |
| 10:SA:198:MET:HE2  | 64:SR:85:VAL:HG12  | 1.83                     | 0.60              |
| 85:L5:261:G:H2'    | 85:L5:262:G:C8     | 2.35                     | 0.60              |
| 85:L5:1709:C:O2    | 85:L5:1716:G:O6    | 2.20                     | 0.60              |
| 85:L5:1977:C:HO2'  | 85:L5:1978:C:P     | 2.25                     | 0.60              |
| 85:L5:2017:A:O2'   | 85:L5:2018:C:O5'   | 2.20                     | 0.60              |
| 85:L5:2614:C:O2'   | 85:L5:2808:G:OP1   | 2.17                     | 0.60              |
| 85:L5:4149:C:OP1   | 45:LZ:60:LYS:NZ    | 2.35                     | 0.60              |
| 85:L5:4635:A:H3'   | 85:L5:4636:U:H4'   | 1.82                     | 0.60              |
| 23:LB:216:MET:HE1  | 23:LB:281:ASN:N    | 2.12                     | 0.60              |
| 24:LC:339:THR:O    | 24:LC:343:GLN:HG2  | 2.02                     | 0.60              |
| 33:LM:108:ASP:HB3  | 35:LO:199:HIS:HE2  | 1.65                     | 0.60              |
| 42:LV:35:LYS:HG2   | 42:LV:67:LYS:HE2   | 1.83                     | 0.60              |
| 54:Li:46:GLU:OE1   | 54:Li:47:VAL:N     | 2.34                     | 0.60              |
| 77:SZ:104:ARG:HG3  | 77:SZ:105:ALA:H    | 1.66                     | 0.60              |
| 79:S2:454:U:H2'    | 79:S2:455:A:H8     | 1.65                     | 0.60              |
| 79:S2:924:G:O6     | 79:S2:1018:U:O4    | 2.19                     | 0.60              |
| 79:S2:1084:A:OP1   | 79:S2:1858:G:O2'   | 2.17                     | 0.60              |
| 11:sB:146:ARG:HB2  | 11:sB:149:GLN:OE1  | 2.02                     | 0.60              |
| 15:sC:209:VAL:HG21 | 15:sC:233:LEU:HD22 | 1.83                     | 0.60              |
| 26:IE:157:HIS:HB3  | 26:IE:160:LYS:HG3  | 1.83                     | 0.60              |
| 27:IF:67:THR:HA    | 27:IF:70:ARG:HG2   | 1.83                     | 0.60              |
| 33:IM:55:MET:SD    | 33:IM:55:MET:N     | 2.68                     | 0.60              |
| 36:IP:54:GLN:HA    | 36:IP:83:TRP:CD1   | 2.37                     | 0.60              |
| 51:lf:52:LYS:NZ    | 85:l5:4751:G:N7    | 2.50                     | 0.60              |
| 57:ll:20:ASN:HD22  | 57:ll:42:ARG:HG3   | 1.67                     | 0.60              |
| 63:lz:165:LEU:HA   | 85:l5:3968:U:H4'   | 1.84                     | 0.60              |
| 63:lz:178:GLU:OE1  | 63:lz:182:ASN:ND2  | 2.34                     | 0.60              |
| 66:sF:43:GLU:OE2   | 66:sF:43:GLU:N     | 2.33                     | 0.60              |
| 71:sT:6:VAL:HG12   | 71:sT:135:ALA:HB2  | 1.84                     | 0.60              |
| 79:s2:106:C:H2'    | 79:s2:107:A:C8     | 2.37                     | 0.60              |
| 79:s2:152:U:C2     | 79:s2:167:G:N2     | 2.70                     | 0.60              |
| 79:s2:1797:U:H2'   | 79:s2:1798:C:C6    | 2.37                     | 0.60              |
| 80:cB:654:PRO:HG2  | 80:cB:696:ASN:HD21 | 1.66                     | 0.60              |
| 83:ls:57:LYS:HA    | 85:l5:2020:U:O3'   | 2.02                     | 0.60              |
| 84:lt:63:THR:HG22  | 84:lt:72:GLU:HG3   | 1.82                     | 0.60              |
| 85:l5:394:G:N2     | 85:l5:397:G:OP2    | 2.29                     | 0.60              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 85:l5:679:C:H2'    | 85:l5:680:G:C8     | 2.36                     | 0.60              |
| 3:SI:190:LEU:H     | 3:SI:190:LEU:HD12  | 1.66                     | 0.60              |
| 4:SL:96:ILE:HG22   | 4:SL:99:TYR:H      | 1.67                     | 0.60              |
| 5:SX:67:ARG:NH1    | 5:SX:114:ASP:OD2   | 2.35                     | 0.60              |
| 16:SN:71:ILE:HD11  | 79:S2:1018:U:H5''  | 1.83                     | 0.60              |
| 85:L5:945:U:OP1    | 24:LC:342:ARG:NH2  | 2.34                     | 0.60              |
| 85:L5:1669:A:N3    | 85:L5:1852:U:O2'   | 2.34                     | 0.60              |
| 85:L5:2353:U:H2'   | 85:L5:2354:G:H8    | 1.67                     | 0.60              |
| 20:L7:114:U:H2'    | 20:L7:115:A:C8     | 2.36                     | 0.60              |
| 26:LE:281:ILE:HD13 | 26:LE:286:LEU:HD11 | 1.84                     | 0.60              |
| 41:LU:79:SER:OG    | 41:LU:80:LYS:N     | 2.34                     | 0.60              |
| 65:SD:223:ILE:HD12 | 65:SD:225:GLU:OE2  | 2.02                     | 0.60              |
| 67:SK:14:LEU:HA    | 67:SK:17:LYS:HE3   | 1.84                     | 0.60              |
| 69:SQ:52:LEU:HB3   | 69:SQ:56:LEU:HD11  | 1.84                     | 0.60              |
| 77:SZ:58:LEU:HA    | 77:SZ:62:VAL:HG23  | 1.83                     | 0.60              |
| 79:S2:1410:C:H2'   | 79:S2:1411:G:H8    | 1.67                     | 0.60              |
| 2:sE:75:LYS:NZ     | 79:s2:122:G:OP1    | 2.34                     | 0.59              |
| 3:sI:3:ILE:O       | 3:sI:30:GLY:N      | 2.35                     | 0.59              |
| 3:sI:110:ARG:HB2   | 3:sI:166:PHE:HZ    | 1.67                     | 0.59              |
| 11:sB:103:MET:HG3  | 11:sB:215:VAL:HG22 | 1.84                     | 0.59              |
| 11:sB:151:ARG:HB3  | 64:sR:133:GLY:N    | 2.16                     | 0.59              |
| 12:sH:77:VAL:HA    | 12:sH:80:VAL:HG22  | 1.83                     | 0.59              |
| 26:lE:226:ARG:NH2  | 85:l5:695:G:H5''   | 2.16                     | 0.59              |
| 27:lF:155:TYR:CE1  | 27:lF:187:MET:HE2  | 2.37                     | 0.59              |
| 29:lH:9:THR:HG21   | 29:lH:54:ARG:HD2   | 1.83                     | 0.59              |
| 38:lR:95:TRP:NE1   | 85:l5:1572:U:H4'   | 2.17                     | 0.59              |
| 41:lU:21:PHE:CZ    | 41:lU:80:LYS:HA    | 2.37                     | 0.59              |
| 41:lU:101:ARG:HB2  | 41:lU:115:PHE:CE2  | 2.37                     | 0.59              |
| 48:lc:36:LYS:HZ2   | 48:lc:40:GLN:HE21  | 1.50                     | 0.59              |
| 50:le:99:ILE:HD12  | 50:le:108:ARG:HB2  | 1.84                     | 0.59              |
| 62:lr:67:ARG:NH2   | 85:l5:667:A:OP2    | 2.34                     | 0.59              |
| 66:sF:195:GLU:OE2  | 66:sF:195:GLU:N    | 2.34                     | 0.59              |
| 66:sF:201:LYS:HD2  | 66:sF:204:ARG:HH22 | 1.67                     | 0.59              |
| 70:sS:137:LYS:HG3  | 70:sS:138:THR:HG23 | 1.84                     | 0.59              |
| 79:s2:1711:U:H2'   | 79:s2:1712:A:H8    | 1.67                     | 0.59              |
| 80:cB:150:ARG:HH22 | 80:cB:199:PRO:HG2  | 1.67                     | 0.59              |
| 80:cB:591:CYS:HB2  | 80:cB:604:MET:SD   | 2.41                     | 0.59              |
| 85:l5:262:G:H2'    | 85:l5:263:G:C8     | 2.37                     | 0.59              |
| 85:l5:494:U:H2'    | 85:l5:495:C:C6     | 2.36                     | 0.59              |
| 85:l5:4127:A:H61   | 85:l5:4156:G:H2'   | 1.67                     | 0.59              |
| 5:SX:36:LEU:HD21   | 79:S2:407:G:N1     | 2.17                     | 0.59              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 5: SX:46: HIS:CE1    | 79: S2:648: A:H1'    | 2.37                     | 0.59              |
| 11: SB:171: ILE:HD11 | 11: SB:197: ILE:HG13 | 1.84                     | 0.59              |
| 11: SB:175: GLU:OE1  | 11: SB:179: ASN:ND2  | 2.35                     | 0.59              |
| 11: SB:219: LYS:NZ   | 61: Lp:89: LEU:O     | 2.24                     | 0.59              |
| 13: SV:17: CYS:HB3   | 13: SV:24: ILE:HD11  | 1.84                     | 0.59              |
| 13: SV:66: ASP:O     | 13: SV:70: LEU:HD23  | 2.01                     | 0.59              |
| 18: SW:4: MET:HE1    | 79: S2:683: G:C4'    | 2.25                     | 0.59              |
| 18: SW:44: HIS:HB3   | 18: SW:46: TYR:HE1   | 1.67                     | 0.59              |
| 85: L5:4419: U:OP1   | 85: L5:4475: G:N2    | 2.35                     | 0.59              |
| 23: LB:77: THR:HG21  | 23: LB:337: VAL:HB   | 1.85                     | 0.59              |
| 24: LC:325: MET:HE2  | 24: LC:325: MET:HA   | 1.85                     | 0.59              |
| 30: LI:99: ILE:HB    | 30: LI:123: GLN:OE1  | 2.02                     | 0.59              |
| 46: La:100: ILE:HD12 | 46: La:101: ILE:H    | 1.67                     | 0.59              |
| 48: Lc:30: GLY:O     | 48: Lc:93: THR:OG1   | 2.19                     | 0.59              |
| 54: Li:2: ALA:N      | 54: Li:5: TYR:HH     | 2.00                     | 0.59              |
| 59: Ln:1: MET:HE2    | 59: Ln:1: MET:N      | 2.17                     | 0.59              |
| 67: SK:97: SER:HB2   | 67: SK:98: ARG:HH11  | 1.67                     | 0.59              |
| 69: SQ:54: PRO:HG2   | 69: SQ:88: ILE:HD11  | 1.83                     | 0.59              |
| 71: ST:11: GLN:HG3   | 71: ST:14: PHE:HD1   | 1.67                     | 0.59              |
| 76: SM:84: LYS:HG3   | 76: SM:88: TRP:CE2   | 2.36                     | 0.59              |
| 79: S2:5: U:H2'      | 79: S2:6: G:H8       | 1.67                     | 0.59              |
| 79: S2:835: C:H4'    | 79: S2:836: G:C8     | 2.36                     | 0.59              |
| 79: S2:1628: C:H2'   | 79: S2:1629: C:C6    | 2.37                     | 0.59              |
| 81: AP:58: A:O2'     | 81: AP:61: C:N4      | 2.35                     | 0.59              |
| 6: sG:223: LYS:HZ1   | 6: sG:227: GLN:HB2   | 1.67                     | 0.59              |
| 11: sB:144: LYS:HB3  | 11: sB:208: HIS:HB3  | 1.84                     | 0.59              |
| 16: sN:14: SER:HB3   | 79: s2:1016: U:H5''  | 1.84                     | 0.59              |
| 17: sO:85: CYS:HB3   | 17: sO:90: ILE:HG23  | 1.82                     | 0.59              |
| 27: lF:93: ILE:HD11  | 27: lF:118: PHE:HA   | 1.84                     | 0.59              |
| 31: lJ:35: ARG:HB3   | 31: lJ:123: ILE:HD12 | 1.83                     | 0.59              |
| 39: lS:8: ARG:NH2    | 85: l5:939: G:O2'    | 2.35                     | 0.59              |
| 44: lY:59: ARG:HA    | 44: lY:63: LYS:HZ3   | 1.67                     | 0.59              |
| 45: lZ:92: ASP:HB3   | 45: lZ:95: VAL:HG12  | 1.82                     | 0.59              |
| 45: lZ:133: LYS:NZ   | 85: l5:2754: G:OP2   | 2.34                     | 0.59              |
| 68: sP:122: THR:O    | 79: s2:1240: A:N6    | 2.34                     | 0.59              |
| 69: sQ:39: LEU:HB3   | 69: sQ:51: LEU:HD21  | 1.83                     | 0.59              |
| 75: sg:217: MET:HE3  | 75: sg:229: THR:HG23 | 1.84                     | 0.59              |
| 79: s2:375: U:H2'    | 79: s2:376: A:H8     | 1.64                     | 0.59              |
| 79: s2:1199: A:H2'   | 79: s2:1200: A:C8    | 2.38                     | 0.59              |
| 79: s2:1275: G:N2    | 79: s2:1506: A:OP2   | 2.30                     | 0.59              |
| 80: cB:595: SER:HA   | 80: cB:724: THR:HG21 | 1.83                     | 0.59              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 82:pE:34:U:HO2'    | 82:pE:35:U:P       | 2.24                     | 0.59              |
| 85:l5:950:G:H2'    | 85:l5:951:G:H8     | 1.68                     | 0.59              |
| 85:l5:2751:G:H2'   | 85:l5:2752:G:H8    | 1.66                     | 0.59              |
| 85:l5:3700:C:O2'   | 85:l5:3774:A:N3    | 2.30                     | 0.59              |
| 85:l5:4951:G:H2'   | 85:l5:4952:G:H8    | 1.67                     | 0.59              |
| 8:SY:18:LEU:HB2    | 8:SY:20:ARG:HD3    | 1.84                     | 0.59              |
| 17:SO:112:ALA:O    | 17:SO:116:LEU:HG   | 2.02                     | 0.59              |
| 18:SW:87:GLU:N     | 18:SW:87:GLU:OE2   | 2.32                     | 0.59              |
| 85:L5:717:U:H2'    | 85:L5:718:C:C6     | 2.37                     | 0.59              |
| 85:L5:1628:C:H2'   | 85:L5:1629:G:C8    | 2.37                     | 0.59              |
| 85:L5:1653:A:OP2   | 46:La:27:LYS:NZ    | 2.34                     | 0.59              |
| 85:L5:4725:C:OP1   | 23:LB:103:LYS:NZ   | 2.36                     | 0.59              |
| 85:L5:5005:G:H2'   | 87:LW:51:TRP:HZ3   | 1.66                     | 0.59              |
| 20:L7:40:U:O2      | 31:LJ:75:ARG:NE    | 2.27                     | 0.59              |
| 20:L7:92:C:H2'     | 20:L7:93:G:C8      | 2.34                     | 0.59              |
| 29:LH:94:SER:OG    | 29:LH:142:ASP:OD1  | 2.20                     | 0.59              |
| 36:LP:140:MET:HE2  | 36:LP:140:MET:N    | 2.17                     | 0.59              |
| 46:La:148:ALA:N    | 54:Li:6:PRO:O      | 2.35                     | 0.59              |
| 65:SD:11:PHE:HE2   | 72:SU:27:ARG:HG2   | 1.67                     | 0.59              |
| 65:SD:27:ARG:O     | 67:SK:61:GLN:NE2   | 2.35                     | 0.59              |
| 79:S2:532:C:N4     | 79:S2:551:U:H3     | 1.99                     | 0.59              |
| 87:LW:100:VAL:O    | 87:LW:104:GLN:NE2  | 2.35                     | 0.59              |
| 1:cH:30:ARG:NH2    | 1:cH:39:GLU:O      | 2.35                     | 0.59              |
| 2:sE:18:TRP:HE1    | 2:sE:42:LEU:HA     | 1.67                     | 0.59              |
| 9:se:36:MET:SD     | 9:se:37:GLN:N      | 2.76                     | 0.59              |
| 17:sO:135:ILE:HD11 | 79:s2:986:G:N2     | 2.17                     | 0.59              |
| 21:l8:28:C:H2'     | 21:l8:29:G:H8      | 1.68                     | 0.59              |
| 24:lC:188:ARG:NH2  | 85:l5:2299:G:O6    | 2.35                     | 0.59              |
| 26:lE:94:LYS:HE2   | 85:l5:688:U:C5'    | 2.32                     | 0.59              |
| 28:lG:161:VAL:HG21 | 28:lG:166:LEU:HD21 | 1.84                     | 0.59              |
| 32:lL:56:ARG:NH1   | 32:lL:74:ARG:O     | 2.34                     | 0.59              |
| 35:lO:62:MET:CE    | 35:lO:70:PRO:HD3   | 2.30                     | 0.59              |
| 35:lO:81:TRP:CE2   | 35:lO:99:LEU:HD11  | 2.37                     | 0.59              |
| 36:lP:42:ARG:HH12  | 36:lP:110:ASP:HA   | 1.67                     | 0.59              |
| 40:lT:70:HIS:NE2   | 85:l5:4327:C:OP1   | 2.36                     | 0.59              |
| 49:ld:102:LEU:HD12 | 49:ld:103:TYR:N    | 2.17                     | 0.59              |
| 56:lk:7:GLU:OE1    | 56:lk:8:ILE:N      | 2.36                     | 0.59              |
| 59:ln:16:LYS:NZ    | 79:s2:1818:A:O2'   | 2.34                     | 0.59              |
| 63:lz:82:ILE:HD12  | 63:lz:83:PRO:HD2   | 1.84                     | 0.59              |
| 64:sR:43:SER:HB2   | 79:s2:1387:G:C5'   | 2.32                     | 0.59              |
| 69:sQ:141:TYR:OH   | 79:s2:1668:U:OP2   | 2.20                     | 0.59              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 70:sS:34:LYS:NZ    | 79:s2:1631:U:O3'   | 2.35                     | 0.59              |
| 79:s2:996:A:H2'    | 79:s2:997:A:H8     | 1.68                     | 0.59              |
| 79:s2:1344:A:H3'   | 79:s2:1371:U:OP1   | 2.02                     | 0.59              |
| 79:s2:1658:G:OP2   | 79:s2:1660:C:N4    | 2.35                     | 0.59              |
| 80:cB:744:ILE:HD11 | 80:cB:787:TYR:HB3  | 1.84                     | 0.59              |
| 82:pE:27:U:H2'     | 82:pE:28:C:C6      | 2.37                     | 0.59              |
| 7:SJ:60:LEU:O      | 7:SJ:70:ARG:NH1    | 2.36                     | 0.59              |
| 17:SO:138:ASP:O    | 79:S2:984:C:H1'    | 2.02                     | 0.59              |
| 85:L5:1368:A:H2'   | 85:L5:1369:C:O4'   | 2.01                     | 0.59              |
| 85:L5:1507:C:H2'   | 85:L5:1508:A:H8    | 1.67                     | 0.59              |
| 85:L5:1514:U:H1'   | 32:LL:10:LEU:HD11  | 1.84                     | 0.59              |
| 85:L5:1876:U:H2'   | 85:L5:1877:G:C8    | 2.37                     | 0.59              |
| 85:L5:3859:G:N7    | 36:LP:25:HIS:HE1   | 2.00                     | 0.59              |
| 85:L5:4071:U:H2'   | 85:L5:4072:C:H6    | 1.67                     | 0.59              |
| 85:L5:4153:C:H2'   | 85:L5:4154:G:C8    | 2.38                     | 0.59              |
| 23:LB:48:GLY:O     | 23:LB:345:LEU:N    | 2.30                     | 0.59              |
| 27:LF:85:ALA:N     | 40:LT:138:ALA:HB2  | 2.16                     | 0.59              |
| 27:LF:110:GLN:OE1  | 27:LF:115:ARG:NH2  | 2.35                     | 0.59              |
| 31:LJ:63:ARG:HH12  | 60:Lo:103:VAL:CG1  | 2.14                     | 0.59              |
| 35:LO:87:MET:HE2   | 35:LO:87:MET:N     | 2.17                     | 0.59              |
| 43:LX:120:ASP:OD1  | 43:LX:121:VAL:N    | 2.35                     | 0.59              |
| 44:LY:32:SER:HB2   | 44:LY:49:ILE:HD11  | 1.82                     | 0.59              |
| 66:SF:175:ASP:OD1  | 66:SF:175:ASP:N    | 2.34                     | 0.59              |
| 70:SS:102:GLY:O    | 70:SS:106:LYS:HB2  | 2.03                     | 0.59              |
| 74:Sd:36:LEU:HD11  | 74:Sd:38:MET:HB3   | 1.84                     | 0.59              |
| 79:S2:1221:G:H2'   | 79:S2:1222:G:C8    | 2.37                     | 0.59              |
| 7:sJ:161:LEU:HA    | 7:sJ:167:GLY:H     | 1.67                     | 0.59              |
| 10:sA:10:MET:CE    | 10:sA:15:VAL:HG11  | 2.32                     | 0.59              |
| 11:sB:226:GLY:HA3  | 85:l5:4100:C:H4'   | 1.83                     | 0.59              |
| 21:l8:110:U:O5'    | 57:ll:8:ARG:NH2    | 2.32                     | 0.59              |
| 22:lA:80:GLU:CD    | 61:lp:76:ALA:HB2   | 2.28                     | 0.59              |
| 22:lA:208:GLU:OE1  | 85:l5:1631:A:H2    | 1.86                     | 0.59              |
| 23:lB:168:MET:HE1  | 23:lB:173:LEU:HD23 | 1.83                     | 0.59              |
| 23:lB:175:GLN:HG3  | 85:l5:4985:U:O3'   | 2.01                     | 0.59              |
| 24:lC:352:ASP:OD1  | 24:lC:353:LYS:N    | 2.36                     | 0.59              |
| 27:lF:187:MET:HA   | 27:lF:190:LEU:HD13 | 1.84                     | 0.59              |
| 31:lJ:99:PHE:HB3   | 31:lJ:159:LYS:HG2  | 1.83                     | 0.59              |
| 34:lN:4:TYR:HD2    | 85:l5:114:G:H5''   | 1.67                     | 0.59              |
| 50:le:86:GLU:OE2   | 50:le:89:LEU:HD22  | 2.02                     | 0.59              |
| 55:lj:34:CYS:SG    | 55:lj:36:LYS:N     | 2.74                     | 0.59              |
| 59:ln:21:ARG:HH22  | 79:s2:1175:G:P     | 2.26                     | 0.59              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 78:sf:103:LEU:HD23 | 78:sf:104:LYS:H    | 1.65                     | 0.59              |
| 79:s2:478:G:H4'    | 80:cB:409:ARG:HH12 | 1.67                     | 0.59              |
| 79:s2:1033:G:N2    | 79:s2:1080:A:HO2'  | 1.99                     | 0.59              |
| 80:cB:37:ASP:HA    | 80:cB:40:VAL:HG12  | 1.83                     | 0.59              |
| 80:cB:174:LEU:O    | 80:cB:178:PHE:HD1  | 1.86                     | 0.59              |
| 84:lt:127:GLY:HA2  | 84:lt:130:LYS:HD2  | 1.84                     | 0.59              |
| 84:lt:139:VAL:HG11 | 85:l5:1976:G:N2    | 2.18                     | 0.59              |
| 85:l5:1683:U:H2'   | 85:l5:1684:A:C8    | 2.38                     | 0.59              |
| 3:SI:149:TYR:O     | 3:SI:153:LYS:HG3   | 2.02                     | 0.59              |
| 5:SX:96:GLU:OE1    | 5:SX:97:ASN:ND2    | 2.35                     | 0.59              |
| 11:SB:35:ALA:HB2   | 11:SB:44:ILE:HD11  | 1.84                     | 0.59              |
| 85:L5:1402:C:C2    | 85:L5:1415:G:N2    | 2.70                     | 0.59              |
| 85:L5:2400:G:H21   | 52:Lg:6:THR:HG22   | 1.68                     | 0.59              |
| 85:L5:2835:A:O2'   | 23:LB:228:TYR:O    | 2.20                     | 0.59              |
| 85:L5:2837:U:OP1   | 23:LB:249:ARG:NH2  | 2.27                     | 0.59              |
| 85:L5:2892:C:H5    | 38:LR:74:ARG:HH12  | 1.50                     | 0.59              |
| 85:L5:4130:C:H2'   | 85:L5:4131:G:C8    | 2.38                     | 0.59              |
| 85:L5:4586:G:OP1   | 35:LO:72:HIS:N     | 2.28                     | 0.59              |
| 85:L5:4630:G:H2'   | 85:L5:4631:G:C8    | 2.37                     | 0.59              |
| 20:L7:49:A:H5''    | 25:LD:224:SER:OG   | 2.03                     | 0.59              |
| 24:LC:138:MET:HE1  | 24:LC:144:ILE:H    | 1.68                     | 0.59              |
| 27:LF:149:SER:O    | 27:LF:153:LEU:HG   | 2.02                     | 0.59              |
| 32:LL:177:LYS:HB3  | 32:LL:180:ALA:HB3  | 1.83                     | 0.59              |
| 40:LT:151:LEU:HD23 | 40:LT:151:LEU:H    | 1.65                     | 0.59              |
| 43:LX:141:ALA:HB3  | 43:LX:144:TYR:CE2  | 2.37                     | 0.59              |
| 44:LY:53:ASP:HB2   | 44:LY:106:ILE:HD11 | 1.83                     | 0.59              |
| 53:Lh:29:SER:O     | 53:Lh:33:VAL:HG23  | 2.03                     | 0.59              |
| 62:Lr:61:VAL:HA    | 62:Lr:81:THR:HA    | 1.82                     | 0.59              |
| 79:S2:604:A:H2'    | 79:S2:605:A:C8     | 2.38                     | 0.59              |
| 79:S2:982:G:H2'    | 79:S2:983:A:C8     | 2.37                     | 0.59              |
| 79:S2:1726:G:N1    | 79:S2:1809:A:N7    | 2.50                     | 0.59              |
| 79:S2:1754:G:N7    | 79:S2:1779:G:N2    | 2.51                     | 0.59              |
| 1:CH:75:LEU:HB3    | 1:CH:79:LYS:HE3    | 1.84                     | 0.59              |
| 10:sA:120:ARG:HH12 | 15:sC:267:GLN:HB3  | 1.66                     | 0.59              |
| 20:l7:92:C:H2'     | 20:l7:93:G:C8      | 2.35                     | 0.59              |
| 27:lF:32:ARG:HA    | 27:lF:35:LYS:HE2   | 1.83                     | 0.59              |
| 35:lO:54:TYR:O     | 35:lO:54:TYR:HD2   | 1.85                     | 0.59              |
| 37:lQ:68:ARG:NH1   | 85:l5:1420:A:H3'   | 2.18                     | 0.59              |
| 38:lR:93:VAL:O     | 38:lR:96:MET:HB2   | 2.02                     | 0.59              |
| 38:lR:108:ARG:NH2  | 85:l5:2899:C:OP1   | 2.30                     | 0.59              |
| 51:lF:36:ARG:HD2   | 51:lF:80:ASN:H     | 1.67                     | 0.59              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 52:lg:97:ILE:HD11  | 85:l5:4122:G:C5    | 2.36                     | 0.59              |
| 54:li:58:MET:HB3   | 54:li:94:LEU:HD11  | 1.82                     | 0.59              |
| 64:sR:52:GLY:HA2   | 79:s2:1454:A:C8    | 2.38                     | 0.59              |
| 69:sQ:14:GLY:HA3   | 69:sQ:86:GLN:NE2   | 2.17                     | 0.59              |
| 70:sS:70:ILE:HD12  | 70:sS:77:TYR:CE1   | 2.38                     | 0.59              |
| 75:sg:15:ASN:HD21  | 79:s2:1472:C:H4'   | 1.65                     | 0.59              |
| 76:sM:44:LYS:HZ3   | 76:sM:47:ALA:HB2   | 1.67                     | 0.59              |
| 80:cB:396:MET:HB2  | 80:cB:485:ILE:HB   | 1.83                     | 0.59              |
| 80:cB:561:LEU:HA   | 80:cB:565:HIS:HB2  | 1.83                     | 0.59              |
| 81:aP:18:G:O2'     | 81:aP:57:G:N2      | 2.35                     | 0.59              |
| 85:l5:161:G:H2'    | 85:l5:162:A:C8     | 2.37                     | 0.59              |
| 85:l5:4063:U:H2'   | 85:l5:4064:C:C2    | 2.38                     | 0.59              |
| 85:l5:4922:C:C4    | 85:l5:4923:C:N4    | 2.70                     | 0.59              |
| 80:CB:55:ARG:HG3   | 80:CB:56:PHE:HD1   | 1.67                     | 0.59              |
| 80:CB:349:ALA:O    | 80:CB:352:GLN:NE2  | 2.35                     | 0.59              |
| 6:SG:31:ARG:NH2    | 79:S2:1745:A:O2'   | 2.35                     | 0.59              |
| 6:SG:144:LEU:O     | 87:LW:94:ARG:NH1   | 2.30                     | 0.59              |
| 7:SJ:135:ILE:H     | 7:SJ:135:ILE:HD12  | 1.67                     | 0.59              |
| 8:SY:104:ARG:HH12  | 79:S2:492:C:H5     | 1.49                     | 0.59              |
| 14:Sa:13:LYS:HD3   | 14:Sa:13:LYS:C     | 2.27                     | 0.59              |
| 15:SC:204:ILE:O    | 15:SC:211:LYS:NZ   | 2.34                     | 0.59              |
| 85:L5:1726:U:H2'   | 85:L5:1727:U:H6    | 1.68                     | 0.59              |
| 85:L5:1942:A:H2'   | 85:L5:1943:A:C8    | 2.37                     | 0.59              |
| 85:L5:4935:C:H2'   | 85:L5:4936:G:H8    | 1.67                     | 0.59              |
| 24:LC:301:ALA:O    | 37:LQ:132:LYS:NZ   | 2.32                     | 0.59              |
| 47:Lb:102:PRO:HA   | 47:Lb:109:ARG:HH22 | 1.67                     | 0.59              |
| 65:SD:105:LEU:HD22 | 65:SD:184:ILE:HG12 | 1.85                     | 0.59              |
| 69:SQ:140:ARG:HB2  | 79:S2:1644:C:H4'   | 1.84                     | 0.59              |
| 79:S2:1658:G:OP2   | 79:S2:1660:C:N4    | 2.35                     | 0.59              |
| 87:LW:81:ALA:HB2   | 87:LW:87:LEU:HD22  | 1.84                     | 0.59              |
| 5:sX:45:SER:OG     | 79:s2:648:A:N3     | 2.28                     | 0.59              |
| 5:sX:68:LYS:HB3    | 5:sX:91:LEU:HD22   | 1.84                     | 0.59              |
| 5:sX:137:LYS:NZ    | 79:s2:30:C:O3'     | 2.32                     | 0.59              |
| 9:se:29:THR:HG21   | 79:s2:524:U:C2     | 2.37                     | 0.59              |
| 10:sA:85:ARG:HE    | 10:sA:86:ALA:N     | 2.01                     | 0.59              |
| 14:sa:90:GLU:OE1   | 14:sa:90:GLU:N     | 2.19                     | 0.59              |
| 18:sW:75:ILE:HG21  | 18:sW:125:ILE:HG13 | 1.84                     | 0.59              |
| 19:sb:55:LEU:HD12  | 19:sb:56:CYS:N     | 2.18                     | 0.59              |
| 23:lB:80:GLU:HG3   | 23:lB:326:VAL:HG13 | 1.85                     | 0.59              |
| 24:lC:5:ARG:NH1    | 24:lC:24:LEU:O     | 2.35                     | 0.59              |
| 26:lE:223:ARG:NH2  | 26:lE:238:GLU:OE2  | 2.36                     | 0.59              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:IO:194:GLU:HA   | 35:IO:197:LYS:HD2  | 1.84                     | 0.59              |
| 43:IX:79:PHE:CZ    | 43:IX:99:ILE:HG21  | 2.37                     | 0.59              |
| 46:la:145:VAL:HG23 | 54:li:5:TYR:CZ     | 2.38                     | 0.59              |
| 52:lg:54:ARG:HH11  | 85:l5:2653:C:H1'   | 1.66                     | 0.59              |
| 54:li:30:ARG:HD2   | 85:l5:327:U:O2'    | 2.02                     | 0.59              |
| 58:lm:100:TYR:O    | 85:l5:4472:G:O2'   | 2.21                     | 0.59              |
| 71:sT:129:ARG:HH22 | 79:s2:1416:C:C5'   | 2.12                     | 0.59              |
| 75:sg:131:LEU:HG   | 75:sg:139:LYS:HD3  | 1.82                     | 0.59              |
| 76:sM:120:ALA:O    | 76:sM:124:ILE:HG12 | 2.02                     | 0.59              |
| 80:cB:369:CYS:SG   | 80:cB:385:ILE:HG13 | 2.42                     | 0.59              |
| 80:cB:753:GLU:HG3  | 80:cB:782:PHE:CE2  | 2.37                     | 0.59              |
| 3:SI:83:TYR:HB3    | 3:SI:101:ILE:HD11  | 1.85                     | 0.59              |
| 3:SI:105:ASP:N     | 3:SI:105:ASP:OD1   | 2.36                     | 0.59              |
| 6:SG:140:ARG:O     | 6:SG:144:LEU:HG    | 2.02                     | 0.59              |
| 10:SA:36:GLN:O     | 10:SA:53:ARG:NH1   | 2.34                     | 0.59              |
| 10:SA:57:LYS:NZ    | 13:SV:70:LEU:HD21  | 2.17                     | 0.59              |
| 18:SW:102:ILE:HB   | 18:SW:113:HIS:HD2  | 1.67                     | 0.59              |
| 85:L5:332:C:H4'    | 34:LN:150:TRP:CE3  | 2.37                     | 0.59              |
| 85:L5:1847:C:H2'   | 85:L5:1848:C:C6    | 2.38                     | 0.59              |
| 85:L5:2301:G:O3'   | 50:Le:81:ASN:ND2   | 2.36                     | 0.59              |
| 85:L5:4153:C:H2'   | 85:L5:4154:G:H8    | 1.68                     | 0.59              |
| 24:LC:204:ARG:NH2  | 24:LC:205:ARG:O    | 2.30                     | 0.59              |
| 31:LJ:51:SER:N     | 31:LJ:69:ALA:O     | 2.35                     | 0.59              |
| 34:LN:123:GLU:HB2  | 34:LN:128:LYS:HA   | 1.84                     | 0.59              |
| 39:LS:46:TYR:O     | 39:LS:50:GLN:HG3   | 2.02                     | 0.59              |
| 45:LZ:117:LYS:HA   | 45:LZ:120:GLU:HG2  | 1.85                     | 0.59              |
| 76:SM:60:MET:SD    | 76:SM:60:MET:N     | 2.75                     | 0.59              |
| 87:IW:2:LYS:HE2    | 87:IW:2:LYS:HA     | 1.85                     | 0.59              |
| 6:sG:162:LEU:HB2   | 6:sG:170:ARG:HG2   | 1.84                     | 0.59              |
| 10:sA:34:MET:O     | 10:sA:38:ILE:HG22  | 2.03                     | 0.59              |
| 12:sH:143:ARG:HG2  | 12:sH:157:HIS:HE1  | 1.67                     | 0.59              |
| 15:sC:60:TRP:CE3   | 15:sC:96:PHE:CE2   | 2.90                     | 0.59              |
| 23:IB:276:HIS:ND1  | 85:l5:4716:C:OP1   | 2.31                     | 0.59              |
| 27:IF:222:LYS:HB3  | 27:IF:231:GLY:HA2  | 1.84                     | 0.59              |
| 30:II:43:VAL:HG23  | 30:II:44:ASP:OD2   | 2.00                     | 0.59              |
| 34:IN:104:GLU:HA   | 34:IN:160:GLU:HG3  | 1.84                     | 0.59              |
| 45:IZ:73:LYS:HE3   | 45:IZ:75:TYR:HE2   | 1.67                     | 0.59              |
| 66:sF:139:VAL:HA   | 73:sc:63:ARG:HH12  | 1.66                     | 0.59              |
| 75:sg:119:GLN:HB3  | 75:sg:131:LEU:HD11 | 1.84                     | 0.59              |
| 75:sg:125:ARG:HD2  | 75:sg:150:TRP:CE3  | 2.38                     | 0.59              |
| 75:sg:256:ILE:HB   | 75:sg:270:LEU:HD12 | 1.85                     | 0.59              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 76:sM:51:VAL:HB    | 76:sM:109:VAL:HG13 | 1.84                     | 0.59              |
| 79:s2:634:A:H2'    | 79:s2:635:G:C8     | 2.37                     | 0.59              |
| 79:s2:848:U:H2'    | 79:s2:849:A:H8     | 1.68                     | 0.59              |
| 79:s2:1644:C:H2'   | 79:s2:1645:C:C6    | 2.37                     | 0.59              |
| 82:pE:38:A:H2'     | 82:pE:39:U:C6      | 2.38                     | 0.59              |
| 83:ls:69:LEU:HD13  | 83:ls:72:ASN:HB3   | 1.83                     | 0.59              |
| 85:l5:62:A:N3      | 85:l5:77:U:O2'     | 2.30                     | 0.59              |
| 85:l5:711:A:H2'    | 85:l5:712:C:C6     | 2.38                     | 0.59              |
| 85:l5:4727:A:H2'   | 85:l5:4728:U:O4'   | 2.02                     | 0.59              |
| 80:CB:48:SER:OG    | 80:CB:49:ALA:N     | 2.34                     | 0.59              |
| 11:SB:214:LYS:HD3  | 11:SB:215:VAL:N    | 2.18                     | 0.59              |
| 19:Sb:33:MET:N     | 19:Sb:33:MET:SD    | 2.76                     | 0.59              |
| 85:L5:1628:C:OP2   | 22:LA:9:ARG:NE     | 2.24                     | 0.59              |
| 85:L5:4089:G:H2'   | 85:L5:4090:G:C8    | 2.38                     | 0.59              |
| 85:L5:4096:C:H1'   | 85:L5:4111:U:N3    | 2.18                     | 0.59              |
| 85:L5:4101:C:H4'   | 85:L5:4107:G:C4    | 2.38                     | 0.59              |
| 85:L5:4474:A:OP2   | 85:L5:4476:C:N4    | 2.28                     | 0.59              |
| 24:LC:189:MET:HE1  | 24:LC:200:ARG:HD2  | 1.84                     | 0.59              |
| 24:LC:237:ILE:HG23 | 24:LC:238:LEU:HD22 | 1.83                     | 0.59              |
| 25:LD:136:ASP:OD1  | 25:LD:137:GLY:N    | 2.35                     | 0.59              |
| 44:LY:22:PRO:HD2   | 44:LY:25:ILE:HD11  | 1.83                     | 0.59              |
| 53:Lh:105:LYS:CB   | 53:Lh:108:GLN:HE21 | 2.06                     | 0.59              |
| 67:SK:3:MET:HG3    | 67:SK:44:HIS:HB3   | 1.84                     | 0.59              |
| 68:SP:43:ARG:NE    | 79:S2:1617:G:O6    | 2.36                     | 0.59              |
| 71:ST:28:LEU:H     | 71:ST:28:LEU:HD12  | 1.68                     | 0.59              |
| 79:S2:516:A:N1     | 79:S2:643:A:O2'    | 2.29                     | 0.59              |
| 79:S2:751:G:H1'    | 79:S2:793:G:H21    | 1.65                     | 0.59              |
| 79:S2:1355:C:H3'   | 79:S2:1356:G:H8    | 1.68                     | 0.59              |
| 79:S2:1392:U:H2'   | 79:S2:1393:G:C8    | 2.38                     | 0.59              |
| 2:sE:69:PHE:CZ     | 8:sY:17:LEU:HD22   | 2.36                     | 0.59              |
| 11:sB:186:ASN:OD1  | 11:sB:187:LYS:N    | 2.36                     | 0.59              |
| 17:sO:76:LEU:HA    | 17:sO:79:GLN:HE21  | 1.68                     | 0.59              |
| 21:l8:23:C:OP1     | 44:IY:15:ARG:NH2   | 2.28                     | 0.59              |
| 21:l8:75:G:H2'     | 21:l8:76:C:H6      | 1.67                     | 0.59              |
| 35:lO:23:VAL:HG23  | 35:lO:33:VAL:HG11  | 1.85                     | 0.59              |
| 35:lO:93:LYS:HE3   | 85:l5:1308:C:C4'   | 2.20                     | 0.59              |
| 42:IV:99:GLU:OE2   | 87:IW:23:ARG:HA    | 2.02                     | 0.59              |
| 43:IX:145:ASP:OD2  | 43:IX:146:ALA:N    | 2.35                     | 0.59              |
| 70:sS:66:ARG:O     | 70:sS:70:ILE:HG12  | 2.02                     | 0.59              |
| 79:s2:559:G:O2'    | 79:s2:560:A:H5''   | 2.03                     | 0.59              |
| 83:ls:148:SER:O    | 83:ls:151:THR:OG1  | 2.19                     | 0.59              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 84:lt:121:LEU:HB3 | 84:lt:129:ILE:HD12 | 1.84                     | 0.59              |
| 85:l5:3607:U:H2'  | 85:l5:3608:A:C8    | 2.38                     | 0.59              |
| 2:SE:94:LYS:HE3   | 8:SY:16:ARG:HB2    | 1.85                     | 0.59              |
| 12:SH:160:LYS:HZ2 | 12:SH:193:GLN:HG2  | 1.68                     | 0.59              |
| 15:SC:138:GLY:HA3 | 15:SC:162:ILE:HD13 | 1.84                     | 0.59              |
| 85:L5:337:U:OP1   | 32:LL:31:ARG:NH1   | 2.35                     | 0.59              |
| 85:L5:364:G:H1'   | 85:L5:365:U:H5     | 1.67                     | 0.59              |
| 85:L5:490:C:N4    | 85:L5:491:G:O6     | 2.35                     | 0.59              |
| 85:L5:683:C:O2'   | 26:LE:100:LYS:NZ   | 2.35                     | 0.59              |
| 85:L5:4101:C:N1   | 85:L5:4106:G:H4'   | 2.17                     | 0.59              |
| 85:L5:4102:C:O5'  | 85:L5:4106:G:C2'   | 2.51                     | 0.59              |
| 85:L5:4457:U:OP1  | 42:LV:50:ASN:ND2   | 2.36                     | 0.59              |
| 85:L5:4674:C:O2'  | 23:LB:282:LYS:NZ   | 2.35                     | 0.59              |
| 23:LB:54:THR:OG1  | 23:LB:55:HIS:N     | 2.35                     | 0.59              |
| 23:LB:222:VAL:O   | 23:LB:343:ARG:NH1  | 2.36                     | 0.59              |
| 23:LB:389:MET:SD  | 23:LB:392:LEU:HD11 | 2.43                     | 0.59              |
| 25:LD:97:ALA:HA   | 25:LD:100:CYS:SG   | 2.42                     | 0.59              |
| 33:LM:16:SER:HB3  | 33:LM:56:GLN:HG3   | 1.83                     | 0.59              |
| 34:LN:10:LEU:HG   | 34:LN:19:MET:HE3   | 1.85                     | 0.59              |
| 45:LZ:14:LEU:HD21 | 45:LZ:81:MET:HB2   | 1.82                     | 0.59              |
| 45:LZ:96:VAL:HG12 | 45:LZ:110:ALA:HB1  | 1.85                     | 0.59              |
| 48:Lc:56:ARG:O    | 48:Lc:60:ILE:HG12  | 2.03                     | 0.59              |
| 51:Lf:33:VAL:HG23 | 51:Lf:38:GLU:HB2   | 1.84                     | 0.59              |
| 56:Lk:58:GLN:OE1  | 56:Lk:58:GLN:N     | 2.33                     | 0.59              |
| 66:SF:168:THR:N   | 66:SF:171:GLU:OE2  | 2.35                     | 0.59              |
| 68:SP:76:VAL:HG12 | 68:SP:94:VAL:HA    | 1.84                     | 0.59              |
| 79:S2:300:U:H2'   | 79:S2:301:A:H8     | 1.68                     | 0.59              |
| 79:S2:609:U:H2'   | 79:S2:610:G:C8     | 2.38                     | 0.59              |
| 10:sA:10:MET:CA   | 10:sA:55:TRP:CH2   | 2.84                     | 0.59              |
| 23:lB:228:TYR:O   | 85:l5:2835:A:O2'   | 2.20                     | 0.59              |
| 26:lE:240:TYR:OH  | 26:lE:246:ARG:NH1  | 2.35                     | 0.59              |
| 32:lL:130:LYS:HD3 | 32:lL:131:PRO:HD2  | 1.85                     | 0.59              |
| 35:lO:18:ARG:O    | 35:lO:22:ILE:HG13  | 2.02                     | 0.59              |
| 40:lT:3:ASN:HD22  | 40:lT:9:ARG:CZ     | 2.16                     | 0.59              |
| 52:lg:54:ARG:CZ   | 85:l5:2682:G:H21   | 2.15                     | 0.59              |
| 61:lp:56:HIS:HD2  | 61:lp:63:THR:HG22  | 1.64                     | 0.59              |
| 63:lz:59:PRO:HG2  | 63:lz:62:LYS:CD    | 2.31                     | 0.59              |
| 64:sR:1:MET:SD    | 79:s2:1680:G:H5'   | 2.42                     | 0.59              |
| 71:sT:7:LYS:NZ    | 79:s2:1426:U:H5'   | 2.17                     | 0.59              |
| 72:sU:98:VAL:O    | 72:sU:102:THR:HG22 | 2.03                     | 0.59              |
| 79:s2:17:C:H2'    | 79:s2:18:C:H6      | 1.68                     | 0.59              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 79:s2:654:A:OP2   | 79:s2:655:A:O2'    | 2.18                     | 0.59              |
| 79:s2:1407:U:H2'  | 79:s2:1408:U:H6    | 1.68                     | 0.59              |
| 79:s2:1545:A:N3   | 79:s2:1671:G:O2'   | 2.32                     | 0.59              |
| 85:l5:174:C:H2'   | 85:l5:175:C:C6     | 2.38                     | 0.59              |
| 85:l5:513:U:H1'   | 85:l5:516:C:H41    | 1.67                     | 0.59              |
| 85:l5:1717:C:H2'  | 85:l5:1718:C:C2    | 2.37                     | 0.59              |
| 85:l5:4071:U:H2'  | 85:l5:4072:C:H6    | 1.66                     | 0.59              |
| 80:CB:631:ARG:HD2 | 80:CB:652:PHE:HZ   | 1.67                     | 0.59              |
| 5:SX:131:LEU:HD21 | 79:S2:29:G:O2'     | 2.03                     | 0.59              |
| 7:SJ:39:ASN:ND2   | 79:S2:642:U:O5'    | 2.36                     | 0.59              |
| 8:SY:104:ARG:NH2  | 79:S2:507:G:OP2    | 2.35                     | 0.59              |
| 18:SW:120:HIS:NE2 | 79:S2:805:U:O3'    | 2.35                     | 0.59              |
| 85:L5:267:G:H2'   | 85:L5:268:G:H8     | 1.68                     | 0.59              |
| 85:L5:495:C:H2'   | 85:L5:496:G:C8     | 2.38                     | 0.59              |
| 85:L5:1604:G:H2'  | 85:L5:1605:G:C8    | 2.38                     | 0.59              |
| 85:L5:2419:C:H2'  | 85:L5:2420:A:H8    | 1.67                     | 0.59              |
| 21:L8:39:G:H1'    | 21:L8:103:A:N6     | 2.17                     | 0.59              |
| 21:L8:95:A:OP1    | 55:Lj:81:GLY:N     | 2.31                     | 0.59              |
| 25:LD:212:MET:HA  | 25:LD:212:MET:HE3  | 1.84                     | 0.59              |
| 48:Lc:14:ILE:O    | 48:Lc:18:LEU:HG    | 2.02                     | 0.59              |
| 64:SR:29:HIS:HA   | 64:SR:32:LYS:HG2   | 1.83                     | 0.59              |
| 66:SF:104:THR:OG1 | 66:SF:106:GLU:CD   | 2.46                     | 0.59              |
| 68:SP:59:ARG:NH2  | 79:S2:1297:U:O4    | 2.36                     | 0.59              |
| 75:Sg:13:GLY:O    | 75:Sg:305:ASN:ND2  | 2.30                     | 0.59              |
| 79:S2:107:A:H2'   | 79:S2:108:G:C8     | 2.37                     | 0.59              |
| 82:PE:16:C:H5''   | 82:PE:60:U:H3      | 1.68                     | 0.59              |
| 87:LW:9:SER:HA    | 87:LW:52:THR:HG23  | 1.83                     | 0.59              |
| 4:sL:73:LEU:HD12  | 4:sL:74:SER:H      | 1.68                     | 0.59              |
| 6:sG:189:ARG:HD2  | 79:s2:332:G:N7     | 2.17                     | 0.59              |
| 15:sC:60:TRP:CD1  | 15:sC:60:TRP:C     | 2.80                     | 0.59              |
| 18:sW:115:GLU:HA  | 18:sW:118:ARG:HB2  | 1.83                     | 0.59              |
| 23:lB:100:ARG:NH1 | 85:l5:4911:A:OP2   | 2.36                     | 0.59              |
| 23:lB:303:ALA:HB1 | 23:lB:368:ILE:HD12 | 1.85                     | 0.59              |
| 25:lD:239:MET:SD  | 25:lD:240:TYR:N    | 2.76                     | 0.59              |
| 29:lH:36:ARG:NH1  | 29:lH:152:GLU:OE1  | 2.36                     | 0.59              |
| 33:lM:51:PRO:O    | 33:lM:55:MET:HE1   | 2.03                     | 0.59              |
| 38:lR:180:LYS:HE2 | 38:lR:180:LYS:HA   | 1.85                     | 0.59              |
| 40:lT:79:GLN:HA   | 40:lT:84:ILE:HG22  | 1.84                     | 0.59              |
| 48:lc:26:LYS:HG2  | 48:lc:97:ILE:HB    | 1.84                     | 0.59              |
| 48:lc:38:ILE:CD1  | 48:lc:63:TYR:HB3   | 2.33                     | 0.59              |
| 64:sR:42:PRO:HA   | 79:s2:1388:A:N7    | 2.17                     | 0.59              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 69:sQ:105:LYS:O    | 69:sQ:108:ILE:HG12 | 2.03                     | 0.59              |
| 75:sg:273:GLU:OE1  | 75:sg:308:ARG:NE   | 2.36                     | 0.59              |
| 76:sM:52:LEU:HG    | 76:sM:78:LYS:NZ    | 2.18                     | 0.59              |
| 77:sZ:85:ARG:O     | 77:sZ:89:GLN:HG2   | 2.03                     | 0.59              |
| 79:s2:17:C:H2'     | 79:s2:18:C:C6      | 2.38                     | 0.59              |
| 79:s2:609:U:H2'    | 79:s2:610:G:H8     | 1.67                     | 0.59              |
| 79:s2:1283:C:H1'   | 79:s2:1287:A:H5'   | 1.85                     | 0.59              |
| 81:aP:3:C:H2'      | 81:aP:4:U:C6       | 2.38                     | 0.59              |
| 80:CB:381:ALA:O    | 80:CB:385:ILE:HG13 | 2.03                     | 0.59              |
| 80:CB:671:TYR:HD1  | 80:CB:709:LEU:HB2  | 1.67                     | 0.59              |
| 3:SI:141:ARG:CZ    | 79:S2:191:A:H5''   | 2.33                     | 0.59              |
| 12:SH:133:LEU:HD23 | 12:SH:134:VAL:HG13 | 1.85                     | 0.59              |
| 85:L5:909:A:N1     | 85:L5:910:G:O6     | 2.35                     | 0.59              |
| 85:L5:958:G:H21    | 26:LE:125:LEU:H    | 1.50                     | 0.59              |
| 85:L5:1315:C:N4    | 85:L5:1316:G:O6    | 2.35                     | 0.59              |
| 21:L8:148:A:H2'    | 21:L8:149:G:C8     | 2.38                     | 0.59              |
| 23:LB:307:TYR:OH   | 23:LB:364:ASP:OD2  | 2.19                     | 0.59              |
| 26:LE:258:LEU:HD22 | 26:LE:261:ILE:HD11 | 1.85                     | 0.59              |
| 33:LM:42:CYS:O     | 33:LM:44:GLN:NE2   | 2.35                     | 0.59              |
| 41:LU:116:GLN:NE2  | 41:LU:117:ILE:O    | 2.36                     | 0.59              |
| 53:Lh:88:THR:HB    | 53:Lh:91:MET:HG3   | 1.84                     | 0.59              |
| 58:Lm:80:PRO:HA    | 58:Lm:83:ARG:NE    | 2.17                     | 0.59              |
| 63:Lz:23:ARG:HH12  | 63:Lz:172:VAL:HB   | 1.67                     | 0.59              |
| 65:SD:27:ARG:NH2   | 79:S2:1498:A:OP2   | 2.36                     | 0.59              |
| 79:S2:352:U:H2'    | 79:S2:353:C:C6     | 2.37                     | 0.59              |
| 79:S2:841:G:HO2'   | 79:S2:842:C:H6     | 1.49                     | 0.59              |
| 79:S2:1217:A:H2'   | 79:S2:1218:C:C6    | 2.38                     | 0.59              |
| 79:S2:1757:G:C8    | 79:S2:1758:G:H1'   | 2.38                     | 0.59              |
| 81:AP:49:C:H2'     | 81:AP:50:U:C6      | 2.38                     | 0.59              |
| 2:sE:86:PHE:CD2    | 2:sE:87:MET:HG3    | 2.38                     | 0.58              |
| 6:sG:183:ARG:NH2   | 79:s2:317:C:OP2    | 2.35                     | 0.58              |
| 8:sY:88:LYS:HB3    | 8:sY:97:TYR:CE2    | 2.38                     | 0.58              |
| 16:sN:38:TYR:HE1   | 16:sN:78:LYS:HG2   | 1.68                     | 0.58              |
| 22:lA:236:GLY:N    | 85:l5:3687:A:O2'   | 2.36                     | 0.58              |
| 42:IV:42:VAL:HG13  | 42:IV:61:VAL:HG12  | 1.84                     | 0.58              |
| 66:sF:22:LYS:HG3   | 66:sF:23:TRP:CD2   | 2.37                     | 0.58              |
| 70:sS:86:ARG:HD2   | 70:sS:106:LYS:HE2  | 1.84                     | 0.58              |
| 79:s2:533:A:H61    | 79:s2:550:C:H42    | 1.51                     | 0.58              |
| 79:s2:1756:C:N4    | 79:s2:1776:G:O6    | 2.36                     | 0.58              |
| 80:cB:116:THR:C    | 80:cB:497:MET:HE1  | 2.28                     | 0.58              |
| 83:ls:27:CYS:SG    | 83:ls:28:PHE:N     | 2.70                     | 0.58              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 85:l5:1183:C:H2'   | 85:l5:1184:A:C8    | 2.38                     | 0.58              |
| 85:l5:1628:C:H2'   | 85:l5:1629:G:C8    | 2.38                     | 0.58              |
| 85:l5:1667:G:N1    | 85:l5:2281:U:OP2   | 2.28                     | 0.58              |
| 85:l5:2540:C:H2'   | 85:l5:2541:G:H8    | 1.68                     | 0.58              |
| 80:CB:290:CYS:HA   | 80:CB:294:LEU:HB2  | 1.84                     | 0.58              |
| 2:SE:126:VAL:HA    | 2:SE:141:THR:HA    | 1.85                     | 0.58              |
| 4:SL:86:ILE:N      | 4:SL:111:VAL:O     | 2.33                     | 0.58              |
| 7:SJ:39:ASN:ND2    | 79:S2:642:U:H3'    | 2.18                     | 0.58              |
| 12:SH:154:ILE:HB   | 12:SH:185:VAL:HG12 | 1.85                     | 0.58              |
| 15:SC:263:LYS:HD3  | 15:SC:264:SER:N    | 2.18                     | 0.58              |
| 85:L5:1701:A:OP1   | 85:L5:1703:C:N4    | 2.36                     | 0.58              |
| 85:L5:1751:A:H2'   | 85:L5:1752:G:H8    | 1.67                     | 0.58              |
| 85:L5:3842:C:H1'   | 42:LV:52:LEU:HD12  | 1.85                     | 0.58              |
| 85:L5:3893:C:H2'   | 85:L5:3894:A:C8    | 2.37                     | 0.58              |
| 85:L5:4622:A:HO2'  | 23:LB:13:SER:HG    | 1.51                     | 0.58              |
| 85:L5:4987:C:OP1   | 23:LB:116:ARG:NH1  | 2.36                     | 0.58              |
| 24:LC:7:LEU:HG     | 24:LC:21:ASN:HB3   | 1.84                     | 0.58              |
| 26:LE:62:MET:HE2   | 26:LE:62:MET:HA    | 1.84                     | 0.58              |
| 27:LF:127:LYS:HG3  | 27:LF:128:ALA:N    | 2.18                     | 0.58              |
| 51:Lf:104:MET:SD   | 51:Lf:104:MET:N    | 2.75                     | 0.58              |
| 64:SR:126:MET:HE1  | 79:S2:1125:C:C1'   | 2.33                     | 0.58              |
| 66:SF:45:TYR:HD1   | 66:SF:45:TYR:O     | 1.86                     | 0.58              |
| 67:SK:8:ARG:NH2    | 79:S2:1314:U:O2'   | 2.36                     | 0.58              |
| 70:SS:30:ILE:H     | 70:SS:30:ILE:HD12  | 1.68                     | 0.58              |
| 79:S2:60:A:N3      | 79:S2:316:G:O2'    | 2.33                     | 0.58              |
| 79:S2:520:A:O2'    | 79:S2:825:A:N3     | 2.36                     | 0.58              |
| 79:S2:634:A:H2'    | 79:S2:635:G:C8     | 2.38                     | 0.58              |
| 79:S2:1620:A:H1'   | 79:S2:1624:U:OP2   | 2.03                     | 0.58              |
| 1:cH:45:ALA:HB1    | 9:se:55:PRO:HB3    | 1.84                     | 0.58              |
| 2:sE:188:ASN:HB3   | 2:sE:191:ARG:HD3   | 1.85                     | 0.58              |
| 3:sI:149:TYR:OH    | 79:s2:190:G:OP1    | 2.11                     | 0.58              |
| 5:sX:126:ALA:O     | 5:sX:128:VAL:N     | 2.36                     | 0.58              |
| 6:sG:22:ARG:HD3    | 6:sG:22:ARG:H      | 1.68                     | 0.58              |
| 21:l8:60:G:O6      | 21:l8:96:C:O2'     | 2.20                     | 0.58              |
| 26:lE:264:ILE:HG13 | 26:lE:267:LEU:HD21 | 1.83                     | 0.58              |
| 32:lL:158:ARG:NH2  | 85:l5:1378:C:N3    | 2.50                     | 0.58              |
| 33:lM:136:LEU:HD12 | 33:lM:137:LYS:NZ   | 2.16                     | 0.58              |
| 39:lS:83:ARG:HH21  | 40:lT:156:TYR:HA   | 1.68                     | 0.58              |
| 47:lB:57:MET:HE1   | 85:l5:1828:C:H1'   | 1.85                     | 0.58              |
| 70:sS:30:ILE:H     | 70:sS:30:ILE:HD12  | 1.69                     | 0.58              |
| 75:sg:42:MET:HE3   | 75:sg:92:LEU:HD11  | 1.85                     | 0.58              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 75:sg:165:ILE:HG12 | 75:sg:179:LEU:HD21 | 1.85                     | 0.58              |
| 77:sZ:47:LEU:HB2   | 77:sZ:80:ARG:H     | 1.68                     | 0.58              |
| 79:s2:556:U:H3'    | 79:s2:557:U:H4'    | 1.84                     | 0.58              |
| 79:s2:1828:C:H2'   | 79:s2:1829:G:C8    | 2.37                     | 0.58              |
| 80:cB:309:LYS:O    | 80:cB:312:THR:OG1  | 2.19                     | 0.58              |
| 2:SE:187:ALA:N     | 79:S2:809:A:OP1    | 2.36                     | 0.58              |
| 6:SG:58:LYS:HA     | 6:SG:107:SER:HB3   | 1.86                     | 0.58              |
| 7:SJ:145:PRO:HD2   | 79:S2:522:A:H5''   | 1.85                     | 0.58              |
| 10:SA:11:LYS:HZ2   | 10:SA:13:GLU:H     | 1.51                     | 0.58              |
| 15:SC:253:PRO:HA   | 15:SC:256:TRP:CD1  | 2.38                     | 0.58              |
| 15:SC:263:LYS:HD3  | 15:SC:264:SER:H    | 1.67                     | 0.58              |
| 16:SN:72:LEU:HD12  | 16:SN:75:LEU:HD23  | 1.85                     | 0.58              |
| 17:SO:102:GLY:O    | 17:SO:106:LYS:NZ   | 2.28                     | 0.58              |
| 85:L5:510:U:H5'    | 46:La:86:THR:HG22  | 1.85                     | 0.58              |
| 85:L5:733:A:N6     | 85:L5:933:G:O6     | 2.32                     | 0.58              |
| 85:L5:1332:C:H5''  | 50:Le:29:VAL:HB    | 1.85                     | 0.58              |
| 85:L5:3880:G:H2'   | 85:L5:3881:G:C8    | 2.38                     | 0.58              |
| 23:LB:369:ASP:OD2  | 87:LW:17:HIS:NE2   | 2.36                     | 0.58              |
| 28:LG:175:ARG:CZ   | 28:LG:230:TYR:HB3  | 2.33                     | 0.58              |
| 33:LM:104:MET:HE3  | 35:LO:199:HIS:CD2  | 2.38                     | 0.58              |
| 41:LU:105:ASN:OD1  | 41:LU:106:SER:N    | 2.36                     | 0.58              |
| 44:LY:58:VAL:HG23  | 44:LY:59:ARG:HG2   | 1.86                     | 0.58              |
| 62:Lr:66:ARG:NH1   | 62:Lr:75:THR:O     | 2.36                     | 0.58              |
| 70:SS:87:GLN:HE21  | 79:S2:1612:G:H1'   | 1.68                     | 0.58              |
| 84:Lt:106:PHE:HA   | 84:Lt:109:ILE:HD13 | 1.86                     | 0.58              |
| 87:IW:113:LYS:HD3  | 87:IW:116:LYS:HE3  | 1.85                     | 0.58              |
| 5:sX:5:ARG:HH21    | 79:s2:1157:G:C1'   | 2.16                     | 0.58              |
| 7:sJ:93:LYS:HB2    | 7:sJ:96:TYR:CE1    | 2.37                     | 0.58              |
| 14:sa:5:ARG:HB3    | 79:s2:1865:C:C6    | 2.37                     | 0.58              |
| 19:sb:42:LYS:HD3   | 19:sb:42:LYS:H     | 1.68                     | 0.58              |
| 23:lB:103:LYS:NZ   | 85:l5:4725:C:OP1   | 2.36                     | 0.58              |
| 25:lD:8:LYS:NZ     | 85:l5:4263:C:O3'   | 2.36                     | 0.58              |
| 26:lE:62:MET:HE2   | 26:lE:62:MET:HA    | 1.85                     | 0.58              |
| 40:lT:35:LYS:N     | 40:lT:38:ASP:OD2   | 2.36                     | 0.58              |
| 57:ll:41:ARG:NH1   | 85:l5:2431:A:OP1   | 2.36                     | 0.58              |
| 62:lr:5:LEU:HD22   | 62:lr:5:LEU:H      | 1.67                     | 0.58              |
| 72:sU:78:ASP:OD1   | 74:sd:54:LYS:NZ    | 2.26                     | 0.58              |
| 78:sf:118:ARG:NE   | 78:sf:134:SER:OG   | 2.35                     | 0.58              |
| 79:s2:940:U:H2'    | 79:s2:941:C:C6     | 2.39                     | 0.58              |
| 79:s2:1749:G:OP2   | 87:IW:74:ARG:NH1   | 2.36                     | 0.58              |
| 80:cB:554:LEU:O    | 80:cB:558:LEU:HD23 | 2.03                     | 0.58              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 85:l5:662:C:N4     | 85:l5:663:G:O6     | 2.37                     | 0.58              |
| 85:l5:2901:G:H2'   | 85:l5:2902:G:H5''  | 1.83                     | 0.58              |
| 85:l5:3964:U:O2'   | 85:l5:4048:A:N1    | 2.35                     | 0.58              |
| 85:L5:262:G:H2'    | 85:L5:263:G:C8     | 2.38                     | 0.58              |
| 85:L5:2623:A:OP1   | 41:LU:101:ARG:NE   | 2.36                     | 0.58              |
| 85:L5:3633:C:H2'   | 85:L5:3634:G:C8    | 2.37                     | 0.58              |
| 85:L5:4537:C:H2'   | 85:L5:4538:G:H8    | 1.66                     | 0.58              |
| 23:LB:332:MET:SD   | 23:LB:332:MET:N    | 2.69                     | 0.58              |
| 24:LC:153:VAL:HG22 | 24:LC:257:PHE:CD1  | 2.38                     | 0.58              |
| 27:LF:154:ILE:HG21 | 27:LF:190:LEU:HD11 | 1.84                     | 0.58              |
| 37:LQ:35:LEU:O     | 37:LQ:39:THR:OG1   | 2.15                     | 0.58              |
| 52:Lg:87:VAL:O     | 52:Lg:91:ILE:HG12  | 2.03                     | 0.58              |
| 61:Lp:25:MET:HE1   | 79:S2:1040:G:H5''  | 1.84                     | 0.58              |
| 79:S2:141:A:H4'    | 79:S2:142:C:H3'    | 1.85                     | 0.58              |
| 79:S2:1206:G:O6    | 79:S2:1208:A:N6    | 2.36                     | 0.58              |
| 79:S2:1713:C:H2'   | 79:S2:1714:U:C6    | 2.38                     | 0.58              |
| 79:S2:1802:C:H2'   | 79:S2:1803:U:H6    | 1.67                     | 0.58              |
| 10:sA:178:LEU:O    | 10:sA:182:VAL:HG22 | 2.02                     | 0.58              |
| 12:sH:42:GLU:N     | 12:sH:42:GLU:OE1   | 2.36                     | 0.58              |
| 22:lA:204:MET:HE1  | 22:lA:208:GLU:OE2  | 2.03                     | 0.58              |
| 25:lD:120:GLU:N    | 25:lD:120:GLU:OE1  | 2.36                     | 0.58              |
| 26:lE:183:ARG:HD2  | 85:l5:4936:G:C4    | 2.38                     | 0.58              |
| 33:lM:6:PHE:H      | 33:lM:11:ARG:NH2   | 2.00                     | 0.58              |
| 43:lX:47:ARG:HA    | 43:lX:47:ARG:HH11  | 1.69                     | 0.58              |
| 44:lY:112:ASP:OD1  | 44:lY:115:ARG:N    | 2.25                     | 0.58              |
| 46:la:131:ARG:NH1  | 46:la:135:GLU:OE2  | 2.37                     | 0.58              |
| 49:ld:54:MET:HA    | 49:ld:54:MET:HE2   | 1.86                     | 0.58              |
| 67:sK:5:LYS:O      | 67:sK:9:ILE:HG12   | 2.03                     | 0.58              |
| 75:sg:59:LEU:HD11  | 75:sg:90:TRP:CD2   | 2.39                     | 0.58              |
| 75:sg:139:LYS:HG3  | 75:sg:140:TYR:N    | 2.18                     | 0.58              |
| 75:sg:249:CYS:HB3  | 75:sg:258:ILE:HG23 | 1.84                     | 0.58              |
| 79:s2:1628:C:H2'   | 79:s2:1629:C:C6    | 2.38                     | 0.58              |
| 80:cB:645:GLU:OE2  | 80:cB:665:ILE:HG22 | 2.04                     | 0.58              |
| 81:aP:1:G:H2'      | 81:aP:2:U:C6       | 2.38                     | 0.58              |
| 81:aP:30:G:H2'     | 81:aP:31:C:H6      | 1.68                     | 0.58              |
| 85:l5:1577:G:O2'   | 85:l5:1612:G:H4'   | 2.03                     | 0.58              |
| 85:l5:1874:A:H4'   | 85:l5:4217:G:H22   | 1.67                     | 0.58              |
| 85:l5:2275:G:H2'   | 85:l5:2276:A:H8    | 1.67                     | 0.58              |
| 3:SI:141:ARG:CZ    | 3:SI:141:ARG:HA    | 2.33                     | 0.58              |
| 6:SG:50:VAL:HG21   | 6:SG:111:LEU:HD12  | 1.84                     | 0.58              |
| 7:SJ:109:ARG:NH1   | 7:SJ:146:SER:OG    | 2.36                     | 0.58              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 8:SY:120:THR:O     | 8:SY:124:ASN:ND2  | 2.23                     | 0.58              |
| 11:SB:168:MET:SD   | 11:SB:169:MET:N   | 2.76                     | 0.58              |
| 12:SH:82:GLU:O     | 12:SH:85:LYS:HG3  | 2.04                     | 0.58              |
| 13:SV:3:ASN:ND2    | 15:SC:175:GLY:O   | 2.33                     | 0.58              |
| 18:SW:19:LYS:NZ    | 79:S2:1152:U:O2'  | 2.34                     | 0.58              |
| 85:L5:1566:C:H2'   | 85:L5:1567:U:H6   | 1.68                     | 0.58              |
| 85:L5:1683:U:H2'   | 85:L5:1684:A:C8   | 2.37                     | 0.58              |
| 85:L5:2029:A:H2'   | 85:L5:2030:A:C8   | 2.38                     | 0.58              |
| 85:L5:2611:A:H2'   | 85:L5:2612:G:C8   | 2.38                     | 0.58              |
| 85:L5:3717:A:H2'   | 85:L5:3718:A:H8   | 1.68                     | 0.58              |
| 85:L5:3788:C:N4    | 85:L5:3812:C:O4'  | 2.36                     | 0.58              |
| 85:L5:4139:G:H21   | 85:L5:4140:C:H41  | 1.51                     | 0.58              |
| 85:L5:4346:U:O2'   | 60:Lo:80:LYS:O    | 2.15                     | 0.58              |
| 85:L5:4638:U:H3'   | 85:L5:4639:G:H21  | 1.67                     | 0.58              |
| 40:LT:111:GLU:O    | 40:LT:115:LYS:HG3 | 2.03                     | 0.58              |
| 42:LV:26:ILE:O     | 42:LV:37:LEU:N    | 2.35                     | 0.58              |
| 76:SM:96:ARG:NE    | 76:SM:97:GLU:OE2  | 2.35                     | 0.58              |
| 78:Sf:102:VAL:HG23 | 78:Sf:104:LYS:NZ  | 2.18                     | 0.58              |
| 79:S2:526:A:H2     | 79:S2:559:G:H22   | 1.49                     | 0.58              |
| 79:S2:882:U:H1'    | 79:S2:905:C:C2    | 2.38                     | 0.58              |
| 79:S2:1501:C:H2'   | 79:S2:1502:C:H6   | 1.67                     | 0.58              |
| 5:sX:59:ALA:HB1    | 5:sX:114:ASP:HB2  | 1.85                     | 0.58              |
| 5:sX:68:LYS:NZ     | 79:s2:617:G:OP2   | 2.29                     | 0.58              |
| 8:sY:8:ARG:NH1     | 79:s2:836:G:OP1   | 2.36                     | 0.58              |
| 10:sA:12:GLU:HA    | 10:sA:15:VAL:HG22 | 1.85                     | 0.58              |
| 11:sB:151:ARG:HB3  | 64:sR:133:GLY:H   | 1.68                     | 0.58              |
| 13:sV:41:LYS:HD3   | 13:sV:41:LYS:N    | 2.17                     | 0.58              |
| 23:lB:124:LYS:NZ   | 85:l5:5063:G:O6   | 2.34                     | 0.58              |
| 27:lF:31:LYS:HE3   | 85:l5:1439:C:P    | 2.43                     | 0.58              |
| 33:lM:38:VAL:HG21  | 33:lM:50:MET:HE3  | 1.86                     | 0.58              |
| 39:lS:26:PRO:HB2   | 39:lS:28:TYR:HE1  | 1.69                     | 0.58              |
| 39:lS:131:GLU:N    | 39:lS:131:GLU:OE1 | 2.36                     | 0.58              |
| 64:sR:10:LYS:HE2   | 79:s2:1367:U:H1'  | 1.85                     | 0.58              |
| 66:sF:135:ARG:NH2  | 66:sF:136:ARG:HG3 | 2.19                     | 0.58              |
| 69:sQ:8:GLN:OE1    | 69:sQ:27:ARG:NH1  | 2.36                     | 0.58              |
| 70:sS:133:GLY:HA2  | 79:s2:1622:U:H4'  | 1.86                     | 0.58              |
| 74:sd:30:LEU:O     | 79:s2:1256:G:N2   | 2.27                     | 0.58              |
| 85:l5:188:G:N2     | 85:l5:189:G:O6    | 2.37                     | 0.58              |
| 85:l5:1089:G:H2'   | 85:l5:1090:G:H8   | 1.68                     | 0.58              |
| 85:l5:1999:A:H2'   | 85:l5:2000:G:C4   | 2.39                     | 0.58              |
| 85:l5:3610:A:H2'   | 85:l5:3611:A:H8   | 1.69                     | 0.58              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 85:l5:3641:U:OP2   | 85:l5:3646:A:N6    | 2.36                     | 0.58              |
| 85:l5:3848:U:H4'   | 85:l5:4634:U:C4    | 2.38                     | 0.58              |
| 80:CB:801:ARG:HG3  | 80:CB:806:GLY:HA2  | 1.84                     | 0.58              |
| 6:SG:32:MET:SD     | 6:SG:32:MET:N      | 2.73                     | 0.58              |
| 6:SG:183:ARG:NH2   | 79:S2:316:G:H3'    | 2.17                     | 0.58              |
| 10:SA:196:GLU:H    | 10:SA:196:GLU:CD   | 2.07                     | 0.58              |
| 11:SB:72:ALA:HB3   | 17:SO:128:ARG:HH22 | 1.68                     | 0.58              |
| 11:SB:144:LYS:HB3  | 11:SB:208:HIS:CG   | 2.38                     | 0.58              |
| 12:SH:18:GLU:N     | 12:SH:18:GLU:OE1   | 2.35                     | 0.58              |
| 12:SH:71:SER:O     | 12:SH:74:LYS:NZ    | 2.36                     | 0.58              |
| 15:SC:169:TYR:OH   | 15:SC:175:GLY:O    | 2.15                     | 0.58              |
| 85:L5:415:G:O6     | 21:L8:20:A:N6      | 2.37                     | 0.58              |
| 85:L5:995:C:O2'    | 85:L5:1049:C:N4    | 2.37                     | 0.58              |
| 85:L5:1824:G:H2'   | 85:L5:1825:A:C8    | 2.38                     | 0.58              |
| 85:L5:1906:U:H2'   | 85:L5:1907:A:H8    | 1.69                     | 0.58              |
| 85:L5:2083:C:OP2   | 37:LQ:14:ARG:NH2   | 2.36                     | 0.58              |
| 85:L5:4742:G:H2'   | 85:L5:4743:G:H8    | 1.68                     | 0.58              |
| 20:L7:37:G:N2      | 20:L7:41:G:N3      | 2.52                     | 0.58              |
| 21:L8:93:C:H3'     | 55:Lj:72:ARG:NH1   | 2.18                     | 0.58              |
| 34:LN:8:GLN:OE1    | 34:LN:50:ARG:NH2   | 2.36                     | 0.58              |
| 55:Lj:74:PHE:HA    | 55:Lj:78:PHE:CE2   | 2.38                     | 0.58              |
| 68:SP:121:ILE:HD12 | 70:SS:120:HIS:HD2  | 1.68                     | 0.58              |
| 71:ST:28:LEU:HD13  | 71:ST:54:TYR:HE1   | 1.68                     | 0.58              |
| 72:SU:23:THR:HG23  | 72:SU:113:GLU:OE1  | 2.02                     | 0.58              |
| 72:SU:50:VAL:HA    | 72:SU:91:LEU:CD2   | 2.32                     | 0.58              |
| 73:Sc:11:LEU:HD22  | 73:Sc:55:VAL:HG22  | 1.84                     | 0.58              |
| 73:Sc:31:ARG:H     | 73:Sc:43:ILE:HD12  | 1.68                     | 0.58              |
| 79:S2:28:U:H2'     | 79:S2:29:G:C8      | 2.37                     | 0.58              |
| 83:Ls:37:SER:HA    | 83:Ls:40:MET:HG3   | 1.84                     | 0.58              |
| 1:cH:109:TYR:HA    | 1:cH:114:ALA:HB2   | 1.84                     | 0.58              |
| 3:sI:150:ASP:O     | 3:sI:153:LYS:HG3   | 2.04                     | 0.58              |
| 3:sI:161:LEU:HD13  | 3:sI:195:LEU:HD12  | 1.85                     | 0.58              |
| 4:sL:73:LEU:HD12   | 4:sL:74:SER:N      | 2.18                     | 0.58              |
| 6:sG:20:ASP:CG     | 6:sG:22:ARG:HE     | 2.11                     | 0.58              |
| 8:sY:25:ILE:HD11   | 8:sY:60:PHE:HZ     | 1.68                     | 0.58              |
| 21:l8:5:U:H2'      | 21:l8:6:C:C6       | 2.38                     | 0.58              |
| 21:l8:96:C:H2'     | 21:l8:97:A:C8      | 2.38                     | 0.58              |
| 24:lC:146:GLU:N    | 24:lC:146:GLU:OE1  | 2.36                     | 0.58              |
| 24:lC:284:MET:CE   | 37:lQ:28:LEU:HB3   | 2.30                     | 0.58              |
| 37:lQ:15:ARG:NH1   | 37:lQ:52:PHE:O     | 2.37                     | 0.58              |
| 48:lc:21:VAL:HG23  | 48:lc:99:PRO:HA    | 1.85                     | 0.58              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 55:lj:43:ARG:NH2  | 85:l5:55:G:OP2     | 2.36                     | 0.58              |
| 58:lm:126:LYS:HE3 | 58:lm:128:LYS:HB3  | 1.85                     | 0.58              |
| 64:sR:45:LYS:HB3  | 79:s2:1369:A:N6    | 2.19                     | 0.58              |
| 70:sS:78:LYS:NZ   | 71:sT:32:GLU:HB2   | 2.18                     | 0.58              |
| 71:sT:41:LYS:NZ   | 79:s2:1568:C:O3'   | 2.31                     | 0.58              |
| 79:s2:544:G:H2'   | 79:s2:545:A:C8     | 2.39                     | 0.58              |
| 79:s2:1447:G:H2'  | 79:s2:1448:A:H8    | 1.68                     | 0.58              |
| 80:cB:184:ASN:O   | 80:cB:188:ILE:HG23 | 2.03                     | 0.58              |
| 80:cB:249:ARG:HA  | 80:cB:252:LYS:HG2  | 1.86                     | 0.58              |
| 81:aP:7:G:HO2'    | 81:aP:49:C:H6      | 1.51                     | 0.58              |
| 82:pE:58:A:O2'    | 82:pE:61:C:N4      | 2.37                     | 0.58              |
| 83:ls:32:ALA:O    | 83:ls:85:ASN:ND2   | 2.37                     | 0.58              |
| 85:l5:93:G:H2'    | 85:l5:94:A:C8      | 2.39                     | 0.58              |
| 85:l5:513:U:O2'   | 85:l5:646:G:O6     | 2.18                     | 0.58              |
| 85:l5:1961:G:O2'  | 85:l5:2025:A:N6    | 2.37                     | 0.58              |
| 85:l5:2468:U:O2   | 85:l5:2506:G:N1    | 2.36                     | 0.58              |
| 85:l5:4629:U:H2'  | 85:l5:4630:G:H8    | 1.68                     | 0.58              |
| 80:CB:145:GLN:OE1 | 80:CB:500:SER:OG   | 2.19                     | 0.58              |
| 80:CB:284:LYS:HD2 | 80:CB:285:LEU:N    | 2.19                     | 0.58              |
| 2:SE:105:THR:O    | 2:SE:245:ARG:NH2   | 2.37                     | 0.58              |
| 4:SL:86:ILE:HG22  | 4:SL:111:VAL:HG12  | 1.84                     | 0.58              |
| 10:SA:33:GLN:HE21 | 13:SV:64:GLU:CD    | 2.12                     | 0.58              |
| 11:SB:33:VAL:HG11 | 11:SB:67:PHE:HE2   | 1.68                     | 0.58              |
| 11:SB:89:GLU:OE1  | 11:SB:99:ASN:N     | 2.36                     | 0.58              |
| 15:SC:68:ARG:HE   | 15:SC:277:HIS:CD2  | 2.22                     | 0.58              |
| 85:L5:452:A:H62   | 85:L5:1293:G:H3'   | 1.68                     | 0.58              |
| 85:L5:1211:G:H2'  | 85:L5:1212:G:H8    | 1.67                     | 0.58              |
| 85:L5:1314:C:O5'  | 50:Le:27:ARG:NH2   | 2.35                     | 0.58              |
| 85:L5:1734:G:N2   | 85:L5:1735:U:O4    | 2.34                     | 0.58              |
| 85:L5:1823:G:H4'  | 25:LD:45:ASN:HB2   | 1.84                     | 0.58              |
| 85:L5:2059:C:H2'  | 85:L5:2060:G:H8    | 1.69                     | 0.58              |
| 85:L5:2377:C:H2'  | 85:L5:2378:G:O4'   | 2.03                     | 0.58              |
| 85:L5:4101:C:C6   | 85:L5:4104:G:H4'   | 2.37                     | 0.58              |
| 85:L5:4742:G:H2'  | 85:L5:4743:G:C8    | 2.39                     | 0.58              |
| 28:LG:38:ASN:ND2  | 28:LG:43:GLN:OE1   | 2.36                     | 0.58              |
| 36:LP:69:ARG:HA   | 36:LP:80:GLN:HA    | 1.85                     | 0.58              |
| 54:Li:43:MET:O    | 54:Li:47:VAL:HG12  | 2.04                     | 0.58              |
| 61:Lp:83:ILE:HD12 | 61:Lp:84:ARG:N     | 2.17                     | 0.58              |
| 74:Sd:8:TRP:HZ3   | 79:S2:1512:C:H5''  | 1.69                     | 0.58              |
| 79:S2:109:U:H2'   | 79:S2:110:U:C6     | 2.39                     | 0.58              |
| 79:S2:1133:A:H2'  | 79:S2:1134:G:H8    | 1.68                     | 0.58              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 79:S2:1174:U:H2'  | 79:S2:1175:G:H8    | 1.69                     | 0.58              |
| 83:Ls:65:ILE:HA   | 83:Ls:69:LEU:HD23  | 1.85                     | 0.58              |
| 1:CH:118:ASN:ND2  | 79:S2:534:G:H4'    | 2.19                     | 0.58              |
| 1:cH:106:ILE:O    | 1:cH:110:GLU:HG3   | 2.04                     | 0.58              |
| 6:sG:54:GLY:C     | 6:sG:110:ASN:OD1   | 2.46                     | 0.58              |
| 8:sY:10:ARG:HG3   | 8:sY:24:VAL:HG13   | 1.85                     | 0.58              |
| 8:sY:107:ARG:NH1  | 79:s2:505:G:H5''   | 2.18                     | 0.58              |
| 13:sV:16:LYS:H    | 15:sC:259:THR:HG21 | 1.67                     | 0.58              |
| 15:sC:63:VAL:O    | 15:sC:64:THR:OG1   | 2.19                     | 0.58              |
| 15:sC:178:HIS:CG  | 15:sC:200:ARG:HD2  | 2.38                     | 0.58              |
| 16:sN:70:LYS:O    | 16:sN:74:ILE:HG12  | 2.04                     | 0.58              |
| 18:sW:30:CYS:HA   | 18:sW:34:ILE:HD11  | 1.83                     | 0.58              |
| 25:ID:37:VAL:HG23 | 25:ID:50:ARG:HD2   | 1.85                     | 0.58              |
| 25:ID:84:PRO:HB3  | 25:ID:89:LYS:HA    | 1.86                     | 0.58              |
| 27:IF:64:MET:H    | 27:IF:64:MET:CE    | 2.16                     | 0.58              |
| 39:IS:61:ILE:H    | 39:IS:61:ILE:HD12  | 1.69                     | 0.58              |
| 64:sR:55:THR:O    | 64:sR:59:LYS:HG2   | 2.03                     | 0.58              |
| 70:sS:26:ILE:O    | 70:sS:30:ILE:HD12  | 2.04                     | 0.58              |
| 71:sT:18:LEU:HD23 | 71:sT:22:LEU:HD11  | 1.84                     | 0.58              |
| 71:sT:104:LEU:O   | 71:sT:108:GLU:HG2  | 2.03                     | 0.58              |
| 73:sc:23:SER:O    | 79:s2:1681:U:O2'   | 2.16                     | 0.58              |
| 75:sg:14:HIS:CE1  | 75:sg:18:VAL:HG22  | 2.36                     | 0.58              |
| 75:sg:65:PHE:HE1  | 75:sg:83:TRP:CD2   | 2.21                     | 0.58              |
| 76:sM:15:ASN:OD1  | 76:sM:16:THR:N     | 2.36                     | 0.58              |
| 79:s2:1201:U:H2'  | 79:s2:1202:U:C6    | 2.39                     | 0.58              |
| 79:s2:1657:G:H2'  | 79:s2:1658:G:H8    | 1.66                     | 0.58              |
| 80:cB:116:THR:HB  | 80:cB:497:MET:CE   | 2.34                     | 0.58              |
| 80:cB:675:ILE:O   | 80:cB:679:VAL:HG12 | 2.03                     | 0.58              |
| 85:l5:120:A:N1    | 85:l5:148:C:O2'    | 2.35                     | 0.58              |
| 85:l5:2478:C:O2   | 85:l5:2591:A:O2'   | 2.21                     | 0.58              |
| 85:l5:2640:G:H2'  | 85:l5:2641:A:H8    | 1.69                     | 0.58              |
| 85:l5:3722:G:H2'  | 85:l5:3723:A:H8    | 1.69                     | 0.58              |
| 85:l5:4524:G:H2'  | 85:l5:4525:C:H6    | 1.69                     | 0.58              |
| 10:SA:164:ASN:OD1 | 10:SA:165:ASN:N    | 2.36                     | 0.58              |
| 14:Sa:15:ARG:HD2  | 14:Sa:15:ARG:H     | 1.69                     | 0.58              |
| 14:Sa:43:ASN:HB2  | 14:Sa:66:LYS:HE3   | 1.86                     | 0.58              |
| 85:L5:312:G:H1    | 85:L5:325:U:H3     | 1.52                     | 0.58              |
| 85:L5:1479:G:H2'  | 85:L5:1480:C:C6    | 2.38                     | 0.58              |
| 85:L5:1879:C:H2'  | 85:L5:1880:G:O4'   | 2.04                     | 0.58              |
| 85:L5:3599:A:H2'  | 85:L5:3600:G:H8    | 1.66                     | 0.58              |
| 85:L5:3938:G:OP1  | 34:LN:24:ARG:NH1   | 2.35                     | 0.58              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 85:L5:4218:U:P     | 40:LT:3:ASN:HD21   | 2.27                     | 0.58              |
| 20:L7:13:A:OP2     | 20:L7:66:G:N2      | 2.35                     | 0.58              |
| 25:LD:256:LYS:NZ   | 25:LD:257:PRO:O    | 2.36                     | 0.58              |
| 27:LF:70:ARG:HG3   | 27:LF:71:MET:HE2   | 1.85                     | 0.58              |
| 30:LI:174:THR:HG22 | 30:LI:176:PHE:H    | 1.68                     | 0.58              |
| 32:LL:181:SER:HA   | 32:LL:184:MET:CE   | 2.34                     | 0.58              |
| 45:LZ:76:ASN:OD1   | 45:LZ:77:TYR:N     | 2.36                     | 0.58              |
| 65:SD:46:THR:O     | 65:SD:84:VAL:HA    | 2.03                     | 0.58              |
| 69:SQ:97:GLN:HG3   | 69:SQ:105:LYS:HE2  | 1.86                     | 0.58              |
| 71:ST:63:HIS:NE2   | 79:S2:1542:C:OP1   | 2.37                     | 0.58              |
| 74:Sd:3:HIS:CE1    | 74:Sd:5:GLN:HB3    | 2.38                     | 0.58              |
| 75:Sg:38:LYS:HA    | 75:Sg:65:PHE:HA    | 1.86                     | 0.58              |
| 79:S2:199:C:O2'    | 79:S2:201:C:OP2    | 2.21                     | 0.58              |
| 79:S2:323:C:O2'    | 79:S2:325:C:N4     | 2.34                     | 0.58              |
| 79:S2:432:G:H2'    | 79:S2:433:A:H8     | 1.68                     | 0.58              |
| 79:S2:1407:U:H2'   | 79:S2:1408:U:H6    | 1.65                     | 0.58              |
| 79:S2:1688:C:H2'   | 79:S2:1689:C:H6    | 1.67                     | 0.58              |
| 1:cH:108:ASP:OD2   | 1:cH:114:ALA:N     | 2.37                     | 0.58              |
| 7:sJ:81:LEU:HD12   | 7:sJ:97:ILE:HD12   | 1.86                     | 0.58              |
| 8:sY:80:ASP:OD2    | 28:LG:225:ASN:HB2  | 2.03                     | 0.58              |
| 11:sB:111:CYS:SG   | 14:sa:68:TYR:HD2   | 2.26                     | 0.58              |
| 16:sN:19:ARG:NH2   | 16:sN:21:SER:OG    | 2.36                     | 0.58              |
| 26:lE:145:THR:O    | 26:lE:148:THR:HG23 | 2.03                     | 0.58              |
| 26:lE:226:ARG:HD2  | 26:lE:226:ARG:N    | 2.19                     | 0.58              |
| 28:IG:90:GLN:NE2   | 28:IG:94:GLN:OE1   | 2.36                     | 0.58              |
| 42:IV:52:LEU:HD23  | 42:IV:52:LEU:H     | 1.69                     | 0.58              |
| 76:sM:60:MET:HA    | 76:sM:63:LYS:HG2   | 1.84                     | 0.58              |
| 79:s2:1405:A:H2'   | 79:s2:1406:G:O4'   | 2.03                     | 0.58              |
| 79:s2:1407:U:H2'   | 79:s2:1408:U:C6    | 2.38                     | 0.58              |
| 80:cB:343:TRP:C    | 80:cB:343:TRP:CD1  | 2.82                     | 0.58              |
| 80:cB:422:SER:O    | 80:cB:425:LEU:HD22 | 2.04                     | 0.58              |
| 85:l5:425:U:H2'    | 85:l5:426:A:H8     | 1.69                     | 0.58              |
| 85:l5:1655:C:OP1   | 85:l5:1679:A:O2'   | 2.20                     | 0.58              |
| 85:l5:4492:U:O2'   | 85:l5:4512:U:O2    | 2.16                     | 0.58              |
| 85:l5:4699:U:H1'   | 85:l5:4700:A:H5''  | 1.84                     | 0.58              |
| 10:SA:110:ASN:OD1  | 79:S2:1350:U:O2'   | 2.21                     | 0.58              |
| 12:SH:170:VAL:HG13 | 12:SH:187:PHE:HD1  | 1.66                     | 0.58              |
| 17:SO:43:HIS:CD2   | 17:SO:55:ARG:HB2   | 2.39                     | 0.58              |
| 85:L5:230:G:OP1    | 44:LY:15:ARG:NH1   | 2.35                     | 0.58              |
| 85:L5:1636:U:H5''  | 85:L5:1637:A:H5'   | 1.86                     | 0.58              |
| 85:L5:2468:U:O2    | 85:L5:2506:G:N1    | 2.37                     | 0.58              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 85:L5:2870:A:H2'   | 85:L5:2871:A:C8    | 2.39                     | 0.58              |
| 85:L5:4096:C:O2'   | 85:L5:4100:C:N3    | 2.35                     | 0.58              |
| 85:L5:4102:C:P     | 85:L5:4106:G:C4    | 2.96                     | 0.58              |
| 85:L5:4967:A:H2'   | 85:L5:4968:A:H8    | 1.67                     | 0.58              |
| 25:LD:232:THR:HG22 | 25:LD:235:MET:SD   | 2.44                     | 0.58              |
| 25:LD:232:THR:OG1  | 25:LD:233:PRO:HD2  | 2.03                     | 0.58              |
| 41:LU:62:THR:HG1   | 41:LU:73:THR:HG1   | 1.52                     | 0.58              |
| 43:LX:90:ILE:HG22  | 43:LX:147:LEU:HD22 | 1.86                     | 0.58              |
| 46:La:71:PRO:HG2   | 46:La:108:TYR:HA   | 1.86                     | 0.58              |
| 64:SR:1:MET:HE1    | 79:S2:1467:C:H3'   | 1.86                     | 0.58              |
| 67:SK:31:LYS:NZ    | 67:SK:36:ALA:O     | 2.25                     | 0.58              |
| 67:SK:90:VAL:O     | 67:SK:95:ARG:NH2   | 2.36                     | 0.58              |
| 70:SS:62:ASP:HA    | 70:SS:65:GLU:OE1   | 2.03                     | 0.58              |
| 75:Sg:20:GLN:OE1   | 75:Sg:69:VAL:N     | 2.37                     | 0.58              |
| 75:Sg:152:SER:OG   | 75:Sg:196:ASN:O    | 2.16                     | 0.58              |
| 75:Sg:287:THR:N    | 75:Sg:301:GLY:O    | 2.37                     | 0.58              |
| 76:SM:44:LYS:HE2   | 78:Sf:129:GLY:HA2  | 1.85                     | 0.58              |
| 79:S2:1372:U:OP1   | 79:S2:1385:G:N2    | 2.31                     | 0.58              |
| 84:Lt:82:ILE:HG13  | 84:Lt:137:GLN:HE22 | 1.68                     | 0.58              |
| 1:cH:71:ASP:OD2    | 1:cH:72:ARG:N      | 2.37                     | 0.58              |
| 4:sL:84:ARG:CD     | 79:s2:374:G:H4'    | 2.30                     | 0.58              |
| 10:sA:124:VAL:HG22 | 10:sA:126:ASP:H    | 1.68                     | 0.58              |
| 15:sC:179:THR:OG1  | 15:sC:180:VAL:N    | 2.36                     | 0.58              |
| 16:sN:112:LYS:O    | 16:sN:116:ILE:HG13 | 2.04                     | 0.58              |
| 22:lA:70:LYS:C     | 22:lA:71:LYS:HD3   | 2.28                     | 0.58              |
| 23:lB:112:ASP:OD1  | 23:lB:113:GLU:N    | 2.36                     | 0.58              |
| 40:lT:74:ILE:HD11  | 40:lT:89:ILE:HD11  | 1.86                     | 0.58              |
| 40:lT:121:GLU:N    | 40:lT:121:GLU:OE1  | 2.37                     | 0.58              |
| 41:lU:80:LYS:HE2   | 41:lU:110:TYR:CE2  | 2.39                     | 0.58              |
| 42:lV:39:ILE:H     | 42:lV:39:ILE:HD12  | 1.69                     | 0.58              |
| 62:lr:108:MET:HA   | 62:lr:111:ILE:HB   | 1.85                     | 0.58              |
| 71:sT:129:ARG:NE   | 71:sT:129:ARG:CA   | 2.54                     | 0.58              |
| 71:sT:134:ILE:HA   | 71:sT:137:GLN:NE2  | 2.18                     | 0.58              |
| 79:s2:51:U:H2'     | 79:s2:52:G:H8      | 1.69                     | 0.58              |
| 79:s2:1354:G:H5'   | 79:s2:1355:C:OP2   | 2.04                     | 0.58              |
| 79:s2:1643:U:H2'   | 79:s2:1644:C:C6    | 2.39                     | 0.58              |
| 80:cB:337:LYS:C    | 80:cB:341:ARG:HH12 | 2.12                     | 0.58              |
| 85:l5:1961:G:N2    | 85:l5:2024:G:O2'   | 2.29                     | 0.58              |
| 85:l5:2448:G:OP2   | 85:l5:2510:G:N1    | 2.30                     | 0.58              |
| 85:l5:5018:C:H2'   | 85:l5:5019:A:C8    | 2.39                     | 0.58              |
| 80:CB:764:ASN:ND2  | 85:L5:2009:A:O4'   | 2.37                     | 0.58              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 13:SV:73:ALA:HB1  | 13:SV:78:ILE:HG13  | 1.85                     | 0.58              |
| 85:L5:253:G:H2'   | 85:L5:254:G:C8     | 2.39                     | 0.58              |
| 85:L5:1351:G:H2'  | 85:L5:1352:C:C6    | 2.39                     | 0.58              |
| 85:L5:2895:A:H2'  | 85:L5:2896:G:C8    | 2.39                     | 0.58              |
| 85:L5:3771:C:H2'  | 85:L5:3772:U:C6    | 2.39                     | 0.58              |
| 85:L5:3965:A:O2'  | 85:L5:4038:C:N3    | 2.37                     | 0.58              |
| 85:L5:4711:C:H2'  | 85:L5:4712:C:H6    | 1.68                     | 0.58              |
| 21:L8:138:C:H2'   | 21:L8:139:G:C8     | 2.39                     | 0.58              |
| 22:LA:108:PRO:HD3 | 61:Lp:90:LYS:HE2   | 1.86                     | 0.58              |
| 25:LD:51:MET:HE2  | 25:LD:146:LEU:HB2  | 1.85                     | 0.58              |
| 29:LH:18:ILE:HD11 | 29:LH:47:LEU:HD21  | 1.83                     | 0.58              |
| 30:LI:87:MET:HE1  | 30:LI:89:VAL:HG13  | 1.86                     | 0.58              |
| 34:LN:189:ARG:O   | 34:LN:193:ARG:HG3  | 2.03                     | 0.58              |
| 44:LY:82:ILE:HB   | 44:LY:85:VAL:HG22  | 1.86                     | 0.58              |
| 52:Lg:65:MET:N    | 52:Lg:65:MET:HE2   | 2.19                     | 0.58              |
| 61:Lp:61:MET:SD   | 61:Lp:61:MET:N     | 2.77                     | 0.58              |
| 64:SR:41:ILE:HD11 | 64:SR:47:ARG:HA    | 1.86                     | 0.58              |
| 70:SS:63:GLU:O    | 70:SS:67:VAL:HG12  | 2.04                     | 0.58              |
| 79:S2:455:A:H2'   | 79:S2:456:C:H6     | 1.69                     | 0.58              |
| 1:CH:131:LYS:HB2  | 1:CH:142:GLU:HB3   | 1.86                     | 0.58              |
| 1:cH:85:ARG:NH2   | 1:cH:91:THR:HA     | 2.18                     | 0.58              |
| 2:sE:87:MET:SD    | 2:sE:142:HIS:NE2   | 2.77                     | 0.58              |
| 3:sI:97:VAL:HG12  | 3:sI:100:CYS:HB3   | 1.85                     | 0.58              |
| 10:sA:7:VAL:HG21  | 13:sV:43:THR:HA    | 1.85                     | 0.58              |
| 11:sB:68:GLU:HB2  | 11:sB:83:LYS:HZ1   | 1.68                     | 0.58              |
| 12:sH:162:GLN:HB3 | 12:sH:165:ASN:HB3  | 1.86                     | 0.58              |
| 15:sC:210:PRO:HD3 | 15:sC:236:PHE:CE2  | 2.38                     | 0.58              |
| 17:sO:117:ARG:O   | 17:sO:121:ARG:HG2  | 2.03                     | 0.58              |
| 18:sW:80:ASP:OD2  | 79:s2:803:C:H4'    | 2.03                     | 0.58              |
| 21:l8:75:G:H2'    | 21:l8:76:C:C6      | 2.39                     | 0.58              |
| 22:lA:3:ARG:HH21  | 85:l5:1628:C:H42   | 1.51                     | 0.58              |
| 22:lA:113:VAL:O   | 22:lA:134:ALA:N    | 2.31                     | 0.58              |
| 25:ID:224:SER:OG  | 25:ID:225:GLN:OE1  | 2.21                     | 0.58              |
| 28:lG:41:ILE:HD12 | 28:lG:41:ILE:H     | 1.69                     | 0.58              |
| 29:IH:15:ASN:OD1  | 29:IH:16:VAL:HG13  | 2.04                     | 0.58              |
| 30:II:11:TYR:O    | 30:II:59:GLN:NE2   | 2.37                     | 0.58              |
| 30:II:55:ASP:CG   | 30:II:162:ARG:HH22 | 2.08                     | 0.58              |
| 41:IU:80:LYS:HG2  | 41:IU:110:TYR:CE2  | 2.39                     | 0.58              |
| 44:IY:58:VAL:O    | 44:IY:63:LYS:NZ    | 2.36                     | 0.58              |
| 45:IZ:115:LYS:O   | 45:IZ:119:GLU:HG3  | 2.03                     | 0.58              |
| 64:sR:3:ARG:NH1   | 79:s2:1467:C:H1'   | 2.18                     | 0.58              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 67:sK:31:LYS:HD2  | 67:sK:36:ALA:O     | 2.04                     | 0.58              |
| 71:sT:102:ARG:NH2 | 79:s2:1566:G:OP2   | 2.33                     | 0.58              |
| 75:sg:296:GLN:O   | 75:sg:311:GLN:NE2  | 2.36                     | 0.58              |
| 77:sZ:62:VAL:HA   | 77:sZ:65:TYR:CE1   | 2.38                     | 0.58              |
| 79:s2:1139:C:H2'  | 79:s2:1140:G:O4'   | 2.04                     | 0.58              |
| 79:s2:1825:A:H62  | 81:aP:37:A:H2      | 1.50                     | 0.58              |
| 85:l5:2406:G:O6   | 85:l5:2785:C:N4    | 2.37                     | 0.58              |
| 85:l5:2869:U:O2'  | 85:l5:2881:A:N7    | 2.32                     | 0.58              |
| 85:l5:3710:G:N2   | 85:l5:3711:A:N7    | 2.51                     | 0.58              |
| 80:CB:45:ILE:CD1  | 80:CB:78:PHE:HB2   | 2.33                     | 0.58              |
| 5:SX:112:VAL:HG23 | 79:S2:621:C:OP1    | 2.02                     | 0.58              |
| 85:L5:246:G:OP2   | 44:LY:132:LYS:NZ   | 2.37                     | 0.58              |
| 85:L5:457:G:H2'   | 85:L5:458:C:C6     | 2.39                     | 0.58              |
| 85:L5:2699:C:H2'  | 85:L5:2700:G:H8    | 1.67                     | 0.58              |
| 85:L5:3710:G:H21  | 85:L5:3713:U:H3    | 1.52                     | 0.58              |
| 85:L5:3967:G:OP2  | 85:L5:3969:G:N2    | 2.37                     | 0.58              |
| 85:L5:4069:U:H2'  | 85:L5:4070:U:C6    | 2.37                     | 0.58              |
| 85:L5:5057:C:H2'  | 85:L5:5058:A:C8    | 2.39                     | 0.58              |
| 20:L7:57:C:H2'    | 20:L7:58:A:C8      | 2.38                     | 0.58              |
| 24:LC:261:ASP:O   | 24:LC:265:GLY:N    | 2.36                     | 0.58              |
| 27:LF:184:ILE:HA  | 27:LF:189:ASP:OD2  | 2.03                     | 0.58              |
| 30:LI:99:ILE:HB   | 30:LI:123:GLN:NE2  | 2.19                     | 0.58              |
| 34:LN:160:GLU:HG2 | 34:LN:161:MET:CE   | 2.34                     | 0.58              |
| 39:LS:80:ILE:HG22 | 39:LS:129:VAL:HG13 | 1.85                     | 0.58              |
| 62:Lr:31:ASN:ND2  | 62:Lr:40:TYR:O     | 2.37                     | 0.58              |
| 69:SQ:81:ILE:O    | 69:SQ:84:ILE:HG13  | 2.03                     | 0.58              |
| 79:S2:1740:C:H2'  | 79:S2:1741:U:C6    | 2.39                     | 0.58              |
| 87:IW:4:GLU:N     | 87:IW:4:GLU:OE1    | 2.37                     | 0.58              |
| 2:sE:149:TYR:HE1  | 6:sG:205:GLU:HG3   | 1.69                     | 0.57              |
| 5:sX:8:ARG:NH1    | 79:s2:682:U:OP2    | 2.37                     | 0.57              |
| 6:sG:57:ASP:OD1   | 6:sG:58:LYS:N      | 2.37                     | 0.57              |
| 18:sW:71:LYS:NZ   | 79:s2:1155:U:O3'   | 2.37                     | 0.57              |
| 22:lA:24:LYS:HG3  | 22:lA:49:ILE:HD12  | 1.85                     | 0.57              |
| 24:lC:114:ARG:NH1 | 85:l5:1359:G:OP1   | 2.36                     | 0.57              |
| 35:lO:59:ARG:NH1  | 85:l5:2046:G:OP1   | 2.37                     | 0.57              |
| 36:lP:57:CYS:H    | 36:lP:72:GLN:HB3   | 1.68                     | 0.57              |
| 45:lZ:68:ILE:O    | 45:lZ:115:LYS:NZ   | 2.35                     | 0.57              |
| 53:lh:78:TYR:OH   | 85:l5:16:G:H4'     | 2.04                     | 0.57              |
| 64:sR:60:ARG:HD3  | 64:sR:66:VAL:HB    | 1.86                     | 0.57              |
| 65:sD:76:ARG:O    | 65:sD:76:ARG:NH1   | 2.37                     | 0.57              |
| 66:sF:139:VAL:HA  | 73:sc:63:ARG:NH1   | 2.18                     | 0.57              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 72:sU:20:ILE:HD12 | 72:sU:115:THR:O    | 2.03                     | 0.57              |
| 75:sg:288:SER:O   | 75:sg:301:GLY:N    | 2.36                     | 0.57              |
| 79:s2:126:G:N3    | 79:s2:181:A:H1'    | 2.18                     | 0.57              |
| 79:s2:442:C:H2'   | 79:s2:443:U:C6     | 2.39                     | 0.57              |
| 79:s2:913:A:H8    | 79:s2:913:A:OP2    | 1.86                     | 0.57              |
| 85:l5:705:G:H2'   | 85:l5:706:C:C6     | 2.39                     | 0.57              |
| 7:SJ:164:PRO:HB3  | 7:SJ:170:PRO:HA    | 1.85                     | 0.57              |
| 10:SA:18:PHE:HA   | 10:SA:173:LEU:HD11 | 1.85                     | 0.57              |
| 16:SN:49:GLN:OE1  | 16:SN:49:GLN:N     | 2.33                     | 0.57              |
| 85:L5:676:C:H2'   | 85:L5:677:G:C8     | 2.39                     | 0.57              |
| 85:L5:2411:C:H2'  | 85:L5:2412:A:H8    | 1.69                     | 0.57              |
| 85:L5:2446:C:O2'  | 85:L5:2745:A:N3    | 2.32                     | 0.57              |
| 85:L5:3770:U:H2'  | 85:L5:3771:C:C6    | 2.39                     | 0.57              |
| 85:L5:4563:U:C2   | 85:L5:4564:A:C8    | 2.92                     | 0.57              |
| 20:L7:87:G:N2     | 20:L7:90:A:OP2     | 2.34                     | 0.57              |
| 38:LR:3:MET:HE2   | 38:LR:3:MET:HA     | 1.86                     | 0.57              |
| 40:LT:115:LYS:HA  | 40:LT:118:GLU:HG2  | 1.84                     | 0.57              |
| 42:LV:61:VAL:O    | 42:LV:79:ALA:N     | 2.28                     | 0.57              |
| 44:LY:47:MET:HE2  | 44:LY:47:MET:HA    | 1.84                     | 0.57              |
| 45:LZ:95:VAL:HG11 | 45:LZ:113:GLU:HG2  | 1.86                     | 0.57              |
| 47:Lb:65:MET:HA   | 47:Lb:68:ARG:HE    | 1.69                     | 0.57              |
| 53:Lh:50:VAL:O    | 53:Lh:54:ILE:HG12  | 2.04                     | 0.57              |
| 54:Li:57:ALA:O    | 54:Li:61:LEU:HG    | 2.04                     | 0.57              |
| 66:SF:87:LEU:HD21 | 69:SQ:47:LEU:HD11  | 1.86                     | 0.57              |
| 77:SZ:74:SER:HA   | 77:SZ:79:ILE:HB    | 1.86                     | 0.57              |
| 79:S2:680:G:H2'   | 79:S2:681:U:C6     | 2.39                     | 0.57              |
| 79:S2:1778:C:H2'  | 79:S2:1779:G:C8    | 2.39                     | 0.57              |
| 81:AP:52:G:H2'    | 81:AP:53:G:H8      | 1.69                     | 0.57              |
| 82:PE:55:U:H2'    | 82:PE:57:A:N7      | 2.18                     | 0.57              |
| 2:sE:19:MET:CE    | 79:s2:846:G:C4     | 2.86                     | 0.57              |
| 13:sV:47:ASN:OD1  | 13:sV:49:GLN:N     | 2.36                     | 0.57              |
| 25:lD:164:LYS:HD3 | 25:lD:180:PHE:HE1  | 1.69                     | 0.57              |
| 29:lH:48:LEU:HD12 | 29:lH:54:ARG:HE    | 1.69                     | 0.57              |
| 32:lL:89:LYS:HB2  | 53:lh:114:TYR:CE2  | 2.39                     | 0.57              |
| 33:lM:30:VAL:O    | 39:lS:98:ARG:NH2   | 2.36                     | 0.57              |
| 39:lS:170:LYS:HE3 | 85:l5:4875:G:H5''  | 1.84                     | 0.57              |
| 64:sR:36:GLU:HG2  | 64:sR:47:ARG:HH22  | 1.69                     | 0.57              |
| 65:sD:189:MET:SD  | 65:sD:189:MET:N    | 2.76                     | 0.57              |
| 68:sP:111:MET:HG2 | 68:sP:119:PHE:CZ   | 2.39                     | 0.57              |
| 79:s2:149:A:H3'   | 79:s2:150:A:H8     | 1.68                     | 0.57              |
| 79:s2:162:C:H2'   | 79:s2:163:U:O4'    | 2.05                     | 0.57              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 79:s2:838:G:O2'    | 79:s2:840:C:O5'    | 2.18                     | 0.57              |
| 85:l5:250:C:H2'    | 85:l5:251:C:C6     | 2.39                     | 0.57              |
| 85:l5:253:G:H2'    | 85:l5:254:G:C8     | 2.39                     | 0.57              |
| 85:l5:356:G:N1     | 85:l5:360:A:OP2    | 2.35                     | 0.57              |
| 85:l5:691:C:H2'    | 85:l5:692:A:C8     | 2.39                     | 0.57              |
| 3:SI:72:CYS:HG     | 3:SI:112:TRP:CG    | 2.21                     | 0.57              |
| 7:SJ:11:LYS:NZ     | 79:S2:24:C:OP1     | 2.31                     | 0.57              |
| 7:SJ:67:ASP:OD1    | 7:SJ:70:ARG:N      | 2.32                     | 0.57              |
| 11:SB:76:ASN:OD1   | 11:SB:77:ASP:N     | 2.36                     | 0.57              |
| 11:SB:225:LEU:HD12 | 11:SB:229:MET:HE2  | 1.86                     | 0.57              |
| 13:SV:33:GLN:NE2   | 13:SV:52:THR:OG1   | 2.27                     | 0.57              |
| 18:SW:23:ARG:NH2   | 19:Sb:5:LYS:O      | 2.36                     | 0.57              |
| 85:L5:444:G:H2'    | 85:L5:445:U:C6     | 2.38                     | 0.57              |
| 85:L5:1202:C:H3'   | 85:L5:1203:G:H4'   | 1.86                     | 0.57              |
| 85:L5:1545:G:H2'   | 85:L5:1546:C:C6    | 2.39                     | 0.57              |
| 85:L5:2250:C:H2'   | 85:L5:2251:G:C8    | 2.39                     | 0.57              |
| 85:L5:2283:G:H2'   | 85:L5:2284:G:H8    | 1.69                     | 0.57              |
| 85:L5:2434:G:O3'   | 43:LX:83:THR:HG21  | 2.03                     | 0.57              |
| 85:L5:2775:C:H2'   | 85:L5:2776:G:H8    | 1.68                     | 0.57              |
| 85:L5:4277:G:H2'   | 85:L5:4278:C:C6    | 2.39                     | 0.57              |
| 85:L5:4929:C:H2'   | 85:L5:4930:C:C6    | 2.40                     | 0.57              |
| 27:LF:238:ASP:OD2  | 27:LF:241:ASN:ND2  | 2.34                     | 0.57              |
| 32:LL:16:LYS:O     | 32:LL:21:ARG:NH2   | 2.35                     | 0.57              |
| 35:LO:173:GLN:HE22 | 35:LO:177:LEU:HD11 | 1.69                     | 0.57              |
| 51:Lf:6:TRP:CE2    | 51:Lf:102:ARG:HD3  | 2.39                     | 0.57              |
| 63:Lz:59:PRO:HG2   | 63:Lz:62:LYS:NZ    | 2.17                     | 0.57              |
| 64:SR:98:VAL:CG1   | 64:SR:117:LEU:HD11 | 2.33                     | 0.57              |
| 65:SD:195:THR:HA   | 65:SD:201:LYS:HD2  | 1.85                     | 0.57              |
| 73:Sc:13:ARG:O     | 73:Sc:33:GLU:N     | 2.35                     | 0.57              |
| 74:Sd:27:ARG:HH12  | 79:S2:1263:U:H4'   | 1.69                     | 0.57              |
| 79:S2:920:A:N7     | 79:S2:1021:U:O4    | 2.37                     | 0.57              |
| 83:Ls:146:LYS:HG3  | 83:Ls:155:LEU:HD21 | 1.85                     | 0.57              |
| 87:IW:113:LYS:O    | 87:IW:116:LYS:HG2  | 2.04                     | 0.57              |
| 6:sG:132:ARG:NH2   | 79:s2:168:C:C6     | 2.72                     | 0.57              |
| 8:sY:10:ARG:HB3    | 79:s2:835:C:H42    | 1.69                     | 0.57              |
| 10:sA:122:LEU:HD12 | 10:sA:123:VAL:N    | 2.19                     | 0.57              |
| 11:sB:144:LYS:CD   | 11:sB:208:HIS:HB3  | 2.34                     | 0.57              |
| 15:sC:104:ASP:HA   | 15:sC:130:ILE:HG22 | 1.85                     | 0.57              |
| 26:lE:103:GLY:O    | 26:lE:105:ARG:NH1  | 2.36                     | 0.57              |
| 29:lH:106:GLN:OE1  | 29:lH:107:GLU:N    | 2.37                     | 0.57              |
| 30:lI:166:HIS:NE2  | 40:lT:158:PHE:CD2  | 2.72                     | 0.57              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:IJ:136:ARG:H    | 31:IJ:139:PHE:HD2  | 1.52                     | 0.57              |
| 37:IQ:159:PRO:HB3  | 37:IQ:188:ASN:O    | 2.04                     | 0.57              |
| 39:IS:163:HIS:O    | 85:I5:1919:G:N2    | 2.30                     | 0.57              |
| 42:IV:88:TYR:CE2   | 42:IV:96:LEU:HD21  | 2.39                     | 0.57              |
| 50:Ie:128:ARG:NH1  | 85:I5:2306:G:OP1   | 2.37                     | 0.57              |
| 52:Ig:65:MET:SD    | 52:Ig:65:MET:N     | 2.77                     | 0.57              |
| 54:li:90:LEU:HD12  | 54:li:94:LEU:HD13  | 1.86                     | 0.57              |
| 63:Iz:75:ASP:OD1   | 63:Iz:75:ASP:N     | 2.36                     | 0.57              |
| 76:sM:52:LEU:HD12  | 76:sM:53:ALA:H     | 1.69                     | 0.57              |
| 79:s2:1741:U:H2'   | 79:s2:1742:C:O4'   | 2.04                     | 0.57              |
| 80:cB:660:ASN:HB3  | 80:cB:683:PHE:HZ   | 1.69                     | 0.57              |
| 85:I5:114:G:H22    | 85:I5:158:A:H61    | 1.51                     | 0.57              |
| 85:I5:907:C:H2'    | 85:I5:908:G:C8     | 2.39                     | 0.57              |
| 85:I5:1979:A:H2    | 85:I5:1987:C:H42   | 1.52                     | 0.57              |
| 85:I5:2693:G:H2'   | 85:I5:2694:G:C2    | 2.39                     | 0.57              |
| 80:CB:689:GLU:OE1  | 80:CB:730:TYR:OH   | 2.14                     | 0.57              |
| 4:SL:13:GLN:NE2    | 4:SL:63:THR:OG1    | 2.29                     | 0.57              |
| 11:SB:139:CYS:SG   | 11:SB:168:MET:HE1  | 2.44                     | 0.57              |
| 11:SB:164:ILE:O    | 11:SB:168:MET:HG3  | 2.05                     | 0.57              |
| 15:SC:272:HIS:CG   | 15:SC:275:LYS:HZ2  | 2.22                     | 0.57              |
| 85:L5:43:U:O2      | 60:Lo:44:LYS:NZ    | 2.37                     | 0.57              |
| 85:L5:332:C:H5'    | 34:LN:150:TRP:HZ3  | 1.69                     | 0.57              |
| 85:L5:1179:U:H3'   | 85:L5:1180:C:H5''  | 1.86                     | 0.57              |
| 85:L5:1801:A:O3'   | 40:LT:102:ARG:NH2  | 2.37                     | 0.57              |
| 85:L5:2694:G:H5'   | 85:L5:2695:A:C2    | 2.39                     | 0.57              |
| 85:L5:4159:C:H2'   | 85:L5:4160:C:C6    | 2.39                     | 0.57              |
| 85:L5:4543:G:H2'   | 85:L5:4544:A:C8    | 2.39                     | 0.57              |
| 24:LC:180:ILE:HD13 | 24:LC:224:ILE:HG21 | 1.86                     | 0.57              |
| 26:LE:150:LEU:HD23 | 26:LE:175:VAL:HG11 | 1.85                     | 0.57              |
| 27:LF:149:SER:OG   | 27:LF:245:ARG:NH2  | 2.35                     | 0.57              |
| 28:LG:177:MET:SD   | 28:LG:177:MET:N    | 2.77                     | 0.57              |
| 32:LL:108:GLU:OE1  | 32:LL:108:GLU:N    | 2.28                     | 0.57              |
| 35:LO:118:MET:HE3  | 35:LO:119:VAL:N    | 2.05                     | 0.57              |
| 36:LP:114:ILE:HG22 | 36:LP:150:LEU:HG   | 1.87                     | 0.57              |
| 63:Lz:23:ARG:HA    | 63:Lz:212:LYS:HG3  | 1.85                     | 0.57              |
| 64:SR:21:TYR:CD1   | 64:SR:58:MET:HE1   | 2.40                     | 0.57              |
| 66:SF:145:ARG:O    | 66:SF:149:GLN:HG3  | 2.03                     | 0.57              |
| 76:SM:124:ILE:O    | 76:SM:128:PHE:HD2  | 1.87                     | 0.57              |
| 79:S2:795:A:H2'    | 79:S2:796:G:C8     | 2.38                     | 0.57              |
| 79:S2:1010:G:H2'   | 79:S2:1011:A:H8    | 1.69                     | 0.57              |
| 79:S2:1377:U:O2'   | 79:S2:1379:A:O5'   | 2.19                     | 0.57              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 79:S2:1701:C:C4   | 82:PE:34:U:H1'     | 2.39                     | 0.57              |
| 81:AP:66:C:H5'    | 81:AP:67:G:OP2     | 2.05                     | 0.57              |
| 82:PE:5:G:H2'     | 82:PE:6:G:C8       | 2.39                     | 0.57              |
| 83:Ls:28:PHE:CE1  | 83:Ls:192:VAL:HG22 | 2.40                     | 0.57              |
| 84:Lt:19:GLY:HA3  | 84:Lt:59:THR:HB    | 1.86                     | 0.57              |
| 1:cH:85:ARG:HH12  | 1:cH:92:GLN:HG3    | 1.69                     | 0.57              |
| 2:sE:18:TRP:NE1   | 2:sE:41:CYS:O      | 2.37                     | 0.57              |
| 3:sI:31:ARG:NH2   | 79:s2:381:C:OP2    | 2.36                     | 0.57              |
| 8:sY:122:LYS:NZ   | 79:s2:152:U:OP2    | 2.38                     | 0.57              |
| 21:l8:58:G:N7     | 55:lj:65:ARG:NH2   | 2.51                     | 0.57              |
| 28:lG:175:ARG:HD2 | 28:lG:230:TYR:CG   | 2.39                     | 0.57              |
| 35:lO:175:MET:HE1 | 85:l5:4873:G:C4    | 2.38                     | 0.57              |
| 40:lT:100:LYS:HB2 | 85:l5:1730:U:H4'   | 1.86                     | 0.57              |
| 47:lb:8:THR:HG22  | 47:lb:10:HIS:H     | 1.69                     | 0.57              |
| 48:lc:36:LYS:HD3  | 48:lc:40:GLN:HG2   | 1.86                     | 0.57              |
| 51:lf:51:TYR:OH   | 85:l5:442:G:OP1    | 2.13                     | 0.57              |
| 56:lk:49:ASP:H    | 56:lk:52:LYS:NZ    | 2.01                     | 0.57              |
| 68:sP:77:LYS:HB2  | 68:sP:102:PHE:CD1  | 2.39                     | 0.57              |
| 75:sg:106:LYS:HE3 | 75:sg:107:ASP:H    | 1.69                     | 0.57              |
| 79:s2:113:G:N1    | 79:s2:292:A:N7     | 2.52                     | 0.57              |
| 79:s2:329:G:H2'   | 79:s2:330:G:C8     | 2.34                     | 0.57              |
| 79:s2:1172:U:H2'  | 79:s2:1173:A:C8    | 2.40                     | 0.57              |
| 79:s2:1629:C:H2'  | 79:s2:1630:A:O4'   | 2.04                     | 0.57              |
| 79:s2:1752:C:N3   | 79:s2:1779:G:N1    | 2.46                     | 0.57              |
| 79:s2:1800:A:H3'  | 79:s2:1801:A:H8    | 1.69                     | 0.57              |
| 80:cB:182:VAL:HA  | 80:cB:185:VAL:HG22 | 1.86                     | 0.57              |
| 83:ls:6:ARG:NH2   | 85:l5:2019:C:OP1   | 2.37                     | 0.57              |
| 85:l5:966:A:OP2   | 85:l5:2092:G:N2    | 2.37                     | 0.57              |
| 85:l5:1091:C:H2'  | 85:l5:1092:G:C8    | 2.38                     | 0.57              |
| 85:l5:1479:G:H2'  | 85:l5:1480:C:C6    | 2.39                     | 0.57              |
| 85:l5:4233:A:C8   | 85:l5:4235:G:C8    | 2.92                     | 0.57              |
| 6:SG:1:MET:HE3    | 6:SG:109:LEU:HB2   | 1.86                     | 0.57              |
| 10:SA:56:GLU:HG3  | 13:SV:80:SER:HB3   | 1.85                     | 0.57              |
| 12:SH:80:VAL:O    | 12:SH:84:GLU:HG2   | 2.04                     | 0.57              |
| 14:Sa:53:ILE:HD12 | 17:SO:120:ALA:HB2  | 1.84                     | 0.57              |
| 14:Sa:88:SER:O    | 14:Sa:92:ARG:N     | 2.34                     | 0.57              |
| 85:L5:158:A:N1    | 85:L5:276:C:O2'    | 2.34                     | 0.57              |
| 85:L5:667:A:O4'   | 62:Lr:46:ARG:NH1   | 2.37                     | 0.57              |
| 85:L5:1979:A:N6   | 85:L5:1984:A:OP1   | 2.35                     | 0.57              |
| 85:L5:2580:U:OP1  | 45:LZ:36:ARG:NH1   | 2.38                     | 0.57              |
| 85:L5:2647:A:H3'  | 85:L5:2648:G:H8    | 1.69                     | 0.57              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 85:L5:2669:C:P     | 38:LR:128:LYS:HZ1  | 2.28                     | 0.57              |
| 85:L5:4038:C:OP2   | 85:L5:4039:G:N2    | 2.38                     | 0.57              |
| 22:LA:30:ARG:NH2   | 22:LA:33:ASP:OD2   | 2.38                     | 0.57              |
| 23:LB:92:TYR:HB3   | 23:LB:99:LEU:HD12  | 1.87                     | 0.57              |
| 33:LM:101:LYS:HB2  | 35:LO:200:GLY:HA3  | 1.84                     | 0.57              |
| 35:LO:126:VAL:HG13 | 35:LO:127:VAL:HG13 | 1.86                     | 0.57              |
| 63:Lz:55:LEU:HD23  | 63:Lz:169:VAL:HG11 | 1.86                     | 0.57              |
| 79:S2:639:C:H2'    | 79:S2:640:A:H8     | 1.69                     | 0.57              |
| 79:S2:1244:U:H2'   | 79:S2:1245:G:C8    | 2.39                     | 0.57              |
| 84:Lt:53:TRP:HD1   | 84:Lt:54:LYS:H     | 1.52                     | 0.57              |
| 1:cH:46:ALA:H      | 9:se:55:PRO:HB3    | 1.69                     | 0.57              |
| 4:sL:105:ARG:HH22  | 79:s2:356:C:P      | 2.27                     | 0.57              |
| 11:sB:160:GLN:NE2  | 79:s2:1122:A:OP1   | 2.35                     | 0.57              |
| 12:sH:174:SER:OG   | 12:sH:185:VAL:O    | 2.17                     | 0.57              |
| 14:sa:90:GLU:H     | 14:sa:90:GLU:CD    | 2.11                     | 0.57              |
| 15:sC:114:LYS:HD3  | 15:sC:114:LYS:N    | 2.16                     | 0.57              |
| 17:sO:14:VAL:N     | 17:sO:15:ILE:HA    | 2.19                     | 0.57              |
| 27:lF:213:LEU:O    | 85:l5:2072:C:O2'   | 2.21                     | 0.57              |
| 29:lH:24:THR:HA    | 29:lH:37:ASP:HA    | 1.86                     | 0.57              |
| 30:lI:76:MET:HA    | 30:lI:76:MET:HE3   | 1.86                     | 0.57              |
| 32:lL:78:LEU:HD11  | 32:lL:88:LYS:HD3   | 1.86                     | 0.57              |
| 39:lS:17:LEU:H     | 39:lS:17:LEU:HD12  | 1.69                     | 0.57              |
| 41:lU:79:SER:OG    | 41:lU:80:LYS:N     | 2.37                     | 0.57              |
| 75:sg:8:ARG:HH21   | 75:sg:47:ARG:HD2   | 1.70                     | 0.57              |
| 79:s2:1776:G:OP2   | 79:s2:1776:G:N2    | 2.34                     | 0.57              |
| 85:l5:466:A:H2'    | 85:l5:467:U:C6     | 2.40                     | 0.57              |
| 85:l5:3870:C:H2'   | 85:l5:3871:A:C8    | 2.39                     | 0.57              |
| 3:SI:132:GLU:N     | 3:SI:132:GLU:OE1   | 2.37                     | 0.57              |
| 15:SC:278:THR:HA   | 15:SC:279:ARG:HD2  | 1.86                     | 0.57              |
| 85:L5:20:U:OP2     | 53:Lh:89:ARG:NH2   | 2.37                     | 0.57              |
| 85:L5:72:C:H5      | 32:LL:67:HIS:CD2   | 2.23                     | 0.57              |
| 85:L5:114:G:N2     | 85:L5:158:A:H61    | 2.01                     | 0.57              |
| 85:L5:229:G:H2'    | 85:L5:230:G:H8     | 1.70                     | 0.57              |
| 85:L5:364:G:H5''   | 55:Lj:56:ARG:NH2   | 2.19                     | 0.57              |
| 85:L5:1867:A:H2'   | 85:L5:1868:A:C8    | 2.40                     | 0.57              |
| 85:L5:2358:G:H2'   | 85:L5:2359:U:O4'   | 2.05                     | 0.57              |
| 85:L5:2608:G:H2'   | 85:L5:2609:G:H8    | 1.68                     | 0.57              |
| 85:L5:3658:C:H2'   | 85:L5:3659:G:C8    | 2.37                     | 0.57              |
| 85:L5:4513:A:H2'   | 85:L5:4514:G:H8    | 1.69                     | 0.57              |
| 85:L5:4868:G:O2'   | 85:L5:4872:G:OP1   | 2.22                     | 0.57              |
| 21:L8:5:U:H2'      | 21:L8:6:C:C6       | 2.40                     | 0.57              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 30:LI:66:GLU:OE2   | 30:LI:69:ARG:NH2   | 2.38                     | 0.57              |
| 76:SM:15:ASN:O     | 76:SM:19:GLN:HG2   | 2.04                     | 0.57              |
| 79:S2:158:A:H1'    | 79:S2:464:A:N7     | 2.19                     | 0.57              |
| 79:S2:1565:C:N4    | 79:S2:1566:G:O6    | 2.38                     | 0.57              |
| 87:LW:6:CYS:HB3    | 87:LW:11:TYR:H     | 1.68                     | 0.57              |
| 1:CH:76:GLU:CD     | 1:CH:76:GLU:H      | 2.13                     | 0.57              |
| 7:sJ:28:GLU:O      | 7:sJ:32:ILE:HG22   | 2.04                     | 0.57              |
| 11:sB:113:MET:HG2  | 11:sB:209:ASP:OD2  | 2.05                     | 0.57              |
| 15:sC:75:ILE:HB    | 15:sC:269:PHE:CE1  | 2.35                     | 0.57              |
| 17:sO:28:PHE:HZ    | 17:sO:127:GLY:HA3  | 1.70                     | 0.57              |
| 22:lA:180:LEU:O    | 22:lA:180:LEU:HD12 | 2.04                     | 0.57              |
| 31:lJ:63:ARG:NH1   | 60:lb:105:GLN:H    | 2.02                     | 0.57              |
| 47:lb:17:HIS:NE2   | 85:l5:1724:G:O4'   | 2.38                     | 0.57              |
| 64:sR:32:LYS:HG2   | 79:s2:1453:C:C2'   | 2.34                     | 0.57              |
| 71:sT:121:ARG:HH21 | 79:s2:1563:G:H5''  | 1.70                     | 0.57              |
| 73:sc:44:ARG:NH2   | 73:sc:63:ARG:HD3   | 2.19                     | 0.57              |
| 75:sg:143:GLN:NE2  | 75:sg:144:ASP:OD2  | 2.38                     | 0.57              |
| 79:s2:637:U:H2'    | 79:s2:638:C:C6     | 2.40                     | 0.57              |
| 79:s2:804:U:H2'    | 79:s2:805:U:C6     | 2.40                     | 0.57              |
| 79:s2:1010:G:H2'   | 79:s2:1011:A:H8    | 1.67                     | 0.57              |
| 79:s2:1769:C:OP2   | 79:s2:1771:G:N1    | 2.38                     | 0.57              |
| 79:s2:1829:G:H1'   | 79:s2:1850:A:H2    | 1.70                     | 0.57              |
| 80:cB:174:LEU:O    | 80:cB:178:PHE:CD1  | 2.57                     | 0.57              |
| 82:pE:22:G:H2'     | 82:pE:23:A:H8      | 1.67                     | 0.57              |
| 85:l5:707:C:O2'    | 85:l5:4943:A:N1    | 2.32                     | 0.57              |
| 85:l5:1273:G:O2'   | 85:l5:1274:A:H5'   | 2.04                     | 0.57              |
| 85:l5:1536:U:H2'   | 85:l5:1537:A:H8    | 1.70                     | 0.57              |
| 80:CB:25:ILE:HD11  | 80:CB:127:VAL:HG22 | 1.85                     | 0.57              |
| 80:CB:669:VAL:HG21 | 80:CB:707:VAL:HG23 | 1.86                     | 0.57              |
| 7:SJ:174:LYS:HG2   | 79:S2:561:A:P      | 2.45                     | 0.57              |
| 11:SB:95:ASN:OD1   | 11:SB:96:CYS:N     | 2.38                     | 0.57              |
| 15:SC:66:LEU:HA    | 15:SC:69:LEU:HD12  | 1.86                     | 0.57              |
| 15:SC:66:LEU:HD12  | 15:SC:67:GLY:N     | 2.20                     | 0.57              |
| 85:L5:184:U:O2'    | 85:L5:189:G:O4'    | 2.22                     | 0.57              |
| 85:L5:373:G:OP2    | 55:Lj:36:LYS:NZ    | 2.37                     | 0.57              |
| 85:L5:2066:C:H4'   | 51:Lf:79:GLY:HA2   | 1.86                     | 0.57              |
| 85:L5:2599:G:N2    | 85:L5:2747:U:O4    | 2.36                     | 0.57              |
| 22:LA:57:PRO:HG2   | 22:LA:170:ALA:HB3  | 1.85                     | 0.57              |
| 28:LG:140:VAL:O    | 28:LG:144:THR:OG1  | 2.17                     | 0.57              |
| 29:LH:135:SER:N    | 29:LH:145:ILE:O    | 2.34                     | 0.57              |
| 38:LR:21:LYS:O     | 38:LR:53:LYS:N     | 2.32                     | 0.57              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 38:LR:98:ARG:O     | 38:LR:101:ILE:HG22 | 2.04                     | 0.57              |
| 47:Lb:65:MET:HA    | 47:Lb:68:ARG:NE    | 2.20                     | 0.57              |
| 66:SF:144:LEU:HD11 | 73:Sc:49:PRO:HG2   | 1.87                     | 0.57              |
| 66:SF:147:VAL:O    | 66:SF:151:ILE:HG12 | 2.05                     | 0.57              |
| 70:SS:118:ARG:HD3  | 70:SS:123:LEU:HD21 | 1.85                     | 0.57              |
| 79:S2:1272:C:H2'   | 79:S2:1273:C:C6    | 2.39                     | 0.57              |
| 79:S2:1736:G:H2'   | 79:S2:1737:G:H8    | 1.68                     | 0.57              |
| 83:Ls:91:THR:HG21  | 83:Ls:98:ILE:HG13  | 1.86                     | 0.57              |
| 2:sE:192:ILE:HD11  | 2:sE:242:LYS:HG2   | 1.86                     | 0.57              |
| 6:sG:216:ARG:O     | 6:sG:218:LYS:N     | 2.36                     | 0.57              |
| 11:sB:40:ASN:ND2   | 11:sB:76:ASN:OD1   | 2.37                     | 0.57              |
| 12:sH:145:ARG:NH2  | 18:sW:52:ILE:HG13  | 2.14                     | 0.57              |
| 14:sa:87:ARG:NH2   | 14:sa:92:ARG:O     | 2.38                     | 0.57              |
| 15:sC:98:LEU:O     | 15:sC:98:LEU:HD12  | 2.03                     | 0.57              |
| 15:sC:123:ARG:NH1  | 79:s2:1358:U:OP1   | 2.37                     | 0.57              |
| 15:sC:278:THR:HA   | 15:sC:279:ARG:HD2  | 1.87                     | 0.57              |
| 20:l7:48:G:O2'     | 25:ID:222:GLN:O    | 2.22                     | 0.57              |
| 28:lG:224:THR:HA   | 28:lG:228:ASP:OD1  | 2.03                     | 0.57              |
| 50:le:82:VAL:HG22  | 50:le:111:ILE:HD13 | 1.87                     | 0.57              |
| 57:ll:22:PRO:HG3   | 85:l5:2431:A:OP1   | 2.05                     | 0.57              |
| 67:sK:28:HIS:CD2   | 74:sd:8:TRP:HE1    | 2.23                     | 0.57              |
| 67:sK:45:VAL:O     | 67:sK:49:MET:HG3   | 2.04                     | 0.57              |
| 69:sQ:78:VAL:HA    | 69:sQ:81:ILE:HG22  | 1.87                     | 0.57              |
| 72:sU:59:LYS:HB3   | 72:sU:84:ILE:HB    | 1.87                     | 0.57              |
| 73:sc:30:VAL:HG23  | 73:sc:32:VAL:HG13  | 1.86                     | 0.57              |
| 75:sg:206:LEU:HD13 | 75:sg:218:LEU:HD11 | 1.87                     | 0.57              |
| 76:sM:78:LYS:HD3   | 76:sM:79:VAL:H     | 1.70                     | 0.57              |
| 79:s2:91:A:H5''    | 79:s2:92:A:H5''    | 1.85                     | 0.57              |
| 79:s2:1718:G:H2'   | 79:s2:1814:G:N2    | 2.20                     | 0.57              |
| 85:l5:1471:U:H2'   | 85:l5:1472:C:C6    | 2.40                     | 0.57              |
| 85:l5:1847:C:H2'   | 85:l5:1848:C:C6    | 2.40                     | 0.57              |
| 85:l5:2611:A:H2'   | 85:l5:2612:G:H8    | 1.69                     | 0.57              |
| 85:l5:2683:C:H2'   | 85:l5:2684:C:H6    | 1.69                     | 0.57              |
| 80:CB:157:MET:HE2  | 80:CB:157:MET:N    | 2.18                     | 0.57              |
| 80:CB:179:GLN:O    | 80:CB:183:GLU:HG2  | 2.04                     | 0.57              |
| 12:SH:182:GLY:HA3  | 79:S2:690:G:C8     | 2.31                     | 0.57              |
| 85:L5:8:U:OP1      | 34:LN:41:ARG:NH1   | 2.37                     | 0.57              |
| 85:L5:4101:C:OP2   | 85:L5:4102:C:H5''  | 2.04                     | 0.57              |
| 85:L5:4186:A:H2'   | 85:L5:4187:G:H8    | 1.70                     | 0.57              |
| 85:L5:4431:U:OP2   | 30:LI:3:ARG:NH2    | 2.37                     | 0.57              |
| 85:L5:4765:G:H21   | 39:LS:173:ASN:ND2  | 2.03                     | 0.57              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 85:L5:5037:U:H2'   | 85:L5:5038:A:C8   | 2.40                     | 0.57              |
| 21:L8:90:C:H2'     | 21:L8:91:A:H8     | 1.70                     | 0.57              |
| 24:LC:32:ILE:HG22  | 24:LC:34:PRO:HD3  | 1.87                     | 0.57              |
| 48:Lc:79:ILE:O     | 48:Lc:83:THR:HG23 | 2.05                     | 0.57              |
| 66:SF:118:ASN:ND2  | 66:SF:180:ALA:O   | 2.37                     | 0.57              |
| 70:SS:49:ASP:C     | 70:SS:50:ILE:HD13 | 2.30                     | 0.57              |
| 70:SS:88:LYS:NZ    | 79:S2:1613:G:OP1  | 2.37                     | 0.57              |
| 71:ST:10:ASN:ND2   | 71:ST:13:GLU:HG2  | 2.19                     | 0.57              |
| 75:Sg:147:HIS:HB3  | 75:Sg:171:ASP:CG  | 2.29                     | 0.57              |
| 76:SM:96:ARG:NH2   | 76:SM:97:GLU:OE1  | 2.37                     | 0.57              |
| 79:S2:1279:C:H2'   | 79:S2:1280:G:C8   | 2.40                     | 0.57              |
| 79:S2:1562:C:H2'   | 79:S2:1563:G:C8   | 2.40                     | 0.57              |
| 6:sG:13:GLN:NE2    | 79:s2:153:G:N3    | 2.51                     | 0.57              |
| 6:sG:44:GLU:HG2    | 6:sG:45:TRP:CE3   | 2.40                     | 0.57              |
| 6:sG:134:GLY:O     | 79:s2:65:C:N4     | 2.38                     | 0.57              |
| 6:sG:162:LEU:O     | 6:sG:169:PRO:HA   | 2.04                     | 0.57              |
| 10:sA:147:LEU:HD13 | 10:sA:174:MET:HE3 | 1.87                     | 0.57              |
| 11:sB:57:ILE:HG22  | 11:sB:59:SER:H    | 1.70                     | 0.57              |
| 19:sb:17:ARG:NH1   | 79:s2:1127:C:O3'  | 2.38                     | 0.57              |
| 25:ID:115:MET:HE1  | 85:l5:1819:G:H1'  | 1.87                     | 0.57              |
| 26:lE:135:GLN:N    | 26:lE:135:GLN:OE1 | 2.38                     | 0.57              |
| 29:lH:50:LYS:HD3   | 29:lH:50:LYS:H    | 1.68                     | 0.57              |
| 29:lH:66:GLU:N     | 29:lH:66:GLU:OE1  | 2.37                     | 0.57              |
| 38:lR:116:ASP:OD2  | 38:lR:117:ARG:N   | 2.29                     | 0.57              |
| 40:lT:110:LYS:NZ   | 85:l5:1807:C:O2'  | 2.37                     | 0.57              |
| 44:lY:30:MET:HE1   | 44:lY:78:TYR:HA   | 1.87                     | 0.57              |
| 47:lb:44:ARG:HH12  | 85:l5:1466:G:P    | 2.28                     | 0.57              |
| 65:sD:27:ARG:NH2   | 79:s2:1498:A:OP1  | 2.37                     | 0.57              |
| 71:sT:26:GLY:C     | 71:sT:27:LYS:HD3  | 2.29                     | 0.57              |
| 78:sf:118:ARG:HB2  | 78:sf:131:PHE:CE1 | 2.39                     | 0.57              |
| 79:s2:62:G:O2'     | 79:s2:172:U:OP1   | 2.21                     | 0.57              |
| 79:s2:508:A:H3'    | 79:s2:509:G:H8    | 1.68                     | 0.57              |
| 80:cB:60:ARG:HG2   | 80:cB:61:LYS:O    | 2.04                     | 0.57              |
| 80:cB:401:MET:HE1  | 80:cB:529:LYS:HE3 | 1.86                     | 0.57              |
| 81:aP:41:G:H2'     | 81:aP:42:A:C8     | 2.40                     | 0.57              |
| 84:lt:114:ARG:HD2  | 84:lt:129:ILE:HB  | 1.87                     | 0.57              |
| 85:l5:210:C:HO2'   | 85:l5:233:U:HO2'  | 1.51                     | 0.57              |
| 85:l5:325:U:H2'    | 85:l5:326:C:C6    | 2.40                     | 0.57              |
| 85:l5:2624:G:H2'   | 85:l5:2625:U:H6   | 1.70                     | 0.57              |
| 85:l5:3873:G:H2'   | 85:l5:3874:G:C8   | 2.39                     | 0.57              |
| 85:l5:3948:C:H5''  | 85:l5:3949:A:OP1  | 2.04                     | 0.57              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 7:SJ:91:LYS:HG3   | 7:SJ:96:TYR:CD2    | 2.40                     | 0.57              |
| 10:SA:174:MET:HA  | 10:SA:174:MET:HE3  | 1.86                     | 0.57              |
| 85:L5:267:G:H2'   | 85:L5:268:G:C8     | 2.39                     | 0.57              |
| 85:L5:2791:C:OP1  | 57:Ll:48:LYS:NZ    | 2.37                     | 0.57              |
| 85:L5:4098:A:H5'  | 85:L5:4099:G:OP2   | 2.05                     | 0.57              |
| 85:L5:4504:C:H2'  | 85:L5:4505:C:C6    | 2.40                     | 0.57              |
| 85:L5:4910:G:H1   | 35:LO:108:ILE:H    | 1.52                     | 0.57              |
| 24:LC:205:ARG:HE  | 24:LC:248:ARG:HH12 | 1.52                     | 0.57              |
| 41:LU:80:LYS:NZ   | 41:LU:106:SER:O    | 2.37                     | 0.57              |
| 42:LV:13:LYS:NZ   | 42:LV:57:VAL:O     | 2.38                     | 0.57              |
| 43:LX:74:TYR:HD1  | 53:Lh:25:LYS:HG3   | 1.69                     | 0.57              |
| 52:Lg:45:ALA:HB3  | 52:Lg:82:MET:SD    | 2.45                     | 0.57              |
| 62:Lr:56:ASP:OD1  | 62:Lr:58:LYS:N     | 2.23                     | 0.57              |
| 68:SP:85:ILE:HD12 | 68:SP:114:HIS:O    | 2.05                     | 0.57              |
| 71:ST:28:LEU:HD13 | 71:ST:54:TYR:CE1   | 2.39                     | 0.57              |
| 72:SU:61:LEU:HD12 | 74:Sd:34:TYR:CZ    | 2.40                     | 0.57              |
| 75:Sg:149:GLU:CD  | 75:Sg:150:TRP:N    | 2.63                     | 0.57              |
| 75:Sg:213:ASP:CG  | 75:Sg:215:GLN:HG2  | 2.29                     | 0.57              |
| 79:S2:531:A:N6    | 79:S2:554:A:H1'    | 2.20                     | 0.57              |
| 79:S2:610:G:H2'   | 79:S2:611:G:H8     | 1.69                     | 0.57              |
| 79:S2:649:U:H2'   | 79:S2:650:A:H8     | 1.70                     | 0.57              |
| 6:sG:131:ARG:NH2  | 6:sG:132:ARG:HE    | 2.02                     | 0.57              |
| 8:sY:119:GLY:HA2  | 79:s2:85:A:H5'     | 1.87                     | 0.57              |
| 16:sN:3:ARG:NH2   | 79:s2:923:G:OP1    | 2.37                     | 0.57              |
| 28:lG:104:PRO:HG2 | 28:lG:194:VAL:HA   | 1.87                     | 0.57              |
| 29:IH:96:TYR:CE2  | 29:IH:142:ASP:OD2  | 2.52                     | 0.57              |
| 35:lO:188:LYS:HD3 | 85:l5:4892:A:H5''  | 1.87                     | 0.57              |
| 40:lT:155:PRO:O   | 40:lT:155:PRO:HD2  | 2.05                     | 0.57              |
| 46:la:76:ASP:HB2  | 46:la:115:GLY:HA3  | 1.87                     | 0.57              |
| 70:sS:39:ARG:HG3  | 71:sT:45:LEU:HD12  | 1.85                     | 0.57              |
| 79:s2:806:U:H2'   | 79:s2:807:G:H8     | 1.70                     | 0.57              |
| 79:s2:1172:U:O2   | 79:s2:1188:A:N7    | 2.37                     | 0.57              |
| 79:s2:1266:C:C4   | 79:s2:1517:G:N2    | 2.73                     | 0.57              |
| 85:l5:173:C:H2'   | 85:l5:174:C:C6     | 2.40                     | 0.57              |
| 85:l5:3893:C:H2'  | 85:l5:3894:A:H8    | 1.69                     | 0.57              |
| 85:l5:4178:A:H2'  | 85:l5:4179:G:H8    | 1.70                     | 0.57              |
| 85:l5:4638:U:H3   | 85:l5:4661:G:H1    | 1.53                     | 0.57              |
| 80:CB:229:ALA:HB2 | 80:CB:256:MET:HE2  | 1.87                     | 0.57              |
| 80:CB:450:THR:OG1 | 80:CB:461:ILE:O    | 2.22                     | 0.57              |
| 3:SI:104:ILE:HG22 | 3:SI:171:LEU:HB2   | 1.87                     | 0.57              |
| 7:SJ:127:ARG:HH21 | 7:SJ:145:PRO:HG2   | 1.69                     | 0.57              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:SB:137:LEU:HD13 | 11:SB:215:VAL:HB   | 1.87                     | 0.57              |
| 14:Sa:43:ASN:HA    | 14:Sa:66:LYS:HA    | 1.87                     | 0.57              |
| 85:L5:38:A:H61     | 85:L5:41:C:H3'     | 1.70                     | 0.57              |
| 85:L5:364:G:H8     | 55:Lj:56:ARG:NH2   | 2.01                     | 0.57              |
| 85:L5:675:C:H2'    | 85:L5:676:C:C6     | 2.39                     | 0.57              |
| 85:L5:1183:C:H2'   | 85:L5:1184:A:C8    | 2.40                     | 0.57              |
| 85:L5:2481:G:H2'   | 85:L5:2482:C:C6    | 2.40                     | 0.57              |
| 85:L5:2557:G:O6    | 85:L5:2570:U:O4    | 2.22                     | 0.57              |
| 85:L5:2753:G:H5''  | 45:LZ:135:ARG:HH12 | 1.70                     | 0.57              |
| 85:L5:2845:A:H61   | 85:L5:3843:C:H42   | 0.70                     | 0.57              |
| 85:L5:4870:G:OP2   | 33:LM:5:ARG:NH1    | 2.37                     | 0.57              |
| 85:L5:4936:G:C4    | 26:LE:183:ARG:HD2  | 2.40                     | 0.57              |
| 22:LA:30:ARG:O     | 22:LA:163:ARG:NH1  | 2.37                     | 0.57              |
| 23:LB:107:ALA:HB2  | 23:LB:201:LEU:HG   | 1.86                     | 0.57              |
| 24:LC:266:THR:N    | 24:LC:269:LYS:O    | 2.37                     | 0.57              |
| 27:LF:30:ILE:HD13  | 27:LF:33:LEU:HD21  | 1.85                     | 0.57              |
| 34:LN:16:SER:OG    | 34:LN:19:MET:HG3   | 2.05                     | 0.57              |
| 34:LN:124:ASP:OD1  | 34:LN:125:SER:N    | 2.38                     | 0.57              |
| 41:LU:25:CYS:O     | 41:LU:68:SER:OG    | 2.23                     | 0.57              |
| 50:Le:68:HIS:CD2   | 62:Lr:22:LYS:HG3   | 2.39                     | 0.57              |
| 70:SS:50:ILE:HD11  | 70:SS:66:ARG:NH2   | 2.17                     | 0.57              |
| 79:S2:1365:G:H2'   | 79:S2:1366:G:H8    | 1.70                     | 0.57              |
| 79:S2:1644:C:H2'   | 79:S2:1645:C:C6    | 2.40                     | 0.57              |
| 4:sL:85:THR:HA     | 4:sL:112:HIS:HA    | 1.87                     | 0.57              |
| 4:sL:91:ASP:HA     | 4:sL:106:HIS:HA    | 1.87                     | 0.57              |
| 4:sL:136:LYS:HZ1   | 79:s2:386:C:P      | 2.28                     | 0.57              |
| 11:sB:149:GLN:HG3  | 64:sR:132:ARG:O    | 2.05                     | 0.57              |
| 21:l8:37:A:H2      | 53:lh:89:ARG:HH12  | 1.51                     | 0.57              |
| 27:lF:60:GLU:O     | 27:lF:63:GLN:N     | 2.28                     | 0.57              |
| 29:lH:4:ILE:H      | 39:lS:144:GLN:HE21 | 1.53                     | 0.57              |
| 45:lZ:38:TYR:HB3   | 85:l5:2656:U:H5''  | 1.86                     | 0.57              |
| 48:lc:22:MET:O     | 48:lc:23:LYS:HG2   | 2.04                     | 0.57              |
| 50:le:16:ARG:NH1   | 85:l5:438:G:OP1    | 2.38                     | 0.57              |
| 71:sT:7:LYS:HE2    | 79:s2:1426:U:H5'   | 1.87                     | 0.57              |
| 71:sT:11:GLN:HB2   | 79:s2:1542:C:H4'   | 1.87                     | 0.57              |
| 71:sT:78:ILE:HG22  | 71:sT:79:TYR:CD2   | 2.40                     | 0.57              |
| 79:s2:21:U:H2'     | 79:s2:22:A:C8      | 2.40                     | 0.57              |
| 79:s2:41:G:OP2     | 79:s2:486:A:N6     | 2.22                     | 0.57              |
| 79:s2:1101:U:H2'   | 79:s2:1102:G:C8    | 2.40                     | 0.57              |
| 79:s2:1372:U:P     | 79:s2:1385:G:H1    | 2.26                     | 0.57              |
| 80:cB:24:VAL:HG12  | 80:cB:104:ASP:HA   | 1.86                     | 0.57              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 80:cB:549:ALA:H    | 80:cB:553:HIS:CD2  | 2.23                     | 0.57              |
| 82:pE:4:C:H2'      | 82:pE:5:G:C8       | 2.39                     | 0.57              |
| 83:ls:12:ASN:O     | 83:ls:16:LYS:HG2   | 2.05                     | 0.57              |
| 85:l5:271:C:H2'    | 85:l5:272:U:H6     | 1.69                     | 0.57              |
| 85:l5:908:G:H2'    | 85:l5:909:A:C8     | 2.39                     | 0.57              |
| 85:l5:2034:G:H2'   | 85:l5:2035:C:C6    | 2.40                     | 0.57              |
| 85:l5:3871:A:H2'   | 85:l5:3872:A:C8    | 2.40                     | 0.57              |
| 85:l5:4108:G:H2'   | 85:l5:4109:G:C8    | 2.40                     | 0.57              |
| 85:l5:4130:C:H2'   | 85:l5:4131:G:C8    | 2.40                     | 0.57              |
| 80:CB:435:THR:HG23 | 80:CB:438:LYS:HE2  | 1.87                     | 0.57              |
| 3:SI:22:HIS:HB3    | 79:S2:433:A:H5''   | 1.87                     | 0.57              |
| 3:SI:126:GLY:H     | 3:SI:128:LYS:HE3   | 1.70                     | 0.57              |
| 6:SG:212:LEU:O     | 6:SG:216:ARG:N     | 2.24                     | 0.57              |
| 12:SH:160:LYS:C    | 12:SH:163:GLN:HE22 | 2.12                     | 0.57              |
| 85:L5:241:G:OP1    | 44:LY:28:LYS:NZ    | 2.36                     | 0.57              |
| 85:L5:273:U:H2'    | 85:L5:274:C:C6     | 2.40                     | 0.57              |
| 85:L5:363:A:N7     | 85:L5:378:A:N6     | 2.53                     | 0.57              |
| 85:L5:365:U:H2'    | 85:L5:366:A:C8     | 2.40                     | 0.57              |
| 85:L5:1857:C:H2'   | 85:L5:1858:A:C8    | 2.39                     | 0.57              |
| 85:L5:1865:G:OP2   | 30:LI:98:ARG:NH2   | 2.29                     | 0.57              |
| 85:L5:2634:C:H2'   | 85:L5:2635:U:H6    | 1.70                     | 0.57              |
| 85:L5:2786:C:O2'   | 85:L5:2787:A:OP2   | 2.18                     | 0.57              |
| 85:L5:2884:G:H2'   | 85:L5:2885:A:H8    | 1.70                     | 0.57              |
| 85:L5:4581:G:O2'   | 23:LB:92:TYR:OH    | 2.20                     | 0.57              |
| 85:L5:4680:G:H2'   | 85:L5:4681:A:C8    | 2.40                     | 0.57              |
| 23:LB:264:PHE:N    | 35:LO:64:THR:O     | 2.31                     | 0.57              |
| 24:LC:331:TYR:CG   | 24:LC:335:MET:HE1  | 2.39                     | 0.57              |
| 32:LL:164:GLU:HB2  | 46:La:100:ILE:HG21 | 1.85                     | 0.57              |
| 47:Lb:103:LYS:HG3  | 47:Lb:104:LEU:HD12 | 1.87                     | 0.57              |
| 74:Sd:6:LEU:HD11   | 79:S2:1301:A:H5''  | 1.87                     | 0.57              |
| 75:Sg:60:ARG:HH22  | 79:S2:1397:U:C2'   | 2.18                     | 0.57              |
| 78:Sf:95:ARG:HH22  | 79:S2:1305:C:H3'   | 1.68                     | 0.57              |
| 79:S2:51:U:H2'     | 79:S2:52:G:H8      | 1.69                     | 0.57              |
| 79:S2:145:G:H2'    | 79:S2:146:G:H8     | 1.70                     | 0.57              |
| 79:S2:573:U:H1'    | 79:S2:576:A:N7     | 2.19                     | 0.57              |
| 79:S2:669:A:H2'    | 79:S2:670:A:C4     | 2.40                     | 0.57              |
| 79:S2:1049:A:OP2   | 79:S2:1068:G:N1    | 2.30                     | 0.57              |
| 79:S2:1781:A:H3'   | 79:S2:1783:C:C2    | 2.39                     | 0.57              |
| 2:sE:16:LYS:NZ     | 79:s2:847:A:H5'    | 2.20                     | 0.56              |
| 5:sX:76:LYS:HE2    | 79:s2:482:G:H5'    | 1.87                     | 0.56              |
| 10:sA:90:PHE:HA    | 10:sA:202:TYR:HH   | 1.70                     | 0.56              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 13:sV:64:GLU:CG    | 19:sb:3:LEU:HD21   | 2.34                     | 0.56              |
| 24:lC:190:ARG:HH22 | 85:l5:2295:C:H3'   | 1.70                     | 0.56              |
| 26:lE:264:ILE:CG1  | 26:lE:267:LEU:HD21 | 2.35                     | 0.56              |
| 40:lT:105:PHE:CE1  | 85:l5:1802:A:H4'   | 2.40                     | 0.56              |
| 40:lT:159:MET:H    | 40:lT:159:MET:CE   | 2.14                     | 0.56              |
| 47:lb:13:SER:HA    | 47:lb:16:TRP:NE1   | 2.20                     | 0.56              |
| 50:le:104:SER:OG   | 85:l5:2305:U:O2'   | 2.21                     | 0.56              |
| 53:lh:32:ARG:HD3   | 53:lh:32:ARG:C     | 2.30                     | 0.56              |
| 56:lk:54:GLU:O     | 56:lk:58:GLN:NE2   | 2.33                     | 0.56              |
| 65:sD:192:TRP:CD2  | 65:sD:203:PRO:HB3  | 2.40                     | 0.56              |
| 75:sg:38:LYS:HA    | 75:sg:65:PHE:HA    | 1.87                     | 0.56              |
| 80:cB:477:GLN:N    | 80:cB:477:GLN:OE1  | 2.38                     | 0.56              |
| 85:l5:664:G:N2     | 85:l5:666:G:O6     | 2.38                     | 0.56              |
| 85:l5:717:U:H2'    | 85:l5:718:C:C6     | 2.40                     | 0.56              |
| 85:l5:733:A:N6     | 85:l5:933:G:O6     | 2.32                     | 0.56              |
| 85:l5:1095:A:H2    | 85:l5:1200:G:C2    | 2.22                     | 0.56              |
| 85:l5:1308:C:H2'   | 85:l5:1309:C:H6    | 1.66                     | 0.56              |
| 85:l5:2413:U:H2'   | 85:l5:2414:G:C8    | 2.40                     | 0.56              |
| 85:l5:2540:C:H2'   | 85:l5:2541:G:C8    | 2.40                     | 0.56              |
| 85:l5:2638:G:N1    | 85:l5:2718:U:H2'   | 2.20                     | 0.56              |
| 85:l5:4153:C:H2'   | 85:l5:4154:G:C8    | 2.40                     | 0.56              |
| 85:l5:4154:G:H2'   | 85:l5:4155:C:C6    | 2.40                     | 0.56              |
| 2:SE:45:ILE:HG13   | 2:SE:61:VAL:HG11   | 1.87                     | 0.56              |
| 5:SX:66:ILE:O      | 5:SX:68:LYS:NZ     | 2.38                     | 0.56              |
| 15:SC:73:MET:SD    | 15:SC:96:PHE:HZ    | 2.28                     | 0.56              |
| 17:SO:33:ILE:HD12  | 17:SO:42:VAL:HA    | 1.87                     | 0.56              |
| 85:L5:920:C:H5''   | 39:LS:74:ARG:CZ    | 2.35                     | 0.56              |
| 85:L5:2748:C:H2'   | 85:L5:2749:C:C6    | 2.40                     | 0.56              |
| 85:L5:4587:G:OP1   | 35:LO:61:ARG:NH1   | 2.38                     | 0.56              |
| 25:LD:39:GLN:OE1   | 25:LD:40:ASP:N     | 2.38                     | 0.56              |
| 26:LE:150:LEU:HD12 | 26:LE:151:ILE:H    | 1.67                     | 0.56              |
| 29:LH:92:MET:HE1   | 29:LH:162:GLN:HB2  | 1.87                     | 0.56              |
| 32:LL:110:LEU:O    | 32:LL:114:VAL:HG12 | 2.05                     | 0.56              |
| 38:LR:21:LYS:HE2   | 38:LR:55:VAL:HA    | 1.86                     | 0.56              |
| 39:LS:140:PRO:HA   | 39:LS:143:LYS:HD2  | 1.87                     | 0.56              |
| 41:LU:56:LEU:HG    | 41:LU:61:VAL:HG13  | 1.86                     | 0.56              |
| 55:Lj:35:GLY:O     | 55:Lj:45:ARG:NH2   | 2.38                     | 0.56              |
| 63:Lz:203:ALA:HA   | 63:Lz:217:TYR:HA   | 1.87                     | 0.56              |
| 63:Lz:214:GLN:N    | 63:Lz:215:ARG:HH21 | 1.94                     | 0.56              |
| 76:SM:24:THR:HG21  | 76:SM:116:LYS:HG2  | 1.87                     | 0.56              |
| 76:SM:28:HIS:CE1   | 76:SM:116:LYS:NZ   | 2.67                     | 0.56              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 79:S2:327:G:H5''   | 79:S2:328:U:C2    | 2.40                     | 0.56              |
| 79:S2:1013:U:H2'   | 79:S2:1014:G:H8   | 1.70                     | 0.56              |
| 79:S2:1094:C:H2'   | 79:S2:1095:C:C6   | 2.40                     | 0.56              |
| 79:S2:1703:C:H2'   | 79:S2:1704:C:O4'  | 2.04                     | 0.56              |
| 2:sE:37:LYS:HB2    | 2:sE:40:GLU:HG2   | 1.86                     | 0.56              |
| 2:sE:125:LYS:O     | 2:sE:142:HIS:N    | 2.37                     | 0.56              |
| 3:sI:77:ARG:HH12   | 3:sI:79:ILE:HG12  | 1.69                     | 0.56              |
| 3:sI:141:ARG:NE    | 79:s2:191:A:OP1   | 2.38                     | 0.56              |
| 6:sG:32:MET:HE1    | 6:sG:66:GLY:H     | 1.70                     | 0.56              |
| 6:sG:76:LEU:HA     | 6:sG:94:ARG:HA    | 1.86                     | 0.56              |
| 7:sJ:128:VAL:HG22  | 7:sJ:132:GLN:HE21 | 1.69                     | 0.56              |
| 10:sA:39:TYR:OH    | 64:sR:104:GLU:OE1 | 2.15                     | 0.56              |
| 25:lD:63:GLN:HB2   | 25:lD:74:ILE:CD1  | 2.35                     | 0.56              |
| 48:lc:77:ASN:CG    | 48:lc:80:GLU:HG2  | 2.30                     | 0.56              |
| 64:sR:32:LYS:CG    | 79:s2:1453:C:H2'  | 2.35                     | 0.56              |
| 69:sQ:4:LYS:HG2    | 79:s2:1423:C:H41  | 1.70                     | 0.56              |
| 75:sg:8:ARG:N      | 75:sg:309:VAL:O   | 2.38                     | 0.56              |
| 75:sg:213:ASP:OD1  | 75:sg:213:ASP:N   | 2.32                     | 0.56              |
| 76:sM:44:LYS:NZ    | 76:sM:47:ALA:HB2  | 2.19                     | 0.56              |
| 79:s2:889:U:OP2    | 79:s2:896:U:N3    | 2.38                     | 0.56              |
| 79:s2:1712:A:H2'   | 79:s2:1713:C:H6   | 1.70                     | 0.56              |
| 80:cB:221:TRP:CE2  | 80:cB:340:MET:HE1 | 2.40                     | 0.56              |
| 81:aP:49:C:H2'     | 81:aP:50:U:H6     | 1.69                     | 0.56              |
| 84:lt:83:LYS:HA    | 84:lt:86:LYS:HE2  | 1.86                     | 0.56              |
| 85:l5:2520:C:H2'   | 85:l5:2521:G:C8   | 2.41                     | 0.56              |
| 85:l5:3963:A:H3'   | 85:l5:3965:A:H5'  | 1.86                     | 0.56              |
| 3:SI:25:ARG:HA     | 79:S2:448:A:H5''  | 1.87                     | 0.56              |
| 3:SI:103:LEU:HD12  | 3:SI:170:LYS:HB3  | 1.86                     | 0.56              |
| 7:SJ:140:GLN:NE2   | 7:SJ:141:VAL:O    | 2.38                     | 0.56              |
| 7:SJ:179:LYS:HA    | 7:SJ:182:GLN:HG2  | 1.87                     | 0.56              |
| 10:SA:145:ILE:HD13 | 10:SA:159:ILE:HB  | 1.87                     | 0.56              |
| 10:SA:177:MET:SD   | 10:SA:177:MET:N   | 2.78                     | 0.56              |
| 85:L5:362:A:OP1    | 57:Ll:34:LYS:NZ   | 2.37                     | 0.56              |
| 85:L5:371:A:O2'    | 85:L5:372:A:O4'   | 2.20                     | 0.56              |
| 85:L5:450:G:H2'    | 85:L5:451:C:C6    | 2.39                     | 0.56              |
| 85:L5:706:C:HO2'   | 85:L5:1298:C:HO2' | 1.47                     | 0.56              |
| 85:L5:976:G:O2'    | 24:LC:333:LYS:NZ  | 2.37                     | 0.56              |
| 85:L5:2372:U:O2'   | 49:Ld:69:ASN:ND2  | 2.35                     | 0.56              |
| 85:L5:2745:A:H2'   | 85:L5:2746:A:H8   | 1.70                     | 0.56              |
| 85:L5:2870:A:H2'   | 85:L5:2871:A:H8   | 1.70                     | 0.56              |
| 85:L5:3952:A:H2'   | 85:L5:3953:G:C8   | 2.40                     | 0.56              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 85:L5:4101:C:H5'  | 85:L5:4107:G:C4'   | 2.35                     | 0.56              |
| 85:L5:4601:U:H2'  | 85:L5:4602:A:H8    | 1.69                     | 0.56              |
| 20:L7:7:G:O3'     | 25:LD:33:ARG:NH2   | 2.37                     | 0.56              |
| 21:L8:8:U:H2'     | 21:L8:9:A:C8       | 2.40                     | 0.56              |
| 24:LC:204:ARG:HE  | 24:LC:205:ARG:H    | 1.52                     | 0.56              |
| 37:LQ:147:GLU:OE1 | 37:LQ:151:HIS:NE2  | 2.38                     | 0.56              |
| 51:Lf:45:LYS:HD2  | 51:Lf:105:LEU:HA   | 1.86                     | 0.56              |
| 51:Lf:50:VAL:HA   | 51:Lf:69:VAL:HG12  | 1.86                     | 0.56              |
| 63:Lz:31:THR:O    | 63:Lz:208:SER:OG   | 2.10                     | 0.56              |
| 75:Sg:201:SER:OG  | 75:Sg:203:ASP:O    | 2.22                     | 0.56              |
| 79:S2:694:G:N7    | 79:S2:696:G:N2     | 2.53                     | 0.56              |
| 79:S2:947:G:H2'   | 79:S2:948:C:H6     | 1.70                     | 0.56              |
| 79:S2:1174:U:H2'  | 79:S2:1175:G:C8    | 2.39                     | 0.56              |
| 79:S2:1210:G:O3'  | 79:S2:1211:G:H5'   | 2.05                     | 0.56              |
| 79:S2:1276:A:C5   | 79:S2:1322:G:H1'   | 2.40                     | 0.56              |
| 83:Ls:63:LYS:HG3  | 83:Ls:68:HIS:HE1   | 1.70                     | 0.56              |
| 2:sE:103:TYR:CE1  | 2:sE:189:LEU:HG    | 2.40                     | 0.56              |
| 2:sE:199:GLU:OE1  | 2:sE:201:HIS:CE1   | 2.58                     | 0.56              |
| 9:se:35:ARG:NH2   | 79:s2:526:A:OP1    | 2.38                     | 0.56              |
| 10:sA:169:HIS:HA  | 10:sA:203:PHE:CE2  | 2.39                     | 0.56              |
| 11:sB:133:TYR:CD1 | 11:sB:221:PRO:HD2  | 2.40                     | 0.56              |
| 18:sW:24:GLN:NE2  | 19:sb:7:LEU:HD12   | 2.18                     | 0.56              |
| 18:sW:71:LYS:HB3  | 18:sW:130:PHE:CE1  | 2.39                     | 0.56              |
| 19:sb:72:ARG:HH12 | 79:s2:1120:U:P     | 2.28                     | 0.56              |
| 23:lB:58:ARG:NH2  | 23:lB:361:GLU:OE1  | 2.37                     | 0.56              |
| 23:lB:116:ARG:NH1 | 85:l5:4987:C:OP1   | 2.37                     | 0.56              |
| 24:lC:36:ILE:HD11 | 85:l5:1350:C:H4'   | 1.87                     | 0.56              |
| 24:lC:161:TYR:CE2 | 24:lC:166:GLU:HB2  | 2.41                     | 0.56              |
| 24:lC:261:ASP:O   | 24:lC:265:GLY:N    | 2.27                     | 0.56              |
| 25:lD:177:THR:HA  | 25:lD:180:PHE:CE2  | 2.40                     | 0.56              |
| 27:lF:148:LYS:HG2 | 27:lF:245:ARG:HH21 | 1.69                     | 0.56              |
| 27:lF:179:LEU:HB3 | 27:lF:184:ILE:HB   | 1.87                     | 0.56              |
| 30:lI:76:MET:HE3  | 30:lI:80:CYS:HB2   | 1.87                     | 0.56              |
| 34:lN:17:ASP:OD1  | 34:lN:20:ARG:NH2   | 2.38                     | 0.56              |
| 35:lO:28:LEU:HD13 | 35:lO:88:LEU:HD22  | 1.87                     | 0.56              |
| 40:lT:68:THR:OG1  | 40:lT:69:GLN:N     | 2.36                     | 0.56              |
| 43:lX:72:ASP:O    | 43:lX:76:ILE:HG13  | 2.04                     | 0.56              |
| 51:lF:100:ARG:NH2 | 85:l5:4753:U:OP1   | 2.36                     | 0.56              |
| 58:lm:104:HIS:CE1 | 85:l5:4697:U:H4'   | 2.40                     | 0.56              |
| 62:lr:93:ILE:HA   | 62:lr:96:MET:HG2   | 1.86                     | 0.56              |
| 63:lz:105:LYS:HE3 | 63:lz:131:ALA:HB1  | 1.86                     | 0.56              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 64:sR:14:ARG:NH2   | 79:s2:1465:A:O2'   | 2.39                     | 0.56              |
| 65:sD:60:GLY:HA3   | 65:sD:65:ARG:H     | 1.70                     | 0.56              |
| 65:sD:106:ARG:HE   | 65:sD:173:ARG:HD3  | 1.68                     | 0.56              |
| 65:sD:136:VAL:HG13 | 65:sD:152:PHE:HD1  | 1.70                     | 0.56              |
| 66:sF:135:ARG:O    | 66:sF:203:ASN:ND2  | 2.39                     | 0.56              |
| 67:sK:27:VAL:HG23  | 67:sK:28:HIS:CD2   | 2.40                     | 0.56              |
| 67:sK:28:HIS:NE2   | 74:sd:7:TYR:OH     | 2.33                     | 0.56              |
| 69:sQ:18:THR:OG1   | 69:sQ:75:GLY:HA2   | 2.05                     | 0.56              |
| 79:s2:222:U:H2'    | 79:s2:223:C:C6     | 2.40                     | 0.56              |
| 79:s2:385:G:N3     | 79:s2:385:G:H5'    | 2.21                     | 0.56              |
| 79:s2:735:C:H5''   | 79:s2:736:C:C2     | 2.41                     | 0.56              |
| 79:s2:882:U:H1'    | 79:s2:905:C:C2     | 2.41                     | 0.56              |
| 79:s2:1103:C:H2'   | 79:s2:1104:G:C8    | 2.40                     | 0.56              |
| 79:s2:1459:G:H2'   | 79:s2:1460:C:C6    | 2.39                     | 0.56              |
| 79:s2:1513:C:H2'   | 79:s2:1514:G:C8    | 2.39                     | 0.56              |
| 79:s2:1544:C:N4    | 79:s2:1589:A:OP2   | 2.38                     | 0.56              |
| 80:cB:178:PHE:O    | 80:cB:181:ILE:HG22 | 2.05                     | 0.56              |
| 80:cB:290:CYS:HA   | 80:cB:294:LEU:CD1  | 2.35                     | 0.56              |
| 84:lt:106:PHE:HA   | 84:lt:109:ILE:HD13 | 1.88                     | 0.56              |
| 85:l5:1199:G:H2'   | 85:l5:1200:G:C8    | 2.40                     | 0.56              |
| 85:l5:1648:C:OP2   | 85:l5:1649:U:O2'   | 2.19                     | 0.56              |
| 85:l5:2634:C:H2'   | 85:l5:2635:U:C6    | 2.40                     | 0.56              |
| 85:l5:2745:A:H2'   | 85:l5:2746:A:C8    | 2.39                     | 0.56              |
| 85:l5:3664:G:H2'   | 85:l5:3665:G:C8    | 2.40                     | 0.56              |
| 85:l5:3827:G:O2'   | 85:l5:3829:G:OP2   | 2.19                     | 0.56              |
| 85:l5:4446:U:O2'   | 85:l5:4450:U:OP1   | 2.21                     | 0.56              |
| 85:l5:4524:G:H2'   | 85:l5:4525:C:C6    | 2.39                     | 0.56              |
| 85:l5:5023:C:H3'   | 85:l5:5024:C:H4'   | 1.87                     | 0.56              |
| 80:CB:395:MET:SD   | 80:CB:417:PHE:HB2  | 2.46                     | 0.56              |
| 80:CB:509:VAL:HB   | 80:CB:570:ILE:HD12 | 1.87                     | 0.56              |
| 80:CB:571:LYS:NZ   | 80:CB:572:LYS:O    | 2.39                     | 0.56              |
| 80:CB:651:CYS:HB3  | 80:CB:680:VAL:HG23 | 1.87                     | 0.56              |
| 6:SG:215:LYS:NZ    | 6:SG:219:GLU:OE1   | 2.39                     | 0.56              |
| 10:SA:80:ARG:O     | 10:SA:84:GLN:NE2   | 2.38                     | 0.56              |
| 14:Sa:82:LYS:NZ    | 79:S2:1209:A:H5''  | 2.20                     | 0.56              |
| 18:SW:12:LYS:HE3   | 79:S2:1152:U:H2'   | 1.86                     | 0.56              |
| 85:L5:1:C:H4'      | 85:L5:2:G:O4'      | 2.05                     | 0.56              |
| 85:L5:62:A:OP1     | 34:LN:172:ARG:NH1  | 2.37                     | 0.56              |
| 85:L5:270:U:H2'    | 85:L5:271:C:C6     | 2.41                     | 0.56              |
| 85:L5:469:C:N3     | 26:LE:105:ARG:NH2  | 2.50                     | 0.56              |
| 85:L5:663:G:H2'    | 85:L5:664:G:C8     | 2.41                     | 0.56              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 85:L5:711:A:H2'    | 85:L5:712:C:C6     | 2.40                     | 0.56              |
| 85:L5:1094:G:O6    | 85:L5:1201:U:O4    | 2.22                     | 0.56              |
| 85:L5:1353:G:N7    | 37:LQ:104:ARG:NH2  | 2.53                     | 0.56              |
| 85:L5:1414:C:H2'   | 85:L5:1415:G:C8    | 2.31                     | 0.56              |
| 85:L5:1566:C:H2'   | 85:L5:1567:U:C6    | 2.39                     | 0.56              |
| 85:L5:1629:G:H1    | 22:LA:208:GLU:CD   | 2.12                     | 0.56              |
| 85:L5:2277:C:H2'   | 85:L5:2278:G:H8    | 1.70                     | 0.56              |
| 85:L5:4105:A:H4'   | 85:L5:4106:G:O4'   | 2.05                     | 0.56              |
| 85:L5:4246:G:H2'   | 85:L5:4247:G:H8    | 1.68                     | 0.56              |
| 85:L5:4765:G:H21   | 39:LS:173:ASN:HD21 | 1.52                     | 0.56              |
| 21:L8:130:C:H2'    | 21:L8:131:G:H8     | 1.70                     | 0.56              |
| 25:LD:33:ARG:O     | 25:LD:37:VAL:HG22  | 2.05                     | 0.56              |
| 25:LD:59:ASP:OD1   | 25:LD:60:ILE:N     | 2.38                     | 0.56              |
| 26:LE:68:MET:HE2   | 26:LE:68:MET:HA    | 1.87                     | 0.56              |
| 27:LF:226:HIS:CD2  | 27:LF:228:VAL:H    | 2.23                     | 0.56              |
| 32:LL:194:ILE:HG23 | 32:LL:198:ARG:HH12 | 1.70                     | 0.56              |
| 34:LN:10:LEU:HA    | 54:Li:44:ILE:CD1   | 2.36                     | 0.56              |
| 34:LN:37:HIS:O     | 34:LN:63:ARG:N     | 2.34                     | 0.56              |
| 35:LO:9:LEU:HB2    | 35:LO:35:VAL:HG22  | 1.87                     | 0.56              |
| 46:La:62:HIS:CD2   | 46:La:64:LYS:HE2   | 2.41                     | 0.56              |
| 49:Ld:23:ARG:HG3   | 49:Ld:121:ASN:HA   | 1.87                     | 0.56              |
| 53:Lh:57:VAL:O     | 53:Lh:61:ILE:HG12  | 2.06                     | 0.56              |
| 54:Li:92:ASN:OD1   | 54:Li:93:VAL:N     | 2.37                     | 0.56              |
| 61:Lp:29:ILE:HD11  | 61:Lp:69:TRP:CD2   | 2.41                     | 0.56              |
| 62:Lr:65:LYS:HB2   | 62:Lr:77:TYR:CE1   | 2.40                     | 0.56              |
| 66:SF:100:ILE:HD11 | 66:SF:178:ILE:HG23 | 1.86                     | 0.56              |
| 66:SF:146:ARG:O    | 66:SF:149:GLN:NE2  | 2.39                     | 0.56              |
| 67:SK:55:ARG:NH1   | 79:S2:1277:C:O3'   | 2.38                     | 0.56              |
| 68:SP:75:VAL:HA    | 68:SP:93:MET:HG3   | 1.85                     | 0.56              |
| 76:SM:79:VAL:HG21  | 76:SM:88:TRP:CH2   | 2.40                     | 0.56              |
| 79:S2:41:G:OP2     | 79:S2:486:A:N6     | 2.34                     | 0.56              |
| 79:S2:455:A:O2'    | 79:S2:1735:A:N3    | 2.35                     | 0.56              |
| 79:S2:1235:G:H5'   | 79:S2:1247:C:H42   | 1.71                     | 0.56              |
| 79:S2:1447:G:H2'   | 79:S2:1448:A:C8    | 2.41                     | 0.56              |
| 79:S2:1511:U:H2'   | 79:S2:1512:C:H6    | 1.70                     | 0.56              |
| 79:S2:1736:G:H2'   | 79:S2:1737:G:C8    | 2.40                     | 0.56              |
| 81:AP:28:U:H2'     | 81:AP:29:C:O4'     | 2.04                     | 0.56              |
| 84:Lt:78:SER:O     | 84:Lt:82:ILE:HG12  | 2.04                     | 0.56              |
| 4:sL:129:GLY:N     | 4:sL:140:PHE:HE1   | 1.98                     | 0.56              |
| 11:sB:146:ARG:HB2  | 11:sB:149:GLN:CD   | 2.31                     | 0.56              |
| 14:sa:44:ILE:HG23  | 14:sa:67:LEU:HG    | 1.86                     | 0.56              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 14:sa:58:VAL:HG12  | 17:sO:125:LYS:HB3  | 1.88                     | 0.56              |
| 18:sW:114:GLU:OE2  | 18:sW:118:ARG:NE   | 2.38                     | 0.56              |
| 20:l7:1:G:H2'      | 20:l7:2:U:O4'      | 2.05                     | 0.56              |
| 21:l8:90:C:H1'     | 44:lY:24:HIS:HB3   | 1.88                     | 0.56              |
| 22:lA:83:HIS:HB3   | 61:lp:64:VAL:HG12  | 1.86                     | 0.56              |
| 23:lB:46:PHE:N     | 23:lB:347:LEU:O    | 2.38                     | 0.56              |
| 34:lN:173:GLY:HA3  | 34:lN:188:ARG:HH12 | 1.69                     | 0.56              |
| 53:lh:78:TYR:CE2   | 85:l5:16:G:O3'     | 2.59                     | 0.56              |
| 55:lj:50:SER:O     | 55:lj:50:SER:OG    | 2.23                     | 0.56              |
| 55:lj:64:MET:SD    | 55:lj:67:LEU:HD23  | 2.46                     | 0.56              |
| 64:sR:98:VAL:HB    | 64:sR:102:THR:OG1  | 2.05                     | 0.56              |
| 66:sF:61:PHE:CE2   | 73:sc:51:ARG:HG3   | 2.40                     | 0.56              |
| 68:sP:100:LYS:NZ   | 79:s2:1240:A:O4'   | 2.37                     | 0.56              |
| 71:sT:125:PRO:O    | 71:sT:129:ARG:HG2  | 2.05                     | 0.56              |
| 79:s2:89:C:H2'     | 79:s2:90:G:H8      | 1.70                     | 0.56              |
| 79:s2:1058:A:O5'   | 82:pE:38:A:H5''    | 2.05                     | 0.56              |
| 80:cB:315:LEU:O    | 80:cB:319:LEU:N    | 2.38                     | 0.56              |
| 80:cB:670:GLN:HG2  | 80:cB:671:TYR:CD2  | 2.40                     | 0.56              |
| 80:cB:746:LEU:HD11 | 80:cB:785:LYS:HB3  | 1.88                     | 0.56              |
| 85:l5:519:C:H1'    | 85:l5:643:C:C2     | 2.40                     | 0.56              |
| 85:l5:1604:G:H2'   | 85:l5:1605:G:C8    | 2.40                     | 0.56              |
| 85:l5:1752:G:H2'   | 85:l5:1753:G:H8    | 1.70                     | 0.56              |
| 85:l5:1857:C:H2'   | 85:l5:1858:A:C8    | 2.40                     | 0.56              |
| 85:l5:2385:U:H2'   | 85:l5:2386:U:C6    | 2.41                     | 0.56              |
| 85:l5:2611:A:H2'   | 85:l5:2612:G:C8    | 2.40                     | 0.56              |
| 85:l5:3689:G:O2'   | 85:l5:3818:U:OP2   | 2.23                     | 0.56              |
| 85:l5:4071:U:H2'   | 85:l5:4072:C:C6    | 2.41                     | 0.56              |
| 85:l5:4935:C:H2'   | 85:l5:4936:G:C8    | 2.41                     | 0.56              |
| 80:CB:159:LYS:HE2  | 80:CB:218:LEU:HG   | 1.86                     | 0.56              |
| 6:SG:137:ARG:HD2   | 6:SG:178:ARG:CZ    | 2.36                     | 0.56              |
| 8:SY:37:LYS:HB3    | 8:SY:60:PHE:CE2    | 2.40                     | 0.56              |
| 8:SY:87:PRO:HB2    | 8:SY:89:HIS:CD2    | 2.40                     | 0.56              |
| 18:SW:34:ILE:O     | 18:SW:38:LEU:HG    | 2.03                     | 0.56              |
| 85:L5:174:C:H2'    | 85:L5:175:C:C6     | 2.41                     | 0.56              |
| 85:L5:221:C:H2'    | 85:L5:222:C:C6     | 2.40                     | 0.56              |
| 85:L5:980:U:H2'    | 85:L5:981:C:C6     | 2.40                     | 0.56              |
| 85:L5:1819:G:N3    | 25:LD:115:MET:HE1  | 2.20                     | 0.56              |
| 85:L5:4071:U:H2'   | 85:L5:4072:C:C6    | 2.40                     | 0.56              |
| 85:L5:4303:C:H3'   | 85:L5:4305:G:H21   | 1.70                     | 0.56              |
| 85:L5:4748:U:H2'   | 85:L5:4749:C:C6    | 2.41                     | 0.56              |
| 85:L5:4884:G:N7    | 26:LE:272:ARG:NH2  | 2.52                     | 0.56              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 85:L5:4988:U:H4'   | 85:L5:4989:U:H5    | 1.70                     | 0.56              |
| 85:L5:5058:A:H2'   | 85:L5:5059:C:H6    | 1.69                     | 0.56              |
| 22:LA:159:SER:O    | 22:LA:162:ASN:ND2  | 2.35                     | 0.56              |
| 31:LJ:20:LEU:HA    | 31:LJ:132:VAL:HG23 | 1.86                     | 0.56              |
| 31:LJ:38:LYS:HA    | 31:LJ:41:GLU:OE2   | 2.06                     | 0.56              |
| 32:LL:79:GLU:HG3   | 32:LL:110:LEU:HD11 | 1.87                     | 0.56              |
| 33:LM:28:VAL:HG13  | 33:LM:37:LEU:HD22  | 1.86                     | 0.56              |
| 34:LN:139:HIS:HB3  | 34:LN:142:ILE:HG12 | 1.87                     | 0.56              |
| 36:LP:40:HIS:NE2   | 36:LP:110:ASP:O    | 2.35                     | 0.56              |
| 39:LS:81:TRP:C     | 39:LS:127:MET:HB2  | 2.30                     | 0.56              |
| 40:LT:14:MET:CE    | 40:LT:58:HIS:HD1   | 2.17                     | 0.56              |
| 45:LZ:92:ASP:OD1   | 45:LZ:94:THR:OG1   | 2.23                     | 0.56              |
| 46:La:78:LEU:HD11  | 46:La:117:LEU:CD1  | 2.35                     | 0.56              |
| 61:Lp:57:CYS:SG    | 61:Lp:59:SER:OG    | 2.63                     | 0.56              |
| 63:Lz:57:SER:HB2   | 63:Lz:172:VAL:HG22 | 1.87                     | 0.56              |
| 63:Lz:110:PHE:HZ   | 63:Lz:128:LEU:HD11 | 1.70                     | 0.56              |
| 79:S2:1633:A:H2'   | 79:S2:1634:A:C8    | 2.40                     | 0.56              |
| 84:Lt:63:THR:CG2   | 84:Lt:70:GLN:HB2   | 2.36                     | 0.56              |
| 3:sI:205:ARG:NE    | 3:sI:205:ARG:O     | 2.39                     | 0.56              |
| 6:sG:32:MET:HE1    | 6:sG:65:GLN:HA     | 1.87                     | 0.56              |
| 10:sA:31:ASP:HB2   | 10:sA:151:ASP:HA   | 1.87                     | 0.56              |
| 10:sA:176:TRP:CE3  | 10:sA:199:PRO:HB3  | 2.41                     | 0.56              |
| 11:sB:149:GLN:HE21 | 79:s2:1123:C:H4'   | 1.71                     | 0.56              |
| 22:lA:36:GLU:HA    | 22:lA:91:GLY:HA2   | 1.86                     | 0.56              |
| 23:lB:282:LYS:HB3  | 23:lB:333:LEU:HD12 | 1.88                     | 0.56              |
| 26:lE:262:LYS:HG2  | 26:lE:268:GLN:HE21 | 1.70                     | 0.56              |
| 32:lL:116:ARG:NH2  | 32:lL:155:MET:O    | 2.33                     | 0.56              |
| 37:lQ:10:ASP:OD1   | 37:lQ:10:ASP:N     | 2.30                     | 0.56              |
| 38:lR:162:ARG:NH2  | 79:s2:873:G:N7     | 2.53                     | 0.56              |
| 41:lU:107:LYS:NZ   | 85:l5:2717:G:H5'   | 2.21                     | 0.56              |
| 49:ld:108:TYR:HE1  | 49:ld:110:PRO:HA   | 1.71                     | 0.56              |
| 51:lf:46:ARG:O     | 51:lf:104:MET:HG2  | 2.05                     | 0.56              |
| 58:lm:94:MET:HE2   | 58:lm:121:LEU:HB3  | 1.86                     | 0.56              |
| 64:sR:126:MET:HE1  | 64:sR:129:LYS:HB2  | 1.87                     | 0.56              |
| 70:sS:112:GLU:HG2  | 70:sS:116:LYS:HZ3  | 1.71                     | 0.56              |
| 71:sT:30:VAL:HG12  | 71:sT:53:PHE:CD2   | 2.41                     | 0.56              |
| 79:s2:89:C:H2'     | 79:s2:90:G:C8      | 2.40                     | 0.56              |
| 79:s2:1389:C:C2    | 79:s2:1390:U:C5    | 2.92                     | 0.56              |
| 79:s2:1700:C:O2    | 79:s2:1834:A:N6    | 2.38                     | 0.56              |
| 80:cB:131:CYS:HB3  | 80:cB:157:MET:CE   | 2.35                     | 0.56              |
| 85:l5:2353:U:H2'   | 85:l5:2354:G:H8    | 1.70                     | 0.56              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 85:l5:2569:G:H2'  | 85:l5:2570:U:C6    | 2.41                     | 0.56              |
| 85:l5:2653:C:H2'  | 85:l5:2654:C:H6    | 1.71                     | 0.56              |
| 6:SG:63:MET:HB3   | 6:SG:98:ARG:HB3    | 1.88                     | 0.56              |
| 7:SJ:109:ARG:HG2  | 7:SJ:146:SER:HA    | 1.88                     | 0.56              |
| 8:SY:122:LYS:NZ   | 79:S2:151:C:H5''   | 2.21                     | 0.56              |
| 8:SY:122:LYS:HZ1  | 79:S2:151:C:H5''   | 1.70                     | 0.56              |
| 16:SN:74:ILE:H    | 16:SN:74:ILE:HD12  | 1.70                     | 0.56              |
| 85:L5:952:G:H2'   | 85:L5:953:C:C6     | 2.41                     | 0.56              |
| 85:L5:1505:C:H2'  | 85:L5:1506:G:H8    | 1.69                     | 0.56              |
| 85:L5:1865:G:P    | 30:LI:98:ARG:HH21  | 2.29                     | 0.56              |
| 85:L5:2610:G:H2'  | 85:L5:2611:A:H8    | 1.70                     | 0.56              |
| 85:L5:2859:G:H21  | 85:L5:3837:C:H1'   | 1.71                     | 0.56              |
| 85:L5:3917:A:H2'  | 85:L5:3918:G:H8    | 1.70                     | 0.56              |
| 85:L5:4507:A:H2'  | 85:L5:4508:C:H6    | 1.71                     | 0.56              |
| 85:L5:4537:C:H2'  | 85:L5:4538:G:C8    | 2.40                     | 0.56              |
| 85:L5:4584:A:H2'  | 85:L5:4585:U:O4'   | 2.06                     | 0.56              |
| 85:L5:4621:C:H2'  | 85:L5:4622:A:H8    | 1.71                     | 0.56              |
| 85:L5:4642:U:H2'  | 85:L5:4643:G:C8    | 2.41                     | 0.56              |
| 85:L5:4699:U:H1'  | 85:L5:4700:A:H5''  | 1.87                     | 0.56              |
| 26:LE:63:TYR:CE1  | 26:LE:68:MET:HB3   | 2.40                     | 0.56              |
| 27:LF:122:PHE:HE2 | 27:LF:145:PRO:HG3  | 1.71                     | 0.56              |
| 30:LI:44:ASP:HA   | 30:LI:171:TRP:HZ2  | 1.70                     | 0.56              |
| 43:LX:105:ASN:O   | 43:LX:109:ILE:HG12 | 2.05                     | 0.56              |
| 66:SF:112:LEU:O   | 66:SF:116:ILE:HG12 | 2.06                     | 0.56              |
| 68:SP:79:HIS:HB2  | 79:S2:1298:G:H1'   | 1.87                     | 0.56              |
| 75:Sg:163:PRO:O   | 75:Sg:178:ASN:HA   | 2.04                     | 0.56              |
| 79:S2:655:A:H4'   | 79:S2:656:G:H3'    | 1.87                     | 0.56              |
| 79:S2:1218:C:H2'  | 79:S2:1219:C:C6    | 2.41                     | 0.56              |
| 4:sL:47:PRO:HB2   | 4:sL:49:GLU:OE2    | 2.05                     | 0.56              |
| 5:sX:85:VAL:HG12  | 5:sX:122:VAL:HB    | 1.88                     | 0.56              |
| 6:sG:74:ARG:HA    | 6:sG:96:SER:HA     | 1.88                     | 0.56              |
| 8:sY:7:ILE:HD11   | 8:sY:25:ILE:HB     | 1.87                     | 0.56              |
| 18:sW:101:PHE:HD1 | 18:sW:112:ASP:OD1  | 1.87                     | 0.56              |
| 23:lB:220:ILE:HB  | 23:lB:346:THR:HB   | 1.88                     | 0.56              |
| 27:lF:236:ARG:HD3 | 27:lF:239:GLN:HB2  | 1.87                     | 0.56              |
| 29:lH:111:LEU:HB2 | 29:lH:127:ARG:HH12 | 1.71                     | 0.56              |
| 33:lM:119:ARG:HD2 | 35:lO:189:ILE:HD12 | 1.88                     | 0.56              |
| 38:lR:145:LEU:HA  | 38:lR:148:ASP:OD2  | 2.06                     | 0.56              |
| 39:lS:83:ARG:HH21 | 40:lT:156:TYR:CA   | 2.18                     | 0.56              |
| 55:lj:11:ARG:NH1  | 85:l5:1534:A:O2'   | 2.38                     | 0.56              |
| 56:lk:24:LYS:NZ   | 85:l5:2696:A:N1    | 2.47                     | 0.56              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 60:lo:54:PRO:C     | 60:lo:55:ILE:HD13  | 2.31                     | 0.56              |
| 64:sR:31:ASN:HB2   | 79:s2:1455:A:OP2   | 2.05                     | 0.56              |
| 75:sg:40:ILE:HB    | 75:sg:59:LEU:HB3   | 1.87                     | 0.56              |
| 79:s2:115:U:H2'    | 79:s2:116:U:C6     | 2.40                     | 0.56              |
| 79:s2:626:G:N2     | 79:s2:626:G:OP2    | 2.38                     | 0.56              |
| 79:s2:822:U:N3     | 79:s2:826:A:N6     | 2.51                     | 0.56              |
| 80:cB:394:LEU:HD12 | 80:cB:418:SER:O    | 2.06                     | 0.56              |
| 85:l5:90:G:OP2     | 85:l5:92:C:N4      | 2.35                     | 0.56              |
| 85:l5:1258:G:H2'   | 85:l5:1259:G:C8    | 2.41                     | 0.56              |
| 85:l5:1825:A:H2'   | 85:l5:1826:G:H8    | 1.71                     | 0.56              |
| 85:l5:3726:A:H2'   | 85:l5:3727:A:C8    | 2.41                     | 0.56              |
| 85:l5:3774:A:H2'   | 85:l5:3775:A:N3    | 2.21                     | 0.56              |
| 85:l5:4499:G:C2    | 85:l5:4529:G:H1'   | 2.41                     | 0.56              |
| 2:SE:125:LYS:HD3   | 2:SE:126:VAL:O     | 2.06                     | 0.56              |
| 4:SL:107:LYS:NZ    | 79:S2:355:G:OP2    | 2.39                     | 0.56              |
| 18:SW:27:ILE:N     | 18:SW:61:ILE:O     | 2.31                     | 0.56              |
| 85:L5:1089:G:H2'   | 85:L5:1090:G:H8    | 1.69                     | 0.56              |
| 85:L5:1444:G:H22   | 85:L5:2103:G:H1    | 1.52                     | 0.56              |
| 85:L5:2562:G:N2    | 85:L5:2565:A:OP2   | 2.38                     | 0.56              |
| 85:L5:2897:G:H2'   | 85:L5:2898:G:C8    | 2.40                     | 0.56              |
| 85:L5:3892:U:O2    | 36:LP:69:ARG:NH2   | 2.38                     | 0.56              |
| 85:L5:4102:C:C5    | 85:L5:4105:A:N7    | 2.73                     | 0.56              |
| 85:L5:4740:G:H1'   | 85:L5:4742:G:H5''  | 1.88                     | 0.56              |
| 22:LA:19:HIS:HD2   | 22:LA:193:ARG:HA   | 1.67                     | 0.56              |
| 43:LX:141:ALA:HB3  | 43:LX:144:TYR:HE2  | 1.71                     | 0.56              |
| 50:Le:6:PRO:HG3    | 50:Le:73:GLY:HA3   | 1.87                     | 0.56              |
| 66:SF:115:ALA:O    | 66:SF:119:SER:OG   | 2.22                     | 0.56              |
| 67:SK:1:MET:SD     | 67:SK:2:LEU:N      | 2.78                     | 0.56              |
| 75:Sg:159:ASN:HD21 | 75:Sg:162:ASN:HD22 | 1.54                     | 0.56              |
| 75:Sg:280:LYS:HE3  | 79:S2:1458:G:H5''  | 1.88                     | 0.56              |
| 79:S2:328:U:O2'    | 79:S2:329:G:O5'    | 2.21                     | 0.56              |
| 79:S2:458:A:H2'    | 79:S2:459:C:H6     | 1.71                     | 0.56              |
| 82:PE:58:A:O2'     | 82:PE:61:C:N4      | 2.38                     | 0.56              |
| 5:sX:95:GLU:OE2    | 5:sX:140:ARG:NH1   | 2.39                     | 0.56              |
| 6:sG:132:ARG:CZ    | 79:s2:168:C:H1'    | 2.36                     | 0.56              |
| 10:sA:66:VAL:HG11  | 10:sA:185:MET:HG2  | 1.88                     | 0.56              |
| 11:sB:159:GLN:NE2  | 79:s2:932:G:OP2    | 2.38                     | 0.56              |
| 17:sO:103:ASN:ND2  | 17:sO:142:ARG:HG3  | 2.21                     | 0.56              |
| 19:sb:81:ARG:NH2   | 19:sb:84:HIS:O     | 2.38                     | 0.56              |
| 45:lZ:74:VAL:HG13  | 45:lZ:101:PHE:HE2  | 1.71                     | 0.56              |
| 46:la:125:LYS:HG3  | 46:la:145:VAL:HG13 | 1.86                     | 0.56              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 47:lb:111:ARG:NH2  | 85:l5:1266:G:OP2  | 2.38                     | 0.56              |
| 47:lb:118:LEU:HD11 | 85:l5:1241:C:C5   | 2.40                     | 0.56              |
| 54:li:45:ARG:NH2   | 54:li:49:GLY:O    | 2.35                     | 0.56              |
| 64:sR:32:LYS:CG    | 79:s2:1454:A:H4'  | 2.34                     | 0.56              |
| 70:sS:78:LYS:HZ1   | 71:sT:32:GLU:HB2  | 1.71                     | 0.56              |
| 79:s2:1094:C:H2'   | 79:s2:1095:C:C6   | 2.41                     | 0.56              |
| 79:s2:1130:G:N2    | 79:s2:1130:G:OP2  | 2.38                     | 0.56              |
| 79:s2:1759:G:N2    | 79:s2:1760:G:O6   | 2.39                     | 0.56              |
| 80:cB:801:ARG:HB3  | 85:l5:4605:A:C4   | 2.39                     | 0.56              |
| 85:l5:162:A:H2'    | 85:l5:163:A:H8    | 1.70                     | 0.56              |
| 85:l5:406:C:O2'    | 85:l5:407:A:OP1   | 2.24                     | 0.56              |
| 85:l5:4151:G:H2'   | 85:l5:4152:G:H8   | 1.71                     | 0.56              |
| 2:SE:97:GLU:N      | 2:SE:97:GLU:OE1   | 2.38                     | 0.56              |
| 3:SI:125:LYS:H     | 3:SI:128:LYS:NZ   | 2.03                     | 0.56              |
| 7:SJ:151:LEU:O     | 7:SJ:155:LYS:NZ   | 2.38                     | 0.56              |
| 10:SA:44:ASP:OD1   | 10:SA:46:ILE:HG13 | 2.05                     | 0.56              |
| 14:Sa:10:ARG:HH22  | 79:S2:1859:A:P    | 2.29                     | 0.56              |
| 85:L5:1241:C:C4    | 85:L5:1242:G:C8   | 2.94                     | 0.56              |
| 85:L5:1509:C:H2'   | 85:L5:1510:G:C8   | 2.40                     | 0.56              |
| 85:L5:2109:G:H2'   | 85:L5:2110:C:C6   | 2.40                     | 0.56              |
| 85:L5:2624:G:H2'   | 85:L5:2625:U:C6   | 2.41                     | 0.56              |
| 85:L5:3689:G:O2'   | 85:L5:3818:U:OP2  | 2.24                     | 0.56              |
| 85:L5:4101:C:O2    | 85:L5:4106:G:O3'  | 2.24                     | 0.56              |
| 85:L5:4478:G:O2'   | 85:L5:4602:A:N1   | 2.37                     | 0.56              |
| 23:LB:108:GLU:OE2  | 23:LB:109:HIS:ND1 | 2.38                     | 0.56              |
| 35:LO:155:THR:O    | 35:LO:158:GLU:HG2 | 2.06                     | 0.56              |
| 69:SQ:41:MET:HE1   | 71:ST:10:ASN:CA   | 2.28                     | 0.56              |
| 71:ST:42:HIS:HB2   | 71:ST:83:GLN:HA   | 1.88                     | 0.56              |
| 74:Sd:10:HIS:HB3   | 74:Sd:12:ARG:HH21 | 1.71                     | 0.56              |
| 77:SZ:65:TYR:HA    | 77:SZ:111:ARG:HE  | 1.71                     | 0.56              |
| 83:Ls:45:MET:CE    | 84:Lt:122:ALA:HA  | 2.35                     | 0.56              |
| 1:cH:43:LYS:HD2    | 1:cH:44:TRP:N     | 2.21                     | 0.56              |
| 5:sX:53:GLU:OE1    | 5:sX:55:VAL:HG23  | 2.06                     | 0.56              |
| 7:sJ:173:VAL:O     | 7:sJ:177:ASN:ND2  | 2.38                     | 0.56              |
| 30:II:55:ASP:O     | 30:II:56:GLU:HG3  | 2.05                     | 0.56              |
| 31:IJ:95:ARG:NH1   | 31:IJ:96:LYS:H    | 2.03                     | 0.56              |
| 33:IM:46:ARG:NE    | 85:l5:937:U:OP1   | 2.38                     | 0.56              |
| 33:IM:90:ARG:HH22  | 85:l5:4869:U:P    | 2.29                     | 0.56              |
| 33:IM:91:TRP:CZ2   | 85:l5:4870:G:H2'  | 2.41                     | 0.56              |
| 41:IU:24:ASP:OD1   | 41:IU:26:THR:HG23 | 2.06                     | 0.56              |
| 47:lb:92:LYS:O     | 47:lb:96:LEU:HG   | 2.05                     | 0.56              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 50:le:107:ASN:ND2  | 85:l5:2303:C:OP1   | 2.39                     | 0.56              |
| 62:lr:70:GLN:HG3   | 62:lr:71:ARG:HG3   | 1.87                     | 0.56              |
| 66:sF:47:LYS:HD2   | 69:sQ:115:TYR:HE1  | 1.71                     | 0.56              |
| 67:sK:17:LYS:HG3   | 67:sK:18:GLU:HG2   | 1.88                     | 0.56              |
| 75:sg:104:HIS:ND1  | 75:sg:126:ASP:OD2  | 2.27                     | 0.56              |
| 79:s2:71:G:H3'     | 79:s2:72:C:H4'     | 1.88                     | 0.56              |
| 79:s2:352:U:H2'    | 79:s2:353:C:C6     | 2.41                     | 0.56              |
| 79:s2:1009:A:H2'   | 79:s2:1010:G:H8    | 1.71                     | 0.56              |
| 79:s2:1096:G:H1    | 79:s2:1136:U:H3    | 1.51                     | 0.56              |
| 79:s2:1360:U:O2'   | 79:s2:1379:A:OP2   | 2.23                     | 0.56              |
| 79:s2:1540:G:H2'   | 79:s2:1541:G:H8    | 1.71                     | 0.56              |
| 79:s2:1678:A:H2'   | 79:s2:1679:A:N3    | 2.21                     | 0.56              |
| 79:s2:1781:A:H5''  | 79:s2:1783:C:N4    | 2.21                     | 0.56              |
| 80:cB:120:ARG:HH11 | 80:cB:372:LEU:HD23 | 1.71                     | 0.56              |
| 85:l5:450:G:H2'    | 85:l5:451:C:C6     | 2.41                     | 0.56              |
| 85:l5:457:G:H2'    | 85:l5:458:C:H6     | 1.69                     | 0.56              |
| 85:l5:677:G:H2'    | 85:l5:678:C:H6     | 1.70                     | 0.56              |
| 85:l5:1845:U:H2'   | 85:l5:1846:G:H8    | 1.70                     | 0.56              |
| 85:l5:1876:U:H2'   | 85:l5:1877:G:C8    | 2.41                     | 0.56              |
| 85:l5:2480:G:H2'   | 85:l5:2481:G:C8    | 2.41                     | 0.56              |
| 80:CB:157:MET:SD   | 80:CB:181:ILE:HG21 | 2.46                     | 0.56              |
| 7:SJ:81:LEU:HA     | 7:SJ:84:ILE:HD12   | 1.88                     | 0.56              |
| 8:SY:61:ARG:NH2    | 8:SY:62:THR:O      | 2.39                     | 0.56              |
| 11:SB:38:MET:SD    | 11:SB:38:MET:N     | 2.79                     | 0.56              |
| 15:SC:242:ASP:O    | 15:SC:246:LYS:NZ   | 2.38                     | 0.56              |
| 85:L5:1179:U:OP2   | 25:LD:289:ARG:NH1  | 2.38                     | 0.56              |
| 85:L5:2053:C:O3'   | 35:LO:18:ARG:NH2   | 2.39                     | 0.56              |
| 85:L5:4151:G:H2'   | 85:L5:4152:G:C8    | 2.41                     | 0.56              |
| 85:L5:4238:G:H2'   | 85:L5:4239:A:H8    | 1.71                     | 0.56              |
| 85:L5:4642:U:H2'   | 85:L5:4643:G:H8    | 1.70                     | 0.56              |
| 85:L5:4714:C:H4'   | 23:LB:351:LEU:HD11 | 1.87                     | 0.56              |
| 85:L5:4990:C:H5''  | 85:L5:4991:U:H5''  | 1.88                     | 0.56              |
| 23:LB:116:ARG:HG2  | 23:LB:177:LYS:HA   | 1.88                     | 0.56              |
| 26:LE:203:ILE:O    | 26:LE:206:VAL:HG22 | 2.06                     | 0.56              |
| 48:Lc:48:LEU:HD21  | 48:Lc:57:LYS:HB2   | 1.87                     | 0.56              |
| 61:Lp:58:GLY:HA2   | 61:Lp:61:MET:HE1   | 1.88                     | 0.56              |
| 70:SS:63:GLU:HA    | 70:SS:66:ARG:HB2   | 1.87                     | 0.56              |
| 72:SU:40:ILE:O     | 72:SU:44:LYS:HG2   | 2.05                     | 0.56              |
| 76:SM:22:LEU:HD12  | 76:SM:23:LYS:HD3   | 1.88                     | 0.56              |
| 79:S2:349:A:H2'    | 79:S2:350:C:C6     | 2.41                     | 0.56              |
| 79:S2:533:A:H2'    | 79:S2:534:G:C8     | 2.41                     | 0.56              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 79:S2:1420:G:O2'  | 79:S2:1421:A:O4'   | 2.23                     | 0.56              |
| 79:S2:1860:A:HO2' | 79:S2:1862:G:H8    | 1.52                     | 0.56              |
| 1:CH:104:GLN:HB2  | 65:SD:178:ARG:HH22 | 1.69                     | 0.56              |
| 1:cH:88:LYS:HB2   | 1:cH:90:LEU:HD23   | 1.88                     | 0.56              |
| 1:cH:91:THR:N     | 1:cH:94:ASP:OD2    | 2.36                     | 0.56              |
| 4:sL:103:GLU:OE2  | 5:sX:11:ARG:NE     | 2.39                     | 0.56              |
| 6:sG:20:ASP:OD2   | 6:sG:23:LYS:N      | 2.32                     | 0.56              |
| 11:sB:136:ARG:CZ  | 79:s2:941:C:H5''   | 2.35                     | 0.56              |
| 15:sC:258:GLU:OE2 | 15:sC:259:THR:N    | 2.38                     | 0.56              |
| 26:lE:244:GLU:OE1 | 26:lE:247:LYS:HB2  | 2.06                     | 0.56              |
| 30:lI:66:GLU:O    | 30:lI:70:ILE:HG12  | 2.06                     | 0.56              |
| 36:lP:18:ARG:HA   | 36:lP:147:GLU:HA   | 1.88                     | 0.56              |
| 41:lU:107:LYS:NZ  | 85:l5:2716:C:O3'   | 2.39                     | 0.56              |
| 42:IV:87:SER:HB3  | 42:IV:97:TYR:HD1   | 1.71                     | 0.56              |
| 48:lc:81:LEU:HD23 | 48:lc:91:VAL:HG23  | 1.88                     | 0.56              |
| 49:ld:64:ILE:HG22 | 49:ld:106:VAL:CG1  | 2.35                     | 0.56              |
| 62:lr:103:ARG:CZ  | 62:lr:106:LEU:HD11 | 2.36                     | 0.56              |
| 64:sR:41:ILE:HA   | 79:s2:1387:G:C5    | 2.41                     | 0.56              |
| 65:sD:32:ASP:OD2  | 65:sD:65:ARG:NH2   | 2.38                     | 0.56              |
| 75:sg:241:PHE:CZ  | 75:sg:248:LEU:HD22 | 2.41                     | 0.56              |
| 79:s2:1073:U:H2'  | 79:s2:1074:C:H6    | 1.71                     | 0.56              |
| 79:s2:1373:C:O2'  | 79:s2:1374:C:O5'   | 2.24                     | 0.56              |
| 79:s2:1392:U:H2'  | 79:s2:1393:G:C8    | 2.41                     | 0.56              |
| 79:s2:1702:G:O6   | 79:s2:1836:G:N2    | 2.38                     | 0.56              |
| 83:ls:98:ILE:HA   | 83:ls:101:MET:SD   | 2.45                     | 0.56              |
| 85:l5:25:A:C8     | 85:l5:341:G:C8     | 2.93                     | 0.56              |
| 85:l5:1175:A:H2   | 85:l5:1185:G:H1    | 1.51                     | 0.56              |
| 85:l5:1414:C:O2'  | 85:l5:1415:G:H5'   | 2.06                     | 0.56              |
| 85:l5:2323:C:H2'  | 85:l5:2324:C:C6    | 2.41                     | 0.56              |
| 4:SL:65:ASN:HB3   | 79:S2:294:U:C4     | 2.40                     | 0.56              |
| 11:SB:224:GLU:OE2 | 11:SB:226:GLY:N    | 2.39                     | 0.56              |
| 12:SH:25:GLN:HA   | 12:SH:28:LEU:HB2   | 1.87                     | 0.56              |
| 14:Sa:10:ARG:NH1  | 79:S2:1859:A:OP1   | 2.32                     | 0.56              |
| 85:L5:690:C:H2'   | 85:L5:691:C:C6     | 2.41                     | 0.56              |
| 85:L5:707:C:O2'   | 85:L5:4943:A:N1    | 2.34                     | 0.56              |
| 85:L5:956:A:H1'   | 85:L5:2076:G:H5''  | 1.88                     | 0.56              |
| 85:L5:1837:A:OP2  | 40:LT:108:ARG:NH1  | 2.37                     | 0.56              |
| 85:L5:2022:C:H2'  | 85:L5:2023:C:O4'   | 2.06                     | 0.56              |
| 85:L5:2045:G:C6   | 35:LO:62:MET:HB2   | 2.41                     | 0.56              |
| 85:L5:2079:G:H2'  | 85:L5:2080:U:C6    | 2.41                     | 0.56              |
| 85:L5:2399:G:N3   | 52:Lg:4:ARG:NH2    | 2.54                     | 0.56              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 85:L5:2438:A:OP1   | 43:LX:106:LYS:NZ   | 2.31                     | 0.56              |
| 85:L5:2843:U:O2'   | 85:L5:4632:U:OP1   | 2.24                     | 0.56              |
| 85:L5:4080:C:H2'   | 85:L5:4081:G:H8    | 1.71                     | 0.56              |
| 85:L5:4101:C:C4    | 85:L5:4106:G:O5'   | 2.59                     | 0.56              |
| 85:L5:4532:U:OP2   | 85:L5:4554:G:N1    | 2.39                     | 0.56              |
| 24:LC:208:CYS:O    | 24:LC:251:ILE:N    | 2.33                     | 0.56              |
| 29:LH:96:TYR:HA    | 29:LH:177:ASP:HB2  | 1.88                     | 0.56              |
| 45:LZ:10:VAL:HG21  | 45:LZ:129:TRP:HZ3  | 1.71                     | 0.56              |
| 66:SF:85:LYS:O     | 66:SF:88:MET:HG3   | 2.05                     | 0.56              |
| 70:SS:88:LYS:HG3   | 70:SS:88:LYS:O     | 2.06                     | 0.56              |
| 75:Sg:40:ILE:HD11  | 75:Sg:66:VAL:HG21  | 1.88                     | 0.56              |
| 76:SM:93:LYS:HG2   | 76:SM:103:VAL:HG13 | 1.88                     | 0.56              |
| 77:SZ:92:LEU:HG    | 77:SZ:109:TYR:OH   | 2.06                     | 0.56              |
| 79:S2:680:G:H2'    | 79:S2:681:U:H6     | 1.71                     | 0.56              |
| 79:S2:786:G:H2'    | 79:S2:787:G:C8     | 2.41                     | 0.56              |
| 79:S2:1136:U:H2'   | 79:S2:1137:U:C6    | 2.41                     | 0.56              |
| 11:sB:90:ASP:HB2   | 11:sB:97:LEU:HD21  | 1.87                     | 0.56              |
| 18:sW:34:ILE:O     | 18:sW:38:LEU:HG    | 2.06                     | 0.56              |
| 19:sb:8:LEU:HD12   | 19:sb:9:HIS:HB2    | 1.88                     | 0.56              |
| 20:l7:7:G:H5''     | 25:ID:22:ARG:HD3   | 1.88                     | 0.56              |
| 23:lB:113:GLU:OE2  | 23:lB:169:ARG:NH1  | 2.30                     | 0.56              |
| 25:ID:2:GLY:HA2    | 85:l5:1778:C:H1'   | 1.88                     | 0.56              |
| 27:lF:67:THR:O     | 27:lF:70:ARG:N     | 2.39                     | 0.56              |
| 31:lJ:35:ARG:HB3   | 31:lJ:123:ILE:HD13 | 1.86                     | 0.56              |
| 36:lP:69:ARG:NH2   | 85:l5:3893:C:H1'   | 2.20                     | 0.56              |
| 41:lU:19:LEU:HD23  | 41:lU:19:LEU:H     | 1.70                     | 0.56              |
| 62:lr:93:ILE:HA    | 62:lr:96:MET:SD    | 2.46                     | 0.56              |
| 63:lz:175:THR:HG22 | 63:lz:177:ASP:H    | 1.71                     | 0.56              |
| 65:sD:206:ASP:OD1  | 65:sD:206:ASP:N    | 2.39                     | 0.56              |
| 71:sT:114:GLU:N    | 71:sT:114:GLU:OE1  | 2.38                     | 0.56              |
| 79:s2:88:G:N2      | 79:s2:499:G:O3'    | 2.39                     | 0.56              |
| 79:s2:1024:A:H2'   | 79:s2:1025:U:C6    | 2.41                     | 0.56              |
| 79:s2:1852:C:H2'   | 79:s2:1853:C:H6    | 1.71                     | 0.56              |
| 80:cB:111:PHE:HD2  | 80:cB:501:VAL:HG13 | 1.71                     | 0.56              |
| 85:l5:186:G:H1'    | 85:l5:1366:G:H21   | 1.71                     | 0.56              |
| 85:l5:1326:A:H2'   | 85:l5:1327:C:C6    | 2.40                     | 0.56              |
| 85:l5:1552:G:O2'   | 85:l5:1574:G:N2    | 2.36                     | 0.56              |
| 85:l5:1825:A:H2'   | 85:l5:1826:G:C8    | 2.41                     | 0.56              |
| 85:l5:2361:G:O2'   | 85:l5:3859:G:O6    | 2.24                     | 0.56              |
| 85:l5:4601:U:H2'   | 85:l5:4602:A:H8    | 1.71                     | 0.56              |
| 85:l5:4630:G:H5'   | 87:lW:19:ARG:NH1   | 2.21                     | 0.56              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 85:l5:4736:C:H2'   | 85:l5:4737:G:H8    | 1.71                     | 0.56              |
| 80:CB:3:ASN:HA     | 80:CB:46:ILE:HA    | 1.88                     | 0.56              |
| 80:CB:4:PHE:HB3    | 8:SY:130:LYS:HE3   | 1.86                     | 0.56              |
| 80:CB:595:SER:HA   | 80:CB:724:THR:HG21 | 1.88                     | 0.56              |
| 80:CB:830:ARG:HH21 | 80:CB:833:GLN:HE22 | 1.53                     | 0.56              |
| 3:SI:126:GLY:N     | 3:SI:128:LYS:HE3   | 2.21                     | 0.56              |
| 4:SL:67:SER:OG     | 79:S2:114:G:OP2    | 2.24                     | 0.56              |
| 6:SG:21:GLU:N      | 6:SG:21:GLU:OE1    | 2.38                     | 0.56              |
| 6:SG:115:LYS:NZ    | 6:SG:116:LYS:O     | 2.39                     | 0.56              |
| 10:SA:61:ALA:O     | 10:SA:65:ILE:HG12  | 2.05                     | 0.56              |
| 19:Sb:20:LYS:HB3   | 19:Sb:29:ASN:HD21  | 1.70                     | 0.56              |
| 85:L5:432:U:OP2    | 85:L5:3888:G:N2    | 2.39                     | 0.56              |
| 85:L5:1270:A:H8    | 85:L5:2106:G:H21   | 1.54                     | 0.56              |
| 85:L5:2034:G:H2'   | 85:L5:2035:C:C6    | 2.41                     | 0.56              |
| 85:L5:2376:A:H2'   | 85:L5:2377:C:C6    | 2.41                     | 0.56              |
| 85:L5:2495:U:H2'   | 85:L5:2496:G:H8    | 1.71                     | 0.56              |
| 85:L5:2693:G:H2'   | 85:L5:2694:G:N2    | 2.20                     | 0.56              |
| 85:L5:3861:A:H2'   | 85:L5:3862:A:H8    | 1.71                     | 0.56              |
| 85:L5:3938:G:N2    | 85:L5:4171:C:OP2   | 2.36                     | 0.56              |
| 85:L5:4233:A:C8    | 85:L5:4235:G:C8    | 2.94                     | 0.56              |
| 21:L8:141:C:OP1    | 34:LN:38:ARG:NH1   | 2.32                     | 0.56              |
| 26:LE:188:ARG:HH11 | 26:LE:217:PHE:HB3  | 1.70                     | 0.56              |
| 27:LF:200:ARG:NE   | 27:LF:203:GLU:OE2  | 2.39                     | 0.56              |
| 30:LI:62:SER:HA    | 30:LI:65:LEU:HD13  | 1.87                     | 0.56              |
| 38:LR:148:ASP:HA   | 38:LR:151:ARG:HD3  | 1.88                     | 0.56              |
| 42:LV:82:ILE:HG22  | 42:LV:83:ARG:HG3   | 1.88                     | 0.56              |
| 45:LZ:51:ARG:HB2   | 45:LZ:65:ARG:HH11  | 1.71                     | 0.56              |
| 45:LZ:52:LYS:O     | 45:LZ:65:ARG:NH1   | 2.39                     | 0.56              |
| 58:Lm:94:MET:HE1   | 58:Lm:123:PRO:HB3  | 1.88                     | 0.56              |
| 65:SD:214:LYS:HZ2  | 65:SD:215:ASP:N    | 1.93                     | 0.56              |
| 70:SS:66:ARG:O     | 70:SS:70:ILE:HG12  | 2.05                     | 0.56              |
| 78:Sf:103:LEU:O    | 78:Sf:104:LYS:HG2  | 2.06                     | 0.56              |
| 79:S2:654:A:OP2    | 79:S2:655:A:O2'    | 2.20                     | 0.56              |
| 79:S2:1511:U:H2'   | 79:S2:1512:C:C6    | 2.40                     | 0.56              |
| 79:S2:1683:C:H2'   | 79:S2:1684:C:H6    | 1.70                     | 0.56              |
| 81:AP:68:G:H2'     | 81:AP:69:A:C8      | 2.41                     | 0.56              |
| 1:cH:84:GLY:HA2    | 1:cH:88:LYS:NZ     | 2.21                     | 0.55              |
| 10:sA:39:TYR:CE1   | 10:sA:40:LYS:HB3   | 2.40                     | 0.55              |
| 11:sB:151:ARG:HH21 | 79:s2:1101:U:P     | 2.30                     | 0.55              |
| 12:sH:21:SER:HA    | 12:sH:25:GLN:HG2   | 1.88                     | 0.55              |
| 12:sH:64:VAL:N     | 12:sH:95:ILE:O     | 2.37                     | 0.55              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 12:sH:69:LEU:O     | 12:sH:73:GLN:HG3   | 2.05                     | 0.55              |
| 17:sO:32:HIS:HA    | 17:sO:96:LYS:HB3   | 1.88                     | 0.55              |
| 26:lE:66:LYS:NZ    | 85:l5:978:G:OP1    | 2.39                     | 0.55              |
| 27:lF:74:MET:CE    | 85:l5:1089:G:H1'   | 2.35                     | 0.55              |
| 29:lH:1:MET:HE3    | 85:l5:1951:G:OP1   | 2.06                     | 0.55              |
| 44:lY:126:ARG:NH2  | 85:l5:197:A:O5'    | 2.39                     | 0.55              |
| 45:lZ:100:VAL:HG13 | 45:lZ:106:LEU:HD23 | 1.88                     | 0.55              |
| 47:lb:56:LYS:HE3   | 85:l5:1812:C:O3'   | 2.05                     | 0.55              |
| 63:lz:54:ARG:NH2   | 63:lz:154:THR:O    | 2.39                     | 0.55              |
| 64:sR:27:ASP:HB3   | 79:s2:1455:A:OP2   | 2.06                     | 0.55              |
| 75:sg:42:MET:HB2   | 75:sg:57:ARG:HB2   | 1.88                     | 0.55              |
| 77:sZ:80:ARG:O     | 79:s2:1598:G:O2'   | 2.20                     | 0.55              |
| 79:s2:373:G:H2'    | 79:s2:374:G:C8     | 2.40                     | 0.55              |
| 79:s2:386:C:H2'    | 79:s2:387:C:C6     | 2.41                     | 0.55              |
| 79:s2:479:C:C2     | 79:s2:480:G:C8     | 2.93                     | 0.55              |
| 79:s2:647:U:H2'    | 79:s2:648:A:C8     | 2.36                     | 0.55              |
| 79:s2:1279:C:H2'   | 79:s2:1280:G:H8    | 1.70                     | 0.55              |
| 79:s2:1558:C:H2'   | 79:s2:1559:C:C6    | 2.41                     | 0.55              |
| 81:aP:26:G:O6      | 81:aP:44:A:N1      | 2.39                     | 0.55              |
| 85:l5:6:C:H2'      | 85:l5:7:C:C6       | 2.41                     | 0.55              |
| 85:l5:725:G:H2'    | 85:l5:726:G:H8     | 1.70                     | 0.55              |
| 85:l5:2579:G:N2    | 85:l5:2582:A:OP2   | 2.26                     | 0.55              |
| 85:l5:2775:C:H2'   | 85:l5:2776:G:C8    | 2.39                     | 0.55              |
| 85:l5:4177:C:H2'   | 85:l5:4178:A:H8    | 1.70                     | 0.55              |
| 7:SJ:27:GLN:HA     | 7:SJ:30:LYS:HD3    | 1.88                     | 0.55              |
| 8:SY:29:HIS:HB2    | 8:SY:32:LYS:HG2    | 1.88                     | 0.55              |
| 8:SY:47:MET:O      | 8:SY:49:LYS:NZ     | 2.39                     | 0.55              |
| 8:SY:47:MET:HE1    | 8:SY:48:TYR:CZ     | 2.40                     | 0.55              |
| 10:SA:10:MET:HG3   | 64:SR:111:PHE:CZ   | 2.40                     | 0.55              |
| 10:SA:35:GLU:HA    | 10:SA:38:ILE:HG22  | 1.88                     | 0.55              |
| 10:SA:143:PRO:HD3  | 13:SV:32:ILE:HD11  | 1.88                     | 0.55              |
| 18:SW:28:ARG:NH1   | 79:S2:922:A:OP1    | 2.39                     | 0.55              |
| 85:L5:138:G:H2'    | 85:L5:139:G:H8     | 1.71                     | 0.55              |
| 85:L5:279:A:H3'    | 34:LN:47:LYS:HZ1   | 1.71                     | 0.55              |
| 85:L5:364:G:O6     | 55:Lj:55:ARG:NH2   | 2.34                     | 0.55              |
| 85:L5:1504:G:H2'   | 85:L5:1505:C:C6    | 2.42                     | 0.55              |
| 85:L5:1806:G:H2'   | 85:L5:1807:C:H6    | 1.71                     | 0.55              |
| 85:L5:2262:G:OP2   | 62:Lr:98:ARG:NH1   | 2.32                     | 0.55              |
| 85:L5:2436:U:H3'   | 43:LX:127:LEU:HD22 | 1.88                     | 0.55              |
| 85:L5:2458:C:O2'   | 85:L5:3671:G:N3    | 2.38                     | 0.55              |
| 85:L5:2621:A:H2'   | 85:L5:2622:G:H8    | 1.70                     | 0.55              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 85:L5:3633:C:H2'   | 85:L5:3634:G:H8    | 1.72                     | 0.55              |
| 85:L5:3948:C:H5''  | 85:L5:3949:A:OP1   | 2.05                     | 0.55              |
| 85:L5:5010:U:H2'   | 85:L5:5011:A:C8    | 2.41                     | 0.55              |
| 22:LA:29:LEU:HA    | 22:LA:76:PHE:CE1   | 2.41                     | 0.55              |
| 24:LC:318:PRO:HB2  | 24:LC:325:MET:HE3  | 1.88                     | 0.55              |
| 34:LN:22:LEU:HD22  | 34:LN:26:ARG:HH12  | 1.72                     | 0.55              |
| 40:LT:84:ILE:HG13  | 47:Lb:24:PRO:HD3   | 1.88                     | 0.55              |
| 47:Lb:55:LYS:O     | 47:Lb:58:GLN:NE2   | 2.38                     | 0.55              |
| 56:Lk:5:ILE:HD11   | 56:Lk:43:TYR:CB    | 2.32                     | 0.55              |
| 62:Lr:4:HIS:O      | 62:Lr:8:MET:HG3    | 2.05                     | 0.55              |
| 64:SR:126:MET:O    | 64:SR:126:MET:HG3  | 2.06                     | 0.55              |
| 70:SS:60:THR:HG22  | 70:SS:62:ASP:H     | 1.71                     | 0.55              |
| 75:Sg:61:GLY:O     | 75:Sg:88:ARG:NH2   | 2.39                     | 0.55              |
| 79:S2:598:G:O2'    | 79:S2:605:A:N1     | 2.36                     | 0.55              |
| 79:S2:1007:C:H2'   | 79:S2:1008:A:C8    | 2.41                     | 0.55              |
| 6:sG:74:ARG:NH2    | 6:sG:94:ARG:O      | 2.38                     | 0.55              |
| 6:sG:147:LEU:HB3   | 6:sG:151:ASP:HB2   | 1.88                     | 0.55              |
| 6:sG:223:LYS:NZ    | 6:sG:227:GLN:HB2   | 2.21                     | 0.55              |
| 10:sA:3:GLY:O      | 10:sA:9:GLN:NE2    | 2.39                     | 0.55              |
| 11:sB:78:GLU:N     | 11:sB:78:GLU:OE1   | 2.39                     | 0.55              |
| 11:sB:148:ASN:OD1  | 79:s2:1123:C:O2'   | 2.23                     | 0.55              |
| 12:sH:137:SER:OG   | 12:sH:138:GLU:N    | 2.36                     | 0.55              |
| 22:lA:50:HIS:HD2   | 85:l5:2741:U:H2'   | 1.70                     | 0.55              |
| 22:lA:152:SER:OG   | 85:l5:3661:G:N7    | 2.39                     | 0.55              |
| 24:lC:195:LYS:HE3  | 85:l5:2333:G:H5''  | 1.87                     | 0.55              |
| 36:lP:112:LEU:HD22 | 36:lP:150:LEU:HD22 | 1.87                     | 0.55              |
| 38:lR:65:LYS:HA    | 38:lR:68:LEU:HD12  | 1.87                     | 0.55              |
| 39:lS:127:MET:HE2  | 40:lT:153:PRO:O    | 2.07                     | 0.55              |
| 40:lT:108:ARG:NH2  | 85:l5:1837:A:OP2   | 2.40                     | 0.55              |
| 46:la:65:ARG:NH2   | 85:l5:86:U:O2'     | 2.40                     | 0.55              |
| 52:lg:11:LEU:O     | 52:lg:18:ASN:ND2   | 2.39                     | 0.55              |
| 54:li:32:ARG:NH1   | 85:l5:309:C:OP2    | 2.39                     | 0.55              |
| 66:sF:23:TRP:HE1   | 66:sF:101:HIS:CG   | 2.24                     | 0.55              |
| 66:sF:167:LYS:HZ2  | 66:sF:171:GLU:HG3  | 1.71                     | 0.55              |
| 71:sT:133:ARG:O    | 71:sT:137:GLN:OE1  | 2.23                     | 0.55              |
| 72:sU:20:ILE:HG23  | 72:sU:91:LEU:HB2   | 1.88                     | 0.55              |
| 79:s2:1073:U:H2'   | 79:s2:1074:C:C6    | 2.41                     | 0.55              |
| 79:s2:1198:G:H2'   | 79:s2:1199:A:C8    | 2.42                     | 0.55              |
| 80:cB:219:HIS:O    | 80:cB:341:ARG:HD3  | 2.05                     | 0.55              |
| 83:ls:116:ILE:HG23 | 83:ls:118:PRO:HD3  | 1.88                     | 0.55              |
| 85:l5:1084:C:H2'   | 85:l5:1085:C:H6    | 1.71                     | 0.55              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 85:l5:1194:G:H2'   | 85:l5:1195:G:C8    | 2.40                     | 0.55              |
| 85:l5:3770:U:H2'   | 85:l5:3771:C:H6    | 1.71                     | 0.55              |
| 85:l5:3967:G:N2    | 85:l5:4055:U:O2    | 2.32                     | 0.55              |
| 85:l5:4584:A:H2'   | 85:l5:4585:U:O4'   | 2.05                     | 0.55              |
| 80:CB:178:PHE:O    | 80:CB:181:ILE:HG22 | 2.06                     | 0.55              |
| 7:SJ:50:LEU:O      | 7:SJ:53:ILE:HG13   | 2.06                     | 0.55              |
| 11:SB:69:VAL:HG11  | 11:SB:74:LEU:HD13  | 1.89                     | 0.55              |
| 11:SB:93:GLY:O     | 28:LG:264:LYS:NZ   | 2.39                     | 0.55              |
| 12:SH:31:GLU:HA    | 12:SH:37:LYS:HE3   | 1.88                     | 0.55              |
| 15:SC:272:HIS:O    | 15:SC:276:THR:HG22 | 2.06                     | 0.55              |
| 16:SN:49:GLN:O     | 16:SN:53:ILE:HG12  | 2.05                     | 0.55              |
| 19:Sb:35:VAL:HG22  | 19:Sb:79:PHE:HB2   | 1.87                     | 0.55              |
| 85:L5:173:C:H5''   | 32:LL:129:ARG:NH1  | 2.17                     | 0.55              |
| 85:L5:1172:C:H1'   | 85:L5:1189:G:H22   | 1.72                     | 0.55              |
| 85:L5:1559:G:H5'   | 38:LR:126:LYS:NZ   | 2.21                     | 0.55              |
| 85:L5:1854:G:N2    | 85:L5:4394:A:O4'   | 2.39                     | 0.55              |
| 85:L5:2626:U:OP2   | 41:LU:92:LYS:NZ    | 2.34                     | 0.55              |
| 85:L5:2891:U:OP2   | 38:LR:74:ARG:NE    | 2.34                     | 0.55              |
| 23:LB:141:ASP:O    | 23:LB:145:GLN:HG2  | 2.07                     | 0.55              |
| 33:LM:14:TYR:O     | 33:LM:56:GLN:N     | 2.37                     | 0.55              |
| 33:LM:118:MET:O    | 33:LM:122:ILE:HG12 | 2.06                     | 0.55              |
| 38:LR:99:MET:SD    | 38:LR:103:ARG:HD2  | 2.45                     | 0.55              |
| 39:LS:173:ASN:OD1  | 39:LS:174:THR:N    | 2.39                     | 0.55              |
| 46:La:4:ARG:HG2    | 46:La:5:LEU:HD12   | 1.87                     | 0.55              |
| 47:Lb:37:PRO:HA    | 47:Lb:40:LEU:HB3   | 1.89                     | 0.55              |
| 49:Ld:46:LEU:O     | 49:Ld:49:ILE:HG22  | 2.07                     | 0.55              |
| 79:S2:17:C:H2'     | 79:S2:18:C:C6      | 2.41                     | 0.55              |
| 79:S2:115:U:H2'    | 79:S2:116:U:C6     | 2.41                     | 0.55              |
| 83:Ls:106:LYS:HD2  | 83:Ls:107:VAL:N    | 2.21                     | 0.55              |
| 87:IW:86:SER:N     | 87:IW:89:ASP:OD2   | 2.39                     | 0.55              |
| 3:sI:54:LYS:NZ     | 79:s2:380:G:OP2    | 2.33                     | 0.55              |
| 3:sI:83:TYR:HB2    | 3:sI:202:ILE:HD11  | 1.86                     | 0.55              |
| 6:sG:200:LYS:NZ    | 6:sG:204:GLU:OE2   | 2.39                     | 0.55              |
| 13:sV:9:VAL:HG21   | 15:sC:177:PRO:HD3  | 1.88                     | 0.55              |
| 15:sC:102:LEU:HD21 | 15:sC:130:ILE:HB   | 1.87                     | 0.55              |
| 20:l7:22:A:H2'     | 20:l7:23:A:C8      | 2.41                     | 0.55              |
| 21:l8:27:U:H2'     | 21:l8:28:C:C6      | 2.42                     | 0.55              |
| 34:lN:14:LYS:HE2   | 34:lN:120:TRP:CZ3  | 2.40                     | 0.55              |
| 34:lN:149:GLN:O    | 34:lN:152:THR:OG1  | 2.18                     | 0.55              |
| 38:lR:5:ARG:NH1    | 85:l5:2385:U:OP1   | 2.40                     | 0.55              |
| 39:lS:92:ASN:HD21  | 40:lT:156:TYR:N    | 2.04                     | 0.55              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 50:le:85:LEU:HD12 | 50:le:111:ILE:HG23 | 1.88                     | 0.55              |
| 64:sR:1:MET:CE    | 64:sR:2:GLY:H      | 2.19                     | 0.55              |
| 65:sD:65:ARG:O    | 65:sD:68:GLU:HG2   | 2.07                     | 0.55              |
| 67:sK:88:GLU:N    | 67:sK:88:GLU:OE2   | 2.38                     | 0.55              |
| 70:sS:75:ARG:NH1  | 70:sS:95:TYR:HB2   | 2.21                     | 0.55              |
| 79:s2:538:U:H2'   | 79:s2:539:C:C6     | 2.40                     | 0.55              |
| 79:s2:1093:A:H2'  | 79:s2:1094:C:H6    | 1.70                     | 0.55              |
| 80:cB:626:GLN:O   | 80:cB:631:ARG:NH2  | 2.29                     | 0.55              |
| 83:ls:40:MET:CE   | 83:ls:41:GLN:HG3   | 2.36                     | 0.55              |
| 85:l5:6:C:H2'     | 85:l5:7:C:H6       | 1.71                     | 0.55              |
| 85:l5:67:C:H41    | 85:l5:325:U:HO2'   | 1.53                     | 0.55              |
| 85:l5:1478:C:H2'  | 85:l5:1479:G:H8    | 1.72                     | 0.55              |
| 85:l5:1645:C:H2'  | 85:l5:1646:A:C8    | 2.41                     | 0.55              |
| 85:l5:1645:C:H2'  | 85:l5:1646:A:H8    | 1.72                     | 0.55              |
| 85:l5:2501:C:H2'  | 85:l5:2502:G:C8    | 2.41                     | 0.55              |
| 85:l5:2658:G:O2'  | 85:l5:2675:G:N2    | 2.35                     | 0.55              |
| 80:CB:48:SER:OG   | 79:S2:464:A:N6     | 2.40                     | 0.55              |
| 2:SE:22:LYS:N     | 79:S2:829:C:OP1    | 2.30                     | 0.55              |
| 17:SO:42:VAL:O    | 17:SO:42:VAL:HG12  | 2.06                     | 0.55              |
| 17:SO:45:THR:HA   | 17:SO:52:THR:HA    | 1.88                     | 0.55              |
| 17:SO:53:ILE:H    | 17:SO:53:ILE:HD12  | 1.71                     | 0.55              |
| 85:L5:385:A:H4'   | 85:L5:386:A:H5'    | 1.87                     | 0.55              |
| 85:L5:1366:G:O2'  | 85:L5:1367:C:O2    | 2.25                     | 0.55              |
| 85:L5:2848:G:O2'  | 85:L5:3838:U:O4    | 2.21                     | 0.55              |
| 85:L5:3671:G:H2'  | 85:L5:3672:G:C2    | 2.41                     | 0.55              |
| 85:L5:4967:A:H2'  | 85:L5:4968:A:C8    | 2.41                     | 0.55              |
| 22:LA:135:THR:HB  | 22:LA:149:LYS:HB3  | 1.88                     | 0.55              |
| 25:LD:144:CYS:O   | 25:LD:173:ILE:HG13 | 2.06                     | 0.55              |
| 27:LF:90:ALA:HB2  | 27:LF:125:LEU:HD11 | 1.88                     | 0.55              |
| 28:LG:116:ALA:O   | 28:LG:120:LYS:HG2  | 2.05                     | 0.55              |
| 36:LP:116:HIS:HD1 | 36:LP:149:ILE:HD12 | 1.71                     | 0.55              |
| 44:LY:19:PHE:O    | 44:LY:26:ARG:NH2   | 2.40                     | 0.55              |
| 60:Lo:82:MET:SD   | 60:Lo:82:MET:N     | 2.80                     | 0.55              |
| 67:SK:67:PHE:HB2  | 67:SK:69:TRP:CH2   | 2.41                     | 0.55              |
| 69:SQ:130:LYS:NZ  | 69:SQ:131:LYS:O    | 2.37                     | 0.55              |
| 79:S2:162:C:H2'   | 79:S2:163:U:O4'    | 2.05                     | 0.55              |
| 79:S2:1545:A:N3   | 79:S2:1671:G:O2'   | 2.30                     | 0.55              |
| 82:PE:5:G:H2'     | 82:PE:6:G:H8       | 1.71                     | 0.55              |
| 1:cH:49:ASN:CG    | 1:cH:51:GLN:HE21   | 2.14                     | 0.55              |
| 6:sG:15:LEU:HD13  | 79:s2:155:G:H4'    | 1.88                     | 0.55              |
| 12:sH:157:HIS:HB3 | 12:sH:190:PRO:HG3  | 1.87                     | 0.55              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 15:sC:112:VAL:HG11 | 15:sC:125:LYS:HG3  | 1.88                     | 0.55              |
| 15:sC:232:THR:O    | 15:sC:235:ASN:N    | 2.39                     | 0.55              |
| 17:sO:95:ILE:HG13  | 17:sO:116:LEU:HD21 | 1.88                     | 0.55              |
| 23:lB:167:GLN:HB3  | 23:lB:169:ARG:HH12 | 1.71                     | 0.55              |
| 23:lB:234:ARG:NH1  | 23:lB:268:ARG:O    | 2.36                     | 0.55              |
| 23:lB:252:ALA:HB3  | 85:l5:4457:U:O2    | 2.07                     | 0.55              |
| 26:lE:183:ARG:NE   | 85:l5:4938:A:OP1   | 2.29                     | 0.55              |
| 27:lF:226:HIS:ND1  | 27:lF:228:VAL:HG23 | 2.21                     | 0.55              |
| 32:lL:129:ARG:NH2  | 85:l5:174:C:OP2    | 2.39                     | 0.55              |
| 34:lN:120:TRP:CD1  | 34:lN:121:VAL:N    | 2.74                     | 0.55              |
| 44:lY:38:LEU:HA    | 44:lY:41:LYS:HG2   | 1.88                     | 0.55              |
| 49:ld:26:THR:HB    | 49:ld:85:ARG:HH11  | 1.71                     | 0.55              |
| 49:ld:61:ASP:HB3   | 49:ld:63:ARG:HH21  | 1.72                     | 0.55              |
| 50:le:102:ASN:HD21 | 85:l5:2308:A:P     | 2.30                     | 0.55              |
| 58:lm:124:LYS:HZ2  | 85:l5:4474:A:P     | 2.30                     | 0.55              |
| 65:sD:45:ARG:HG3   | 65:sD:85:GLU:OE2   | 2.06                     | 0.55              |
| 65:sD:205:PRO:HG2  | 79:s2:1388:A:C2    | 2.42                     | 0.55              |
| 70:sS:4:VAL:HA     | 77:sZ:51:ASP:HA    | 1.88                     | 0.55              |
| 79:s2:12:U:H2'     | 79:s2:13:C:H6      | 1.72                     | 0.55              |
| 79:s2:165:G:OP2    | 79:s2:165:G:N2     | 2.37                     | 0.55              |
| 80:cB:45:ILE:HD13  | 80:cB:78:PHE:CD1   | 2.42                     | 0.55              |
| 80:cB:79:TYR:CE2   | 80:cB:81:LEU:HD13  | 2.42                     | 0.55              |
| 85:l5:387:G:HO2'   | 85:l5:412:G:H1     | 1.53                     | 0.55              |
| 85:l5:996:G:N2     | 85:l5:1048:G:OP1   | 2.35                     | 0.55              |
| 85:l5:1294:A:H1'   | 85:l5:1296:G:N1    | 2.20                     | 0.55              |
| 85:l5:2656:U:C4    | 85:l5:2657:G:C6    | 2.95                     | 0.55              |
| 85:l5:3732:A:H2'   | 85:l5:3733:A:C8    | 2.41                     | 0.55              |
| 80:CB:174:LEU:HD12 | 80:CB:174:LEU:H    | 1.72                     | 0.55              |
| 80:CB:347:GLY:O    | 80:CB:351:LEU:HB2  | 2.05                     | 0.55              |
| 2:SE:247:THR:OG1   | 2:SE:250:GLU:OE1   | 2.22                     | 0.55              |
| 7:SJ:137:VAL:N     | 7:SJ:140:GLN:O     | 2.40                     | 0.55              |
| 8:SY:94:HIS:ND1    | 8:SY:94:HIS:O      | 2.34                     | 0.55              |
| 11:SB:52:THR:HG23  | 11:SB:57:ILE:HA    | 1.88                     | 0.55              |
| 15:SC:78:LEU:HD13  | 15:SC:98:LEU:HD11  | 1.89                     | 0.55              |
| 85:L5:152:U:H2'    | 85:L5:153:G:H8     | 1.72                     | 0.55              |
| 85:L5:229:G:OP1    | 44:LY:11:ARG:NH1   | 2.37                     | 0.55              |
| 85:L5:667:A:N1     | 24:LC:291:ARG:NH2  | 2.51                     | 0.55              |
| 85:L5:1340:C:H2'   | 85:L5:1341:U:H6    | 1.70                     | 0.55              |
| 85:L5:1511:U:H2'   | 85:L5:1512:G:C8    | 2.36                     | 0.55              |
| 85:L5:1534:A:H1'   | 55:Lj:11:ARG:HH21  | 1.71                     | 0.55              |
| 85:L5:2353:U:H2'   | 85:L5:2354:G:C8    | 2.41                     | 0.55              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 85:L5:2481:G:H2'  | 85:L5:2482:C:H6    | 1.71                     | 0.55              |
| 85:L5:3833:C:H2'  | 85:L5:3834:C:H6    | 1.70                     | 0.55              |
| 85:L5:4098:A:OP1  | 85:L5:4100:C:N4    | 2.35                     | 0.55              |
| 85:L5:4102:C:O5'  | 85:L5:4106:G:C4    | 2.60                     | 0.55              |
| 85:L5:4300:U:H2'  | 85:L5:4301:U:C6    | 2.42                     | 0.55              |
| 23:LB:29:VAL:HG12 | 23:LB:31:SER:H     | 1.70                     | 0.55              |
| 26:LE:188:ARG:HD3 | 26:LE:217:PHE:HB2  | 1.87                     | 0.55              |
| 34:LN:160:GLU:OE1 | 34:LN:160:GLU:N    | 2.28                     | 0.55              |
| 42:LV:31:ASN:OD1  | 42:LV:116:ALA:N    | 2.30                     | 0.55              |
| 43:LX:108:GLN:HA  | 43:LX:111:GLN:HE21 | 1.71                     | 0.55              |
| 61:Lp:47:MET:HA   | 61:Lp:47:MET:HE2   | 1.88                     | 0.55              |
| 65:SD:11:PHE:CE2  | 72:SU:27:ARG:HG2   | 2.42                     | 0.55              |
| 69:SQ:15:ARG:HG2  | 69:SQ:20:THR:HG22  | 1.88                     | 0.55              |
| 75:Sg:298:LEU:N   | 75:Sg:310:TRP:O    | 2.36                     | 0.55              |
| 79:S2:12:U:H2'    | 79:S2:13:C:C6      | 2.41                     | 0.55              |
| 79:S2:329:G:H2'   | 79:S2:330:G:C8     | 2.41                     | 0.55              |
| 87:IW:20:ARG:NH1  | 87:IW:30:GLN:HB2   | 2.22                     | 0.55              |
| 1:CH:85:ARG:O     | 1:CH:89:GLY:N      | 2.40                     | 0.55              |
| 1:cH:43:LYS:HE2   | 9:se:46:VAL:HB     | 1.88                     | 0.55              |
| 10:sA:111:GLN:OE1 | 10:sA:111:GLN:N    | 2.31                     | 0.55              |
| 10:sA:123:VAL:HA  | 10:sA:145:ILE:HG22 | 1.89                     | 0.55              |
| 10:sA:174:MET:HE1 | 10:sA:175:TRP:CD2  | 2.41                     | 0.55              |
| 14:sa:28:ARG:HH11 | 17:sO:147:ARG:HA   | 1.70                     | 0.55              |
| 15:sC:189:GLY:N   | 79:s2:1355:C:H42   | 1.87                     | 0.55              |
| 19:sb:13:GLU:O    | 19:sb:17:ARG:CB    | 2.54                     | 0.55              |
| 23:lB:61:ASP:N    | 23:lB:61:ASP:OD2   | 2.38                     | 0.55              |
| 25:lD:173:ILE:O   | 25:lD:175:HIS:ND1  | 2.36                     | 0.55              |
| 28:lG:177:MET:HE2 | 28:lG:177:MET:C    | 2.31                     | 0.55              |
| 34:lN:12:ARG:NH2  | 85:l5:279:A:OP2    | 2.36                     | 0.55              |
| 44:lY:100:HIS:CG  | 44:lY:101:PRO:HD2  | 2.42                     | 0.55              |
| 45:lZ:73:LYS:CE   | 45:lZ:75:TYR:HE2   | 2.20                     | 0.55              |
| 49:ld:64:ILE:O    | 49:ld:64:ILE:HD12  | 2.07                     | 0.55              |
| 57:ll:44:TRP:CH2  | 57:ll:45:ARG:HD2   | 2.42                     | 0.55              |
| 64:sR:126:MET:SD  | 64:sR:126:MET:O    | 2.65                     | 0.55              |
| 66:sF:165:ASN:OD1 | 66:sF:166:ILE:N    | 2.39                     | 0.55              |
| 67:sK:90:VAL:HB   | 67:sK:94:LEU:HD23  | 1.88                     | 0.55              |
| 72:sU:62:ARG:HH21 | 79:s2:1548:G:H5'   | 1.71                     | 0.55              |
| 79:s2:1013:U:H2'  | 79:s2:1014:G:H8    | 1.72                     | 0.55              |
| 79:s2:1101:U:H2'  | 79:s2:1102:G:H8    | 1.71                     | 0.55              |
| 80:cB:66:ARG:HG3  | 80:cB:68:ILE:HD12  | 1.89                     | 0.55              |
| 80:cB:254:GLU:HA  | 80:cB:257:MET:CG   | 2.34                     | 0.55              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 80:cB:348:ASP:OD2  | 80:cB:349:ALA:N    | 2.40                     | 0.55              |
| 83:ls:160:LEU:HD11 | 83:ls:175:LEU:HD21 | 1.88                     | 0.55              |
| 85:l5:271:C:H2'    | 85:l5:272:U:C6     | 2.41                     | 0.55              |
| 85:l5:952:G:H2'    | 85:l5:953:C:C6     | 2.42                     | 0.55              |
| 85:l5:1304:C:H2'   | 85:l5:1305:C:C6    | 2.40                     | 0.55              |
| 85:l5:2102:G:H1'   | 85:l5:2103:G:N7    | 2.22                     | 0.55              |
| 80:CB:216:SER:OG   | 80:CB:221:TRP:NE1  | 2.39                     | 0.55              |
| 80:CB:394:LEU:HD11 | 80:CB:396:MET:HE1  | 1.87                     | 0.55              |
| 80:CB:653:GLY:HA2  | 80:CB:660:ASN:HB2  | 1.89                     | 0.55              |
| 2:SE:149:TYR:HE1   | 6:SG:205:GLU:HG2   | 1.70                     | 0.55              |
| 3:SI:6:ASP:OD1     | 3:SI:7:ASN:N       | 2.40                     | 0.55              |
| 3:SI:85:ALA:O      | 4:SL:8:ARG:NE      | 2.36                     | 0.55              |
| 4:SL:136:LYS:NZ    | 79:S2:372:U:P      | 2.79                     | 0.55              |
| 6:SG:156:TYR:HE1   | 87:LW:101:ARG:CZ   | 2.19                     | 0.55              |
| 11:SB:214:LYS:HD3  | 11:SB:214:LYS:C    | 2.31                     | 0.55              |
| 12:SH:82:GLU:O     | 12:SH:86:LYS:HG2   | 2.06                     | 0.55              |
| 12:SH:98:ARG:O     | 79:S2:913:A:N6     | 2.37                     | 0.55              |
| 14:Sa:28:ARG:NH2   | 14:Sa:74:CYS:CB    | 2.63                     | 0.55              |
| 14:Sa:70:LYS:HZ3   | 79:S2:987:A:H5''   | 1.71                     | 0.55              |
| 85:L5:1269:G:N1    | 85:L5:2106:G:H1'   | 2.19                     | 0.55              |
| 85:L5:1279:A:O2'   | 85:L5:1281:G:N7    | 2.37                     | 0.55              |
| 85:L5:1380:G:N2    | 85:L5:1381:U:O4    | 2.33                     | 0.55              |
| 85:L5:1457:G:O2'   | 37:LQ:75:ARG:NH2   | 2.34                     | 0.55              |
| 85:L5:1645:C:OP1   | 24:LC:80:ARG:NH2   | 2.39                     | 0.55              |
| 85:L5:2632:U:H2'   | 85:L5:2633:U:C6    | 2.40                     | 0.55              |
| 85:L5:3642:A:C5    | 55:Lj:3:LYS:HB3    | 2.42                     | 0.55              |
| 85:L5:4096:C:P     | 85:L5:4109:G:HO2'  | 2.29                     | 0.55              |
| 85:L5:4288:C:O2'   | 85:L5:4321:U:OP1   | 2.25                     | 0.55              |
| 85:L5:4993:G:H2'   | 85:L5:4994:G:H8    | 1.71                     | 0.55              |
| 24:LC:146:GLU:N    | 24:LC:146:GLU:OE1  | 2.40                     | 0.55              |
| 30:LI:47:PRO:HB3   | 30:LI:171:TRP:CH2  | 2.42                     | 0.55              |
| 31:LJ:39:VAL:HA    | 31:LJ:42:GLN:HG2   | 1.88                     | 0.55              |
| 31:LJ:93:GLU:HG2   | 31:LJ:173:ILE:HB   | 1.89                     | 0.55              |
| 31:LJ:121:PRO:HD3  | 70:SS:101:ASN:HB3  | 1.88                     | 0.55              |
| 40:LT:111:GLU:HA   | 40:LT:114:GLN:OE1  | 2.07                     | 0.55              |
| 66:SF:55:ARG:O     | 66:SF:62:ARG:NH2   | 2.40                     | 0.55              |
| 70:SS:63:GLU:H     | 70:SS:63:GLU:CD    | 2.12                     | 0.55              |
| 70:SS:88:LYS:HB3   | 70:SS:95:TYR:HE1   | 1.72                     | 0.55              |
| 79:S2:511:U:H2'    | 79:S2:512:A:C8     | 2.42                     | 0.55              |
| 79:S2:925:G:O6     | 79:S2:1017:U:O4    | 2.24                     | 0.55              |
| 79:S2:1687:C:H2'   | 79:S2:1688:C:H6    | 1.71                     | 0.55              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:sE:16:LYS:O     | 2:sE:19:MET:HB2    | 2.07                     | 0.55              |
| 8:sY:15:ASN:ND2   | 8:sY:20:ARG:O      | 2.40                     | 0.55              |
| 10:sA:56:GLU:HG3  | 13:sV:80:SER:HB2   | 1.89                     | 0.55              |
| 11:sB:121:ILE:O   | 11:sB:140:VAL:HA   | 2.06                     | 0.55              |
| 11:sB:145:LYS:HA  | 64:sR:135:VAL:H    | 1.71                     | 0.55              |
| 15:sC:187:ARG:HD3 | 15:sC:192:LEU:HD12 | 1.88                     | 0.55              |
| 16:sN:64:ARG:NH2  | 79:s2:919:A:OP2    | 2.38                     | 0.55              |
| 23:lB:76:VAL:HG21 | 23:lB:332:MET:SD   | 2.47                     | 0.55              |
| 25:lD:17:GLN:NE2  | 40:lT:22:HIS:O     | 2.37                     | 0.55              |
| 26:lE:93:THR:HG23 | 26:lE:106:VAL:HG22 | 1.87                     | 0.55              |
| 26:lE:220:LYS:NZ  | 26:lE:221:LYS:O    | 2.33                     | 0.55              |
| 28:lG:79:ALA:O    | 28:lG:82:GLN:NE2   | 2.34                     | 0.55              |
| 30:lI:193:ASP:OD2 | 85:l5:1750:G:N2    | 2.39                     | 0.55              |
| 34:lN:42:PRO:HG3  | 34:lN:53:TYR:HE2   | 1.72                     | 0.55              |
| 36:lP:67:VAL:HB   | 36:lP:80:GLN:HE21  | 1.72                     | 0.55              |
| 38:lR:71:ARG:NE   | 85:l5:3605:C:OP2   | 2.40                     | 0.55              |
| 44:lY:52:ASP:HB2  | 44:lY:110:LYS:HD3  | 1.89                     | 0.55              |
| 56:lk:30:ASP:OD1  | 56:lk:30:ASP:N     | 2.39                     | 0.55              |
| 60:lo:61:LYS:NZ   | 85:l5:4337:C:H42   | 2.05                     | 0.55              |
| 63:lz:107:TYR:CE1 | 63:lz:110:PHE:HD1  | 2.24                     | 0.55              |
| 64:sR:5:ARG:HG3   | 79:s2:1368:U:O4'   | 2.06                     | 0.55              |
| 64:sR:49:LYS:HZ2  | 79:s2:1368:U:HO2'  | 1.47                     | 0.55              |
| 69:sQ:104:SER:HA  | 69:sQ:107:GLU:HG2  | 1.89                     | 0.55              |
| 75:sg:253:GLY:HA2 | 75:sg:285:GLN:HE22 | 1.71                     | 0.55              |
| 79:s2:609:U:H2'   | 79:s2:610:G:C8     | 2.41                     | 0.55              |
| 79:s2:1512:C:H2'  | 79:s2:1513:C:C6    | 2.42                     | 0.55              |
| 80:cB:221:TRP:CD2 | 80:cB:340:MET:HE1  | 2.42                     | 0.55              |
| 85:l5:256:G:H2'   | 85:l5:257:C:C6     | 2.42                     | 0.55              |
| 85:l5:266:C:O2'   | 85:l5:267:G:H8     | 1.88                     | 0.55              |
| 85:l5:1461:C:H2'  | 85:l5:1462:A:H8    | 1.72                     | 0.55              |
| 85:l5:1876:U:H2'  | 85:l5:1877:G:H8    | 1.71                     | 0.55              |
| 85:l5:2570:U:H2'  | 85:l5:2571:C:C6    | 2.42                     | 0.55              |
| 85:l5:4239:A:H2'  | 85:l5:4240:G:C8    | 2.42                     | 0.55              |
| 80:CB:691:ALA:HA  | 80:CB:730:TYR:CE1  | 2.39                     | 0.55              |
| 5:SX:138:LYS:NZ   | 79:S2:30:C:OP1     | 2.37                     | 0.55              |
| 7:SJ:27:GLN:O     | 7:SJ:31:LEU:HG     | 2.05                     | 0.55              |
| 11:SB:142:PHE:H   | 11:SB:210:VAL:HG12 | 1.72                     | 0.55              |
| 16:SN:55:ARG:HH11 | 79:S2:1017:U:H5'   | 1.72                     | 0.55              |
| 85:L5:55:G:OP2    | 55:Lj:43:ARG:NH2   | 2.40                     | 0.55              |
| 85:L5:209:U:OP1   | 44:LY:63:LYS:NZ    | 2.33                     | 0.55              |
| 85:L5:443:G:OP1   | 51:Lf:68:ARG:NH2   | 2.39                     | 0.55              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 85:L5:993:G:H22    | 85:L5:1050:C:H2'   | 1.72                     | 0.55              |
| 85:L5:1754:U:H2'   | 85:L5:1755:C:H6    | 1.70                     | 0.55              |
| 85:L5:1950:U:H2'   | 85:L5:1951:G:C8    | 2.41                     | 0.55              |
| 85:L5:2108:G:H2'   | 85:L5:2109:G:C8    | 2.41                     | 0.55              |
| 85:L5:2810:U:H2'   | 85:L5:2811:G:O4'   | 2.07                     | 0.55              |
| 85:L5:2869:U:O2'   | 85:L5:2881:A:N7    | 2.34                     | 0.55              |
| 85:L5:4242:U:H3    | 85:L5:4281:A:H2    | 1.53                     | 0.55              |
| 85:L5:5002:U:OP2   | 23:LB:385:LYS:NZ   | 2.34                     | 0.55              |
| 23:LB:47:LEU:HD23  | 23:LB:84:MET:HE3   | 1.88                     | 0.55              |
| 26:LE:67:ALA:HB1   | 26:LE:70:LYS:HE2   | 1.88                     | 0.55              |
| 31:LJ:63:ARG:NH2   | 31:LJ:64:ARG:O     | 2.31                     | 0.55              |
| 34:LN:11:TRP:HA    | 34:LN:19:MET:HE1   | 1.89                     | 0.55              |
| 43:LX:83:THR:O     | 43:LX:86:ALA:N     | 2.40                     | 0.55              |
| 45:LZ:87:VAL:HG12  | 45:LZ:127:ASN:HD22 | 1.70                     | 0.55              |
| 46:La:133:ALA:O    | 46:La:137:ILE:HG12 | 2.06                     | 0.55              |
| 53:Lh:56:ARG:O     | 53:Lh:60:VAL:HG23  | 2.06                     | 0.55              |
| 63:Lz:198:TRP:CG   | 63:Lz:199:GLN:H    | 2.23                     | 0.55              |
| 74:Sd:22:ARG:HG2   | 74:Sd:38:MET:HB2   | 1.89                     | 0.55              |
| 75:Sg:257:LYS:HD3  | 75:Sg:259:TRP:CZ3  | 2.38                     | 0.55              |
| 1:CH:99:ILE:HG13   | 1:CH:124:ILE:HG22  | 1.89                     | 0.55              |
| 3:sI:97:VAL:HG22   | 3:sI:98:LYS:H      | 1.72                     | 0.55              |
| 4:sL:81:LYS:HZ3    | 79:s2:394:G:P      | 2.30                     | 0.55              |
| 5:sX:67:ARG:NH2    | 5:sX:114:ASP:OD2   | 2.36                     | 0.55              |
| 7:sJ:108:ARG:NH2   | 7:sJ:154:GLN:OE1   | 2.39                     | 0.55              |
| 11:sB:84:PHE:HB3   | 11:sB:86:LEU:CD1   | 2.36                     | 0.55              |
| 22:lA:96:LEU:HD11  | 61:lp:86:LEU:HD11  | 1.89                     | 0.55              |
| 27:lF:184:ILE:HA   | 27:lF:189:ASP:OD1  | 2.07                     | 0.55              |
| 28:lG:29:ASN:ND2   | 28:lG:31:LEU:HB3   | 2.20                     | 0.55              |
| 29:lH:5:LEU:HB2    | 29:lH:60:TRP:CZ3   | 2.41                     | 0.55              |
| 34:lN:192:TRP:NE1  | 85:l5:48:G:O5'     | 2.40                     | 0.55              |
| 37:lQ:4:ASP:C      | 37:lQ:5:ILE:HD13   | 2.32                     | 0.55              |
| 40:lT:129:LYS:NZ   | 85:l5:1836:G:O5'   | 2.37                     | 0.55              |
| 42:lV:123:LYS:CA   | 42:lV:139:ILE:HD11 | 2.36                     | 0.55              |
| 44:lY:54:GLU:HA    | 44:lY:69:LYS:HA    | 1.87                     | 0.55              |
| 66:sF:44:LYS:HZ3   | 69:sQ:114:GLN:HE22 | 1.55                     | 0.55              |
| 68:sP:43:ARG:HH12  | 79:s2:1615:U:H3'   | 1.71                     | 0.55              |
| 69:sQ:31:LEU:HD23  | 69:sQ:67:ASP:HB3   | 1.89                     | 0.55              |
| 70:sS:121:ARG:NH2  | 79:s2:1611:G:OP2   | 2.39                     | 0.55              |
| 75:sg:170:TRP:HA   | 75:sg:194:TYR:HB2  | 1.89                     | 0.55              |
| 75:sg:272:GLN:OE1  | 75:sg:272:GLN:N    | 2.34                     | 0.55              |
| 78:sf:130:VAL:HG22 | 79:s2:1310:U:OP1   | 2.06                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 79:s2:328:U:H5''  | 87:IW:113:LYS:HZ1 | 1.71                     | 0.55              |
| 79:s2:924:G:H1    | 79:s2:1018:U:H3   | 1.55                     | 0.55              |
| 79:s2:1419:C:O2'  | 79:s2:1420:G:N3   | 2.40                     | 0.55              |
| 80:cB:330:LYS:HE2 | 80:cB:334:PRO:HB2 | 1.89                     | 0.55              |
| 82:pE:56:C:H3'    | 82:pE:57:A:C8     | 2.42                     | 0.55              |
| 82:pE:70:G:H2'    | 82:pE:71:G:C8     | 2.42                     | 0.55              |
| 84:lt:53:TRP:CE2  | 84:lt:56:LEU:HD21 | 2.42                     | 0.55              |
| 84:lt:61:LYS:HD3  | 84:lt:72:GLU:HB3  | 1.88                     | 0.55              |
| 85:l5:210:C:O2'   | 85:l5:233:U:O2'   | 2.20                     | 0.55              |
| 85:l5:926:G:H2'   | 85:l5:927:G:C8    | 2.41                     | 0.55              |
| 85:l5:1875:C:H2'  | 85:l5:1876:U:C6   | 2.42                     | 0.55              |
| 85:l5:2373:C:H2'  | 85:l5:2374:A:C8   | 2.42                     | 0.55              |
| 85:l5:3937:C:OP2  | 85:l5:3938:G:O2'  | 2.23                     | 0.55              |
| 8:SY:57:VAL:HG22  | 8:SY:60:PHE:HE1   | 1.71                     | 0.55              |
| 18:SW:23:ARG:NE   | 18:SW:24:GLN:HG2  | 2.22                     | 0.55              |
| 85:L5:368:C:H2'   | 85:L5:369:G:C8    | 2.41                     | 0.55              |
| 85:L5:429:A:H2'   | 85:L5:430:G:H8    | 1.70                     | 0.55              |
| 85:L5:1309:C:H2'  | 85:L5:1310:C:C6   | 2.42                     | 0.55              |
| 85:L5:1336:G:H2'  | 85:L5:2346:C:N4   | 2.22                     | 0.55              |
| 85:L5:1628:C:H5'' | 22:LA:15:VAL:HG21 | 1.87                     | 0.55              |
| 85:L5:1950:U:H2'  | 85:L5:1951:G:H8   | 1.70                     | 0.55              |
| 85:L5:2344:U:H2'  | 46:La:9:ARG:HH22  | 1.71                     | 0.55              |
| 85:L5:3887:C:OP2  | 35:LO:85:ARG:NH2  | 2.40                     | 0.55              |
| 85:L5:4944:C:O2   | 51:Lf:67:THR:OG1  | 2.24                     | 0.55              |
| 20:L7:61:G:H5''   | 25:LD:271:MET:HE1 | 1.89                     | 0.55              |
| 25:LD:205:ALA:O   | 25:LD:208:MET:SD  | 2.64                     | 0.55              |
| 31:LJ:9:GLU:OE2   | 31:LJ:10:ASN:ND2  | 2.39                     | 0.55              |
| 33:LM:100:ARG:HE  | 35:LO:198:THR:C   | 2.14                     | 0.55              |
| 55:Lj:39:TYR:O    | 55:Lj:39:TYR:CG   | 2.59                     | 0.55              |
| 72:SU:67:LYS:HD3  | 72:SU:76:THR:HG22 | 1.88                     | 0.55              |
| 75:Sg:66:VAL:HA   | 75:Sg:82:SER:HA   | 1.88                     | 0.55              |
| 75:Sg:104:HIS:CE1 | 75:Sg:130:LYS:HG2 | 2.42                     | 0.55              |
| 75:Sg:199:THR:N   | 75:Sg:208:ALA:O   | 2.38                     | 0.55              |
| 78:Sf:132:MET:CE  | 78:Sf:139:HIS:HB3 | 2.31                     | 0.55              |
| 79:S2:389:A:H2'   | 79:S2:390:C:C6    | 2.42                     | 0.55              |
| 79:S2:979:C:H2'   | 79:S2:980:A:C8    | 2.41                     | 0.55              |
| 79:S2:1199:A:H2'  | 79:S2:1200:A:H8   | 1.69                     | 0.55              |
| 79:S2:1356:G:H2'  | 79:S2:1357:A:C8   | 2.41                     | 0.55              |
| 81:AP:50:U:O2     | 81:AP:64:G:N2     | 2.26                     | 0.55              |
| 6:sG:20:ASP:HB3   | 6:sG:23:LYS:HB2   | 1.88                     | 0.55              |
| 9:se:32:ALA:HB2   | 79:s2:525:A:H5''  | 1.88                     | 0.55              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 18:sW:57:ARG:CZ   | 19:sb:26:GLN:HE22  | 2.20                     | 0.55              |
| 19:sb:51:GLN:NE2  | 79:s2:927:C:O2'    | 2.40                     | 0.55              |
| 26:lE:112:MET:HE2 | 85:l5:2261:G:H4'   | 1.88                     | 0.55              |
| 27:lF:85:ALA:H    | 40:lT:138:ALA:HB2  | 1.71                     | 0.55              |
| 36:lP:40:HIS:NE2  | 36:lP:110:ASP:O    | 2.37                     | 0.55              |
| 54:li:23:LYS:NZ   | 85:l5:160:G:OP2    | 2.40                     | 0.55              |
| 55:lj:55:ARG:NH2  | 85:l5:364:G:O6     | 2.39                     | 0.55              |
| 61:lp:57:CYS:SG   | 61:lp:59:SER:OG    | 2.65                     | 0.55              |
| 63:lz:31:THR:HA   | 63:lz:171:HIS:CD2  | 2.42                     | 0.55              |
| 64:sR:13:ALA:HB1  | 64:sR:54:VAL:HG22  | 1.88                     | 0.55              |
| 65:sD:80:PRO:O    | 65:sD:83:SER:OG    | 2.16                     | 0.55              |
| 79:s2:1174:U:H2'  | 79:s2:1175:G:C8    | 2.42                     | 0.55              |
| 79:s2:1686:G:H2'  | 79:s2:1687:C:C6    | 2.42                     | 0.55              |
| 79:s2:1845:A:H2'  | 79:s2:1846:G:C8    | 2.41                     | 0.55              |
| 80:cB:594:LYS:HZ2 | 80:cB:596:PRO:HA   | 1.71                     | 0.55              |
| 83:ls:13:TYR:CE1  | 83:ls:60:MET:HE2   | 2.42                     | 0.55              |
| 85:l5:1074:G:H3'  | 85:l5:1075:G:H8    | 1.71                     | 0.55              |
| 85:l5:1669:A:N3   | 85:l5:1852:U:O2'   | 2.36                     | 0.55              |
| 85:l5:2373:C:H2'  | 85:l5:2374:A:H8    | 1.71                     | 0.55              |
| 85:l5:3870:C:H2'  | 85:l5:3871:A:H8    | 1.71                     | 0.55              |
| 85:l5:4054:C:H5'' | 85:l5:4055:U:C5    | 2.41                     | 0.55              |
| 85:l5:4680:G:H2'  | 85:l5:4681:A:H8    | 1.71                     | 0.55              |
| 80:CB:42:LYS:HE2  | 80:CB:347:GLY:N    | 2.09                     | 0.55              |
| 80:CB:84:ASN:HB2  | 80:CB:88:PHE:CZ    | 2.41                     | 0.55              |
| 80:CB:503:PRO:HG3 | 80:CB:535:GLN:HE22 | 1.72                     | 0.55              |
| 80:CB:671:TYR:HB2 | 80:CB:709:LEU:HD22 | 1.89                     | 0.55              |
| 6:SG:217:MET:O    | 6:SG:221:LYS:HG2   | 2.07                     | 0.55              |
| 11:SB:105:LEU:HG  | 11:SB:106:THR:O    | 2.07                     | 0.55              |
| 16:SN:50:ILE:O    | 16:SN:54:LEU:HG    | 2.07                     | 0.55              |
| 85:L5:189:G:H2'   | 85:L5:190:G:C8     | 2.42                     | 0.55              |
| 85:L5:271:C:H2'   | 85:L5:272:U:H6     | 1.71                     | 0.55              |
| 85:L5:282:C:H1'   | 85:L5:306:A:N6     | 2.21                     | 0.55              |
| 85:L5:727:C:H2'   | 85:L5:728:U:C6     | 2.42                     | 0.55              |
| 85:L5:1726:U:H2'  | 85:L5:1727:U:C6    | 2.42                     | 0.55              |
| 85:L5:2081:C:H2'  | 85:L5:2082:G:C8    | 2.42                     | 0.55              |
| 85:L5:4112:C:H41  | 85:L5:4116:C:C1'   | 2.17                     | 0.55              |
| 85:L5:4638:U:H3   | 85:L5:4661:G:H1    | 1.54                     | 0.55              |
| 85:L5:4645:C:OP2  | 38:LR:62:ARG:NH1   | 2.40                     | 0.55              |
| 20:L7:64:G:H2'    | 20:L7:65:G:C8      | 2.41                     | 0.55              |
| 22:LA:109:GLU:OE1 | 22:LA:139:HIS:ND1  | 2.40                     | 0.55              |
| 30:LI:209:TRP:O   | 30:LI:212:LEU:HD12 | 2.07                     | 0.55              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:LJ:113:ILE:HG21 | 31:LJ:119:TYR:HB2  | 1.87                     | 0.55              |
| 34:LN:6:TYR:CE1    | 54:Li:40:VAL:HG13  | 2.42                     | 0.55              |
| 34:LN:160:GLU:H    | 34:LN:160:GLU:CD   | 2.14                     | 0.55              |
| 47:Lb:102:PRO:HA   | 47:Lb:109:ARG:NH2  | 2.22                     | 0.55              |
| 51:Lf:35:ALA:HA    | 51:Lf:81:SER:HA    | 1.88                     | 0.55              |
| 53:Lh:107:GLN:O    | 53:Lh:110:LYS:HG2  | 2.06                     | 0.55              |
| 63:Lz:53:VAL:HG11  | 63:Lz:185:LEU:HD13 | 1.89                     | 0.55              |
| 79:S2:383:G:H2'    | 79:S2:384:U:C6     | 2.41                     | 0.55              |
| 79:S2:1281:G:C6    | 79:S2:1282:A:C6    | 2.95                     | 0.55              |
| 83:Ls:7:ALA:HA     | 83:Ls:10:LYS:HE2   | 1.88                     | 0.55              |
| 1:CH:73:VAL:CG1    | 1:CH:114:ALA:HB3   | 2.36                     | 0.55              |
| 3:sI:72:CYS:HA     | 3:sI:74:ARG:HH21   | 1.71                     | 0.55              |
| 6:sG:131:ARG:O     | 87:lW:83:THR:HG23  | 2.06                     | 0.55              |
| 10:sA:38:ILE:HD12  | 10:sA:48:ILE:O     | 2.07                     | 0.55              |
| 10:sA:215:GLN:CD   | 10:sA:215:GLN:H    | 2.15                     | 0.55              |
| 11:sB:68:GLU:HB2   | 11:sB:83:LYS:NZ    | 2.22                     | 0.55              |
| 14:sa:32:LYS:NZ    | 79:s2:989:C:O2'    | 2.39                     | 0.55              |
| 16:sN:39:LYS:HA    | 16:sN:42:LYS:HZ2   | 1.72                     | 0.55              |
| 18:sW:66:THR:CG2   | 18:sW:68:ARG:HG2   | 2.37                     | 0.55              |
| 20:l7:4:U:H2'      | 20:l7:5:A:C8       | 2.42                     | 0.55              |
| 20:l7:22:A:H2'     | 20:l7:23:A:H8      | 1.71                     | 0.55              |
| 20:l7:110:G:H2'    | 20:l7:111:C:C6     | 2.41                     | 0.55              |
| 21:l8:25:G:H2'     | 21:l8:26:C:H6      | 1.71                     | 0.55              |
| 23:lB:55:HIS:CE1   | 87:lW:16:GLY:HA3   | 2.42                     | 0.55              |
| 23:lB:74:GLU:OE2   | 23:lB:285:TYR:OH   | 2.24                     | 0.55              |
| 24:lC:283:LYS:HZ3  | 37:lQ:24:TYR:HB2   | 1.71                     | 0.55              |
| 24:lC:337:ARG:NH1  | 26:lE:55:GLY:O     | 2.36                     | 0.55              |
| 26:lE:176:THR:HB   | 26:lE:186:LEU:HD13 | 1.89                     | 0.55              |
| 27:lF:237:GLU:N    | 27:lF:237:GLU:OE2  | 2.39                     | 0.55              |
| 29:lH:183:GLU:OE2  | 29:lH:184:LYS:N    | 2.40                     | 0.55              |
| 30:lI:38:ARG:NH1   | 30:lI:83:ASP:OD2   | 2.39                     | 0.55              |
| 34:lN:96:ARG:HH22  | 34:lN:104:GLU:CD   | 2.15                     | 0.55              |
| 46:la:35:ALA:HB2   | 85:l5:38:A:H5''    | 1.89                     | 0.55              |
| 53:lh:81:LEU:HD23  | 53:lh:84:ARG:HD2   | 1.88                     | 0.55              |
| 56:lk:4:LYS:NZ     | 85:l5:2691:U:O2'   | 2.28                     | 0.55              |
| 60:lo:99:ARG:NH1   | 60:lo:99:ARG:O     | 2.37                     | 0.55              |
| 65:sD:167:TYR:OH   | 65:sD:192:TRP:HB2  | 2.07                     | 0.55              |
| 68:sP:32:GLN:HA    | 68:sP:35:GLN:OE1   | 2.06                     | 0.55              |
| 70:sS:85:ASN:OD1   | 79:s2:1630:A:O2'   | 2.22                     | 0.55              |
| 75:sg:88:ARG:NH1   | 75:sg:100:ARG:HH21 | 2.05                     | 0.55              |
| 76:sM:17:ALA:O     | 76:sM:20:GLU:HG3   | 2.07                     | 0.55              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 79:s2:543:C:H3'    | 79:s2:544:G:C8     | 2.41                     | 0.55              |
| 79:s2:561:A:H2'    | 79:s2:562:U:O4'    | 2.07                     | 0.55              |
| 79:s2:1202:U:H2'   | 79:s2:1203:G:H8    | 1.72                     | 0.55              |
| 79:s2:1359:U:C2    | 79:s2:1360:U:C5    | 2.95                     | 0.55              |
| 79:s2:1467:C:C2    | 79:s2:1468:C:C5    | 2.95                     | 0.55              |
| 79:s2:1756:C:OP2   | 79:s2:1757:G:N2    | 2.33                     | 0.55              |
| 80:cB:79:TYR:CG    | 80:cB:351:LEU:HD13 | 2.42                     | 0.55              |
| 80:cB:158:ASN:N    | 80:cB:158:ASN:OD1  | 2.40                     | 0.55              |
| 80:cB:216:SER:OG   | 80:cB:221:TRP:NE1  | 2.40                     | 0.55              |
| 80:cB:255:ASP:OD1  | 80:cB:256:MET:N    | 2.40                     | 0.55              |
| 85:l5:1511:U:H2'   | 85:l5:1512:G:C8    | 2.41                     | 0.55              |
| 85:l5:2616:C:C2    | 85:l5:2722:G:N2    | 2.75                     | 0.55              |
| 85:l5:3916:G:H2'   | 85:l5:3917:A:H8    | 1.72                     | 0.55              |
| 85:l5:4679:G:H2'   | 85:l5:4680:G:C8    | 2.42                     | 0.55              |
| 80:CB:348:ASP:O    | 80:CB:352:GLN:HG3  | 2.06                     | 0.55              |
| 4:SL:82:MET:HE1    | 79:S2:394:G:O3'    | 2.06                     | 0.55              |
| 6:SG:31:ARG:HH22   | 79:S2:1746:U:P     | 2.30                     | 0.55              |
| 6:SG:70:HIS:HA     | 6:SG:98:ARG:HH12   | 1.72                     | 0.55              |
| 12:SH:190:PRO:HB2  | 12:SH:193:GLN:HE22 | 1.71                     | 0.55              |
| 15:SC:208:PRO:O    | 15:SC:212:LYS:HG2  | 2.06                     | 0.55              |
| 85:L5:746:A:H2'    | 85:L5:747:A:C8     | 2.42                     | 0.55              |
| 85:L5:1360:G:H2'   | 85:L5:1361:G:H8    | 1.72                     | 0.55              |
| 85:L5:2461:G:O3'   | 34:LN:108:ARG:NH1  | 2.40                     | 0.55              |
| 85:L5:4743:G:H2'   | 85:L5:4744:A:C8    | 2.42                     | 0.55              |
| 85:L5:4912:G:N2    | 23:LB:156:TYR:OH   | 2.40                     | 0.55              |
| 25:LD:60:ILE:HG12  | 25:LD:93:THR:HA    | 1.88                     | 0.55              |
| 36:LP:117:ILE:HG13 | 36:LP:148:MET:HE3  | 1.87                     | 0.55              |
| 48:Lc:23:LYS:HD2   | 48:Lc:23:LYS:C     | 2.32                     | 0.55              |
| 60:Lo:66:ILE:H     | 60:Lo:66:ILE:HD12  | 1.71                     | 0.55              |
| 64:SR:106:LEU:HA   | 64:SR:109:LEU:HD23 | 1.88                     | 0.55              |
| 66:SF:175:ASP:O    | 66:SF:178:ILE:HG13 | 2.07                     | 0.55              |
| 70:SS:12:ILE:HD11  | 70:SS:19:ASN:HD21  | 1.71                     | 0.55              |
| 71:ST:20:ALA:C     | 71:ST:24:LYS:NZ    | 2.65                     | 0.55              |
| 75:Sg:196:ASN:N    | 75:Sg:210:GLY:O    | 2.32                     | 0.55              |
| 79:S2:14:C:H2'     | 79:S2:15:U:C6      | 2.42                     | 0.55              |
| 79:S2:433:A:H2'    | 79:S2:434:G:C8     | 2.42                     | 0.55              |
| 79:S2:838:G:H1'    | 79:S2:839:C:H3'    | 1.87                     | 0.55              |
| 82:PE:72:C:H2'     | 82:PE:73:G:H8      | 1.72                     | 0.55              |
| 84:Lt:16:ARG:HG2   | 84:Lt:18:THR:HG22  | 1.89                     | 0.55              |
| 84:Lt:55:GLY:H     | 84:Lt:59:THR:HG23  | 1.72                     | 0.55              |
| 2:sE:94:LYS:HD2    | 2:sE:95:THR:HG23   | 1.88                     | 0.55              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 6:sG:52:ILE:HD12   | 6:sG:109:LEU:HD21  | 1.89                     | 0.55              |
| 10:sA:62:ALA:HB1   | 10:sA:181:GLU:OE1  | 2.07                     | 0.55              |
| 12:sH:12:ASN:ND2   | 12:sH:16:PRO:O     | 2.38                     | 0.55              |
| 12:sH:65:PRO:HG2   | 12:sH:68:GLN:HB2   | 1.89                     | 0.55              |
| 12:sH:82:GLU:HG3   | 12:sH:86:LYS:HE3   | 1.89                     | 0.55              |
| 13:sV:30:ALA:C     | 13:sV:60:ARG:HH22  | 2.14                     | 0.55              |
| 15:sC:253:PRO:HA   | 15:sC:256:TRP:CD2  | 2.42                     | 0.55              |
| 16:sN:48:SER:OG    | 79:s2:1017:U:O2    | 2.23                     | 0.55              |
| 23:lB:216:MET:HE2  | 23:lB:216:MET:HA   | 1.88                     | 0.55              |
| 37:lQ:49:LYS:NZ    | 85:l5:1693:U:OP2   | 2.40                     | 0.55              |
| 40:lT:44:GLY:HA2   | 40:lT:95:HIS:HB3   | 1.88                     | 0.55              |
| 42:IV:30:ASP:OD2   | 42:IV:32:THR:OG1   | 2.22                     | 0.55              |
| 66:sF:127:ARG:HH12 | 73:sc:66:ARG:CZ    | 2.19                     | 0.55              |
| 70:sS:35:GLY:HA3   | 70:sS:99:LEU:HA    | 1.88                     | 0.55              |
| 70:sS:112:GLU:O    | 70:sS:116:LYS:NZ   | 2.39                     | 0.55              |
| 75:sg:165:ILE:HG22 | 75:sg:177:TRP:HD1  | 1.70                     | 0.55              |
| 75:sg:216:ALA:N    | 75:sg:230:LEU:O    | 2.39                     | 0.55              |
| 77:sZ:66:LYS:HB3   | 77:sZ:111:ARG:HG2  | 1.88                     | 0.55              |
| 79:s2:562:U:H2'    | 79:s2:563:G:C8     | 2.42                     | 0.55              |
| 79:s2:1666:C:H2'   | 79:s2:1667:U:C6    | 2.42                     | 0.55              |
| 80:cB:776:VAL:HG23 | 80:cB:778:GLY:H    | 1.71                     | 0.55              |
| 80:cB:829:SER:OG   | 80:cB:831:PRO:HG2  | 2.07                     | 0.55              |
| 84:lt:123:ARG:HB3  | 84:lt:129:ILE:HD11 | 1.89                     | 0.55              |
| 85:l5:1408:G:O2'   | 85:l5:1411:C:O2    | 2.24                     | 0.55              |
| 85:l5:1754:U:H2'   | 85:l5:1755:C:H6    | 1.72                     | 0.55              |
| 85:l5:1779:U:H2'   | 85:l5:1780:A:C8    | 2.41                     | 0.55              |
| 85:l5:1800:U:H2'   | 85:l5:1801:A:H8    | 1.72                     | 0.55              |
| 85:l5:3832:U:H2'   | 85:l5:3833:C:H6    | 1.70                     | 0.55              |
| 85:l5:3938:G:N2    | 85:l5:4171:C:OP2   | 2.39                     | 0.55              |
| 85:l5:4059:C:O2'   | 85:l5:4060:U:H5'   | 2.07                     | 0.55              |
| 85:l5:4520:G:H2'   | 85:l5:4521:U:O4'   | 2.07                     | 0.55              |
| 80:CB:27:HIS:HB2   | 80:CB:139:THR:HG23 | 1.88                     | 0.55              |
| 3:SI:202:ILE:HG22  | 3:SI:205:ARG:HH21  | 1.72                     | 0.55              |
| 7:SJ:19:PRO:HA     | 7:SJ:24:ARG:HH21   | 1.72                     | 0.55              |
| 8:SY:40:ILE:O      | 8:SY:44:LEU:HG     | 2.07                     | 0.55              |
| 10:SA:66:VAL:HA    | 10:SA:186:ARG:NH2  | 2.22                     | 0.55              |
| 14:Sa:28:ARG:HG2   | 17:SO:147:ARG:HA   | 1.88                     | 0.55              |
| 85:L5:1890:G:N2    | 85:L5:1890:G:OP2   | 2.40                     | 0.55              |
| 85:L5:2018:C:H2'   | 85:L5:2019:C:C6    | 2.42                     | 0.55              |
| 85:L5:2041:A:N7    | 85:L5:4434:C:O2'   | 2.40                     | 0.55              |
| 85:L5:2274:C:H5''  | 24:LC:312:ARG:HB3  | 1.89                     | 0.55              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 85:L5:2519:U:OP2   | 52:Lg:36:LYS:NZ    | 2.40                     | 0.55              |
| 85:L5:2621:A:H2'   | 85:L5:2622:G:C8    | 2.41                     | 0.55              |
| 85:L5:2705:G:H22   | 85:L5:2710:C:H5    | 1.54                     | 0.55              |
| 21:L8:137:A:H2'    | 21:L8:138:C:C6     | 2.42                     | 0.55              |
| 22:LA:68:ARG:HG3   | 22:LA:70:LYS:HG3   | 1.87                     | 0.55              |
| 23:LB:254:ILE:HD12 | 23:LB:262:VAL:HG11 | 1.87                     | 0.55              |
| 24:LC:206:GLY:O    | 24:LC:248:ARG:NH2  | 2.40                     | 0.55              |
| 31:LJ:164:ARG:O    | 31:LJ:168:GLN:NE2  | 2.38                     | 0.55              |
| 36:LP:36:ILE:HD11  | 36:LP:44:ALA:HB1   | 1.89                     | 0.55              |
| 39:LS:29:ARG:HB2   | 40:LT:148:PRO:HB2  | 1.89                     | 0.55              |
| 66:SF:127:ARG:HH12 | 73:Sc:66:ARG:HH12  | 1.55                     | 0.55              |
| 71:ST:77:LYS:HD3   | 71:ST:94:ARG:HH21  | 1.72                     | 0.55              |
| 71:ST:84:ARG:NH1   | 79:S2:1605:G:OP1   | 2.31                     | 0.55              |
| 75:Sg:240:CYS:SG   | 75:Sg:291:TRP:CD1  | 3.00                     | 0.55              |
| 79:S2:5:U:H2'      | 79:S2:6:G:C8       | 2.42                     | 0.55              |
| 79:S2:594:A:H4'    | 79:S2:595:U:H5'    | 1.90                     | 0.55              |
| 79:S2:746:C:H2'    | 79:S2:747:U:C6     | 2.42                     | 0.55              |
| 82:PE:15:G:N2      | 82:PE:21:A:H1'     | 2.22                     | 0.55              |
| 5:sX:67:ARG:HG3    | 5:sX:115:ILE:HD11  | 1.89                     | 0.54              |
| 7:sJ:84:ILE:O      | 7:sJ:108:ARG:NH2   | 2.37                     | 0.54              |
| 14:sa:5:ARG:HH21   | 79:s2:1864:U:H3'   | 1.71                     | 0.54              |
| 15:sC:187:ARG:NH2  | 15:sC:189:GLY:O    | 2.40                     | 0.54              |
| 16:sN:92:ILE:HG21  | 16:sN:149:LEU:CD1  | 2.36                     | 0.54              |
| 17:sO:96:LYS:NZ    | 17:sO:130:GLU:OE2  | 2.40                     | 0.54              |
| 20:l7:37:G:H2'     | 20:l7:38:U:C6      | 2.41                     | 0.54              |
| 22:lA:21:LYS:NZ    | 85:l5:2448:G:O2'   | 2.27                     | 0.54              |
| 24:lC:179:ASP:OD2  | 24:lC:207:PRO:HD3  | 2.07                     | 0.54              |
| 28:lG:50:ASP:OD2   | 28:lG:51:LEU:N     | 2.39                     | 0.54              |
| 34:lN:124:ASP:HB3  | 34:lN:127:TYR:H    | 1.72                     | 0.54              |
| 35:lO:12:ARG:HD3   | 35:lO:37:ARG:CZ    | 2.37                     | 0.54              |
| 35:lO:43:ILE:HG23  | 35:lO:136:ALA:HB3  | 1.89                     | 0.54              |
| 35:lO:159:LYS:O    | 35:lO:163:LYS:HG2  | 2.07                     | 0.54              |
| 37:lQ:30:LYS:HE3   | 62:lr:8:MET:HE1    | 1.89                     | 0.54              |
| 37:lQ:30:LYS:HE3   | 62:lr:8:MET:CE     | 2.38                     | 0.54              |
| 60:lo:61:LYS:HZ3   | 85:l5:4337:C:N4    | 2.06                     | 0.54              |
| 64:sR:17:ILE:HD11  | 64:sR:54:VAL:HA    | 1.90                     | 0.54              |
| 69:sQ:81:ILE:HA    | 69:sQ:84:ILE:HG12  | 1.89                     | 0.54              |
| 74:sd:44:ARG:HH22  | 79:s2:1337:C:H5'   | 1.71                     | 0.54              |
| 79:s2:12:U:H2'     | 79:s2:13:C:C6      | 2.42                     | 0.54              |
| 79:s2:825:A:H2'    | 79:s2:826:A:C8     | 2.42                     | 0.54              |
| 79:s2:1281:G:C6    | 79:s2:1282:A:C6    | 2.95                     | 0.54              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 79:s2:1310:U:H2'   | 79:s2:1311:C:H6   | 1.72                     | 0.54              |
| 79:s2:1558:C:H2'   | 79:s2:1559:C:H6   | 1.72                     | 0.54              |
| 79:s2:1726:G:H2'   | 79:s2:1727:G:C8   | 2.42                     | 0.54              |
| 79:s2:1758:G:N2    | 79:s2:1772:C:OP1  | 2.34                     | 0.54              |
| 80:cB:396:MET:SD   | 80:cB:416:VAL:HA  | 2.47                     | 0.54              |
| 83:ls:102:LEU:HD11 | 83:ls:187:LEU:HB2 | 1.89                     | 0.54              |
| 85:l5:128:C:H2'    | 85:l5:129:C:C6    | 2.42                     | 0.54              |
| 85:l5:956:A:N7     | 85:l5:1283:G:O2'  | 2.30                     | 0.54              |
| 85:l5:1708:G:H2'   | 85:l5:1709:C:H3'  | 1.89                     | 0.54              |
| 85:l5:1855:G:O6    | 85:l5:1880:G:N2   | 2.39                     | 0.54              |
| 85:l5:2274:C:H2'   | 85:l5:2275:G:C8   | 2.43                     | 0.54              |
| 2:SE:36:HIS:ND1    | 2:SE:85:GLY:HA3   | 2.22                     | 0.54              |
| 2:SE:122:LYS:O     | 2:SE:161:GLN:NE2  | 2.39                     | 0.54              |
| 3:SI:31:ARG:HH21   | 79:S2:380:G:H5''  | 1.72                     | 0.54              |
| 7:SJ:32:ILE:HA     | 7:SJ:37:LEU:CD1   | 2.37                     | 0.54              |
| 11:SB:108:ASP:OD1  | 11:SB:109:LYS:N   | 2.40                     | 0.54              |
| 15:SC:60:TRP:HH2   | 15:SC:93:ILE:HG22 | 1.72                     | 0.54              |
| 16:SN:62:GLN:HB2   | 16:SN:65:PHE:HE2  | 1.70                     | 0.54              |
| 19:Sb:49:HIS:ND1   | 19:Sb:69:GLY:O    | 2.40                     | 0.54              |
| 85:L5:69:A:H5'     | 85:L5:100:C:O2'   | 2.07                     | 0.54              |
| 85:L5:926:G:H2'    | 85:L5:927:G:H8    | 1.72                     | 0.54              |
| 85:L5:1985:G:N2    | 85:L5:2003:G:O2'  | 2.35                     | 0.54              |
| 85:L5:4072:C:H2'   | 85:L5:4073:A:H8   | 1.71                     | 0.54              |
| 85:L5:4420:U:O4    | 85:L5:4475:G:N2   | 2.40                     | 0.54              |
| 21:L8:137:A:H2'    | 21:L8:138:C:H6    | 1.71                     | 0.54              |
| 22:LA:57:PRO:HG2   | 22:LA:170:ALA:CB  | 2.36                     | 0.54              |
| 22:LA:61:VAL:HG13  | 22:LA:74:GLU:OE2  | 2.07                     | 0.54              |
| 23:LB:199:GLU:OE2  | 23:LB:200:ARG:NH2 | 2.41                     | 0.54              |
| 24:LC:287:THR:CG2  | 62:Lr:5:LEU:HD21  | 2.34                     | 0.54              |
| 34:LN:120:TRP:HE1  | 34:LN:123:GLU:HB3 | 1.72                     | 0.54              |
| 53:Lh:31:LEU:HD13  | 53:Lh:47:ILE:HG13 | 1.88                     | 0.54              |
| 60:Lo:3:ASN:HA     | 60:Lo:92:GLU:O    | 2.07                     | 0.54              |
| 66:SF:129:GLY:O    | 66:SF:135:ARG:NH2 | 2.29                     | 0.54              |
| 78:Sf:113:LYS:HD3  | 78:Sf:114:ILE:N   | 2.22                     | 0.54              |
| 79:S2:89:C:O2      | 79:S2:499:G:H4'   | 2.08                     | 0.54              |
| 79:S2:321:C:H2'    | 79:S2:322:C:C6    | 2.41                     | 0.54              |
| 79:S2:980:A:H2'    | 79:S2:981:A:C8    | 2.42                     | 0.54              |
| 79:S2:1380:C:H2'   | 79:S2:1381:G:C8   | 2.41                     | 0.54              |
| 79:S2:1729:U:O2    | 79:S2:1805:G:N2   | 2.31                     | 0.54              |
| 81:AP:1:G:H2'      | 81:AP:2:U:H6      | 1.72                     | 0.54              |
| 2:sE:19:MET:HE1    | 79:s2:846:G:C5    | 2.41                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:sL:7:GLU:OE1     | 79:s2:375:U:H4'    | 2.07                     | 0.54              |
| 6:sG:50:VAL:HG23   | 6:sG:113:ILE:HG13  | 1.89                     | 0.54              |
| 13:sV:40:ASP:OD1   | 13:sV:44:GLY:N     | 2.40                     | 0.54              |
| 19:sb:11:SER:OG    | 19:sb:14:GLU:HG2   | 2.07                     | 0.54              |
| 20:l7:110:G:H2'    | 20:l7:111:C:H6     | 1.72                     | 0.54              |
| 23:lB:95:THR:HG23  | 23:lB:97:ARG:N     | 2.22                     | 0.54              |
| 26:lE:62:MET:SD    | 26:lE:66:LYS:NZ    | 2.74                     | 0.54              |
| 29:lH:120:GLU:OE2  | 85:l5:4612:C:H1'   | 2.07                     | 0.54              |
| 36:lP:94:MET:CG    | 36:lP:148:MET:HE1  | 2.35                     | 0.54              |
| 39:lS:45:TRP:NE1   | 39:lS:61:ILE:HD11  | 2.22                     | 0.54              |
| 42:lV:131:ARG:O    | 42:lV:134:SER:OG   | 2.24                     | 0.54              |
| 62:lr:24:THR:HG22  | 85:l5:2289:C:N4    | 2.22                     | 0.54              |
| 66:sF:88:MET:HE3   | 79:s2:1535:U:H1'   | 1.89                     | 0.54              |
| 69:sQ:45:ARG:HH12  | 71:sT:10:ASN:ND2   | 2.04                     | 0.54              |
| 77:sZ:101:SER:HB3  | 77:sZ:108:ILE:HG22 | 1.89                     | 0.54              |
| 79:s2:79:A:H2'     | 79:s2:80:G:O4'     | 2.06                     | 0.54              |
| 79:s2:666:U:H2'    | 79:s2:667:U:C6     | 2.42                     | 0.54              |
| 79:s2:1801:A:H2'   | 79:s2:1802:C:H6    | 1.72                     | 0.54              |
| 83:ls:77:LYS:O     | 83:ls:80:PRO:HD2   | 2.08                     | 0.54              |
| 83:ls:157:ASP:OD1  | 83:ls:157:ASP:N    | 2.41                     | 0.54              |
| 85:l5:1080:C:N3    | 85:l5:1220:G:N1    | 2.54                     | 0.54              |
| 85:l5:2683:C:H2'   | 85:l5:2684:C:C6    | 2.42                     | 0.54              |
| 85:l5:3813:A:N3    | 85:l5:4538:G:O2'   | 2.34                     | 0.54              |
| 85:l5:4080:C:H2'   | 85:l5:4081:G:C8    | 2.42                     | 0.54              |
| 10:SA:149:ASN:O    | 10:SA:152:SER:OG   | 2.24                     | 0.54              |
| 11:SB:162:ARG:HH12 | 79:S2:1005:G:P     | 2.30                     | 0.54              |
| 12:SH:143:ARG:HE   | 18:SW:53:ILE:HD13  | 1.72                     | 0.54              |
| 15:SC:252:THR:OG1  | 15:SC:254:ASP:OD1  | 2.20                     | 0.54              |
| 85:L5:85:G:O2'     | 85:L5:97:G:O6      | 2.21                     | 0.54              |
| 85:L5:156:G:OP1    | 53:Lh:109:ARG:NH2  | 2.39                     | 0.54              |
| 85:L5:310:G:H2'    | 85:L5:311:G:C8     | 2.42                     | 0.54              |
| 85:L5:425:U:H2'    | 85:L5:426:A:H8     | 1.71                     | 0.54              |
| 85:L5:444:G:H2'    | 85:L5:445:U:H6     | 1.72                     | 0.54              |
| 85:L5:1802:A:N3    | 40:LT:130:ARG:NH2  | 2.44                     | 0.54              |
| 85:L5:3667:C:OP1   | 22:LA:234:LYS:HE3  | 2.07                     | 0.54              |
| 85:L5:4039:G:N2    | 85:L5:4050:A:O2'   | 2.39                     | 0.54              |
| 85:L5:4088:C:H2'   | 85:L5:4089:G:C8    | 2.42                     | 0.54              |
| 85:L5:4549:G:H2'   | 85:L5:4550:G:H8    | 1.71                     | 0.54              |
| 85:L5:4622:A:H2'   | 85:L5:4623:G:C8    | 2.42                     | 0.54              |
| 22:LA:56:ALA:HB2   | 22:LA:130:SER:HB2  | 1.88                     | 0.54              |
| 23:LB:325:GLU:N    | 23:LB:325:GLU:OE1  | 2.40                     | 0.54              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 24:LC:266:THR:OG1 | 24:LC:269:LYS:N    | 2.40                     | 0.54              |
| 28:LG:109:GLU:HA  | 28:LG:112:GLN:HG3  | 1.89                     | 0.54              |
| 33:LM:131:GLN:CD  | 35:LO:177:LEU:HD13 | 2.32                     | 0.54              |
| 39:LS:32:ILE:HD11 | 39:LS:40:ALA:HA    | 1.88                     | 0.54              |
| 62:Lr:7:TRP:HB2   | 62:Lr:44:ILE:HD13  | 1.89                     | 0.54              |
| 64:SR:1:MET:HE3   | 79:S2:1468:C:O5'   | 2.08                     | 0.54              |
| 70:SS:35:GLY:N    | 79:S2:1631:U:OP1   | 2.40                     | 0.54              |
| 74:Sd:25:SER:O    | 74:Sd:25:SER:OG    | 2.26                     | 0.54              |
| 79:S2:106:C:H2'   | 79:S2:107:A:C8     | 2.42                     | 0.54              |
| 83:Ls:27:CYS:HB3  | 83:Ls:193:PHE:HB3  | 1.88                     | 0.54              |
| 2:sE:134:LYS:N    | 79:s2:298:G:OP1    | 2.41                     | 0.54              |
| 4:sL:59:LYS:NZ    | 79:s2:374:G:OP1    | 2.41                     | 0.54              |
| 6:sG:106:LEU:HD21 | 6:sG:109:LEU:HB2   | 1.89                     | 0.54              |
| 10:sA:90:PHE:CD1  | 10:sA:90:PHE:C     | 2.84                     | 0.54              |
| 16:sN:17:PRO:HD3  | 19:sb:28:PRO:HG3   | 1.89                     | 0.54              |
| 21:l8:71:A:H2'    | 44:lY:50:ARG:HH12  | 1.72                     | 0.54              |
| 21:l8:90:C:H2'    | 21:l8:91:A:H8      | 1.72                     | 0.54              |
| 23:IB:145:GLN:HA  | 23:IB:148:LYS:HZ3  | 1.73                     | 0.54              |
| 25:ID:41:LYS:NZ   | 40:lT:32:ARG:O     | 2.38                     | 0.54              |
| 25:ID:45:ASN:HB2  | 85:l5:1823:G:H4'   | 1.90                     | 0.54              |
| 26:IE:94:LYS:NZ   | 85:l5:688:U:OP1    | 2.40                     | 0.54              |
| 27:IF:48:LYS:NZ   | 85:l5:1238:A:O3'   | 2.41                     | 0.54              |
| 27:IF:49:LEU:HD12 | 47:lb:100:ALA:HB3  | 1.88                     | 0.54              |
| 30:II:46:PHE:HB2  | 30:II:139:ARG:HE   | 1.72                     | 0.54              |
| 30:II:74:LYS:NZ   | 85:l5:4415:A:O2'   | 2.35                     | 0.54              |
| 30:II:188:LYS:HA  | 30:II:188:LYS:HE3  | 1.90                     | 0.54              |
| 32:IL:4:SER:OG    | 32:IL:5:ARG:N      | 2.39                     | 0.54              |
| 34:IN:169:ARG:NH2 | 85:l5:63:G:OP1     | 2.40                     | 0.54              |
| 35:IO:10:ASP:OD2  | 35:IO:37:ARG:NH2   | 2.39                     | 0.54              |
| 37:IQ:75:ARG:NH2  | 85:l5:1457:G:O2'   | 2.40                     | 0.54              |
| 38:IR:2:SER:OG    | 38:IR:3:MET:N      | 2.40                     | 0.54              |
| 43:IX:96:LEU:HB2  | 43:IX:138:VAL:HG23 | 1.89                     | 0.54              |
| 62:lr:108:MET:CE  | 85:l5:2263:A:H5''  | 2.37                     | 0.54              |
| 71:sT:5:THR:HG23  | 71:sT:7:LYS:HG2    | 1.89                     | 0.54              |
| 79:s2:198:U:H1'   | 79:s2:202:G:H1     | 1.72                     | 0.54              |
| 79:s2:1093:A:H2'  | 79:s2:1094:C:C6    | 2.42                     | 0.54              |
| 79:s2:1393:G:H2'  | 79:s2:1394:G:C8    | 2.43                     | 0.54              |
| 80:cB:88:PHE:CE1  | 80:cB:226:LYS:NZ   | 2.75                     | 0.54              |
| 84:lt:48:LYS:HZ3  | 84:lt:52:ASP:HA    | 1.71                     | 0.54              |
| 84:lt:149:HIS:NE2 | 85:l5:1993:C:H4'   | 2.22                     | 0.54              |
| 85:l5:221:C:H2'   | 85:l5:222:C:C6     | 2.41                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 85:l5:1881:C:H5'   | 85:l5:2281:U:H1'   | 1.89                     | 0.54              |
| 85:l5:2480:G:H2'   | 85:l5:2481:G:H8    | 1.72                     | 0.54              |
| 85:l5:2508:U:H2'   | 85:l5:2509:C:H6    | 1.72                     | 0.54              |
| 85:l5:3615:G:N2    | 87:lW:44:ARG:HH22  | 2.01                     | 0.54              |
| 85:l5:4098:A:N1    | 85:l5:4112:C:N4    | 2.55                     | 0.54              |
| 85:l5:4504:C:H2'   | 85:l5:4505:C:C6    | 2.42                     | 0.54              |
| 80:CB:78:PHE:O     | 80:CB:79:TYR:HD2   | 1.90                     | 0.54              |
| 2:SE:19:MET:HG2    | 2:SE:19:MET:O      | 2.07                     | 0.54              |
| 7:SJ:137:VAL:HG22  | 7:SJ:138:ARG:HG2   | 1.89                     | 0.54              |
| 15:SC:75:ILE:CD1   | 15:SC:80:GLU:OE2   | 2.52                     | 0.54              |
| 85:L5:14:C:H5''    | 43:LX:56:ARG:HD3   | 1.89                     | 0.54              |
| 85:L5:270:U:H2'    | 85:L5:271:C:H6     | 1.71                     | 0.54              |
| 85:L5:452:A:H4'    | 85:L5:453:G:H5'    | 1.88                     | 0.54              |
| 85:L5:1908:A:H2'   | 85:L5:1909:G:O4'   | 2.07                     | 0.54              |
| 85:L5:3687:A:O2'   | 22:LA:236:GLY:N    | 2.40                     | 0.54              |
| 85:L5:3774:A:H2'   | 85:L5:3775:A:N3    | 2.22                     | 0.54              |
| 85:L5:3937:C:H3'   | 85:L5:3938:G:H2'   | 1.89                     | 0.54              |
| 85:L5:4070:U:H2'   | 85:L5:4071:U:H6    | 1.72                     | 0.54              |
| 27:LF:126:ASN:O    | 27:LF:130:ILE:HG12 | 2.07                     | 0.54              |
| 28:LG:151:LYS:O    | 28:LG:151:LYS:NZ   | 2.41                     | 0.54              |
| 33:LM:28:VAL:HG23  | 33:LM:64:PHE:HE1   | 1.72                     | 0.54              |
| 45:LZ:36:ARG:HB2   | 45:LZ:40:HIS:CE1   | 2.42                     | 0.54              |
| 65:SD:161:GLY:HA3  | 79:S2:1388:A:H61   | 1.72                     | 0.54              |
| 68:SP:112:ILE:HD12 | 68:SP:112:ILE:H    | 1.70                     | 0.54              |
| 76:SM:36:ARG:HH22  | 78:Sf:103:LEU:HA   | 1.72                     | 0.54              |
| 79:S2:670:A:O2'    | 79:S2:1163:C:O2'   | 2.25                     | 0.54              |
| 79:S2:1206:G:H1'   | 79:S2:1834:A:C4    | 2.42                     | 0.54              |
| 79:S2:1802:C:H2'   | 79:S2:1803:U:C6    | 2.41                     | 0.54              |
| 83:Ls:194:ASP:N    | 83:Ls:194:ASP:OD1  | 2.40                     | 0.54              |
| 87:lW:114:GLU:HA   | 87:lW:117:LYS:HD2  | 1.89                     | 0.54              |
| 2:sE:37:LYS:HD2    | 79:s2:345:U:H5''   | 1.88                     | 0.54              |
| 4:sL:75:GLY:N      | 4:sL:126:VAL:O     | 2.39                     | 0.54              |
| 7:sJ:145:PRO:HD2   | 79:s2:522:A:H5''   | 1.90                     | 0.54              |
| 20:l7:37:G:N2      | 20:l7:41:G:N3      | 2.55                     | 0.54              |
| 20:l7:58:A:H2'     | 20:l7:59:G:C8      | 2.43                     | 0.54              |
| 23:lB:214:ASP:OD1  | 23:lB:363:ILE:HG12 | 2.08                     | 0.54              |
| 29:lH:28:LYS:HE2   | 29:lH:28:LYS:HA    | 1.89                     | 0.54              |
| 41:lU:21:PHE:HB3   | 41:lU:72:VAL:CG2   | 2.37                     | 0.54              |
| 63:lz:23:ARG:O     | 63:lz:212:LYS:NZ   | 2.41                     | 0.54              |
| 63:lz:209:THR:HA   | 85:l5:4052:C:H1'   | 1.89                     | 0.54              |
| 64:sR:14:ARG:NH2   | 79:s2:1373:C:H1'   | 2.23                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 65:sD:8:LYS:NZ     | 79:s2:1549:U:OP2   | 2.39                     | 0.54              |
| 65:sD:90:LYS:NZ    | 65:sD:92:ALA:HA    | 2.22                     | 0.54              |
| 65:sD:139:SER:O    | 65:sD:183:GLY:N    | 2.32                     | 0.54              |
| 68:sP:135:ALA:HA   | 79:s2:1524:G:H1'   | 1.89                     | 0.54              |
| 70:sS:36:VAL:HG13  | 70:sS:40:TYR:CE1   | 2.43                     | 0.54              |
| 73:sc:21:THR:N     | 73:sc:27:CYS:O     | 2.38                     | 0.54              |
| 76:sM:106:CYS:SG   | 76:sM:107:SER:N    | 2.80                     | 0.54              |
| 79:s2:24:C:O2'     | 79:s2:25:A:H8      | 1.89                     | 0.54              |
| 79:s2:452:G:H2'    | 79:s2:453:C:H6     | 1.72                     | 0.54              |
| 79:s2:909:G:H2'    | 79:s2:910:G:C8     | 2.43                     | 0.54              |
| 79:s2:1004:U:H2'   | 79:s2:1005:G:C8    | 2.41                     | 0.54              |
| 79:s2:1142:G:H21   | 79:s2:1145:A:H62   | 1.55                     | 0.54              |
| 79:s2:1474:A:H2'   | 79:s2:1475:G:N9    | 2.23                     | 0.54              |
| 80:cB:109:VAL:HG11 | 85:l5:4605:A:O2'   | 2.08                     | 0.54              |
| 80:cB:152:LYS:HG3  | 80:cB:359:PRO:HG2  | 1.90                     | 0.54              |
| 80:cB:761:GLY:C    | 80:cB:765:ARG:HE   | 2.14                     | 0.54              |
| 85:l5:286:U:H2'    | 85:l5:287:U:C6     | 2.42                     | 0.54              |
| 85:l5:407:A:O2'    | 85:l5:410:A:OP1    | 2.22                     | 0.54              |
| 85:l5:3969:G:N7    | 85:l5:4051:C:N4    | 2.55                     | 0.54              |
| 85:l5:5018:C:H2'   | 85:l5:5019:A:H8    | 1.71                     | 0.54              |
| 7:SJ:104:ASP:OD1   | 7:SJ:104:ASP:N     | 2.40                     | 0.54              |
| 10:SA:109:THR:HG21 | 79:S2:1378:A:H61   | 1.72                     | 0.54              |
| 10:SA:158:ASP:O    | 13:SV:69:ILE:HD11  | 2.07                     | 0.54              |
| 85:L5:307:A:N3     | 85:L5:310:G:O2'    | 2.40                     | 0.54              |
| 85:L5:665:C:H4'    | 85:L5:666:G:H5'    | 1.88                     | 0.54              |
| 85:L5:966:A:OP2    | 85:L5:2092:G:N2    | 2.40                     | 0.54              |
| 85:L5:1522:G:H2'   | 85:L5:1653:A:H61   | 1.72                     | 0.54              |
| 85:L5:1615:C:H2'   | 85:L5:1616:U:C6    | 2.43                     | 0.54              |
| 85:L5:1780:A:N3    | 30:LI:198:LYS:NZ   | 2.41                     | 0.54              |
| 85:L5:2411:C:H2'   | 85:L5:2412:A:C8    | 2.42                     | 0.54              |
| 85:L5:2539:C:H2'   | 85:L5:2540:C:C6    | 2.43                     | 0.54              |
| 85:L5:3883:U:H2'   | 85:L5:3884:U:C6    | 2.43                     | 0.54              |
| 85:L5:4691:A:H2'   | 85:L5:4692:A:O4'   | 2.07                     | 0.54              |
| 23:LB:119:TYR:OH   | 23:LB:128:LYS:N    | 2.40                     | 0.54              |
| 31:LJ:36:ALA:HB2   | 31:LJ:126:TYR:CZ   | 2.43                     | 0.54              |
| 35:LO:10:ASP:HB2   | 35:LO:117:ARG:HB3  | 1.89                     | 0.54              |
| 41:LU:83:LEU:HD12  | 41:LU:84:LYS:N     | 2.23                     | 0.54              |
| 49:Ld:33:ILE:HD12  | 49:Ld:45:ALA:HB2   | 1.88                     | 0.54              |
| 52:Lg:94:ALA:O     | 52:Lg:98:GLU:HG2   | 2.07                     | 0.54              |
| 63:Lz:123:ILE:HG23 | 63:Lz:124:LEU:HD23 | 1.89                     | 0.54              |
| 63:Lz:171:HIS:NE2  | 63:Lz:173:LYS:HB2  | 2.22                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 72:SU:90:ASP:O     | 72:SU:91:LEU:HD23  | 2.07                     | 0.54              |
| 72:SU:98:VAL:HA    | 72:SU:101:ILE:HG12 | 1.90                     | 0.54              |
| 75:Sg:45:LEU:O     | 75:Sg:47:ARG:NH1   | 2.38                     | 0.54              |
| 79:S2:186:C:H2'    | 79:S2:187:G:C8     | 2.42                     | 0.54              |
| 79:S2:1198:G:H2'   | 79:S2:1199:A:C8    | 2.42                     | 0.54              |
| 79:S2:1568:C:H2'   | 79:S2:1569:A:C8    | 2.43                     | 0.54              |
| 79:S2:1712:A:H2'   | 79:S2:1713:C:H6    | 1.69                     | 0.54              |
| 81:AP:50:U:H2'     | 81:AP:51:C:H6      | 1.72                     | 0.54              |
| 7:sJ:140:GLN:NE2   | 7:sJ:141:VAL:O     | 2.41                     | 0.54              |
| 10:sA:23:THR:HG21  | 10:sA:173:LEU:HD23 | 1.88                     | 0.54              |
| 11:sB:151:ARG:N    | 64:sR:133:GLY:H    | 2.05                     | 0.54              |
| 12:sH:129:ILE:HD11 | 12:sH:177:TYR:HE1  | 1.72                     | 0.54              |
| 12:sH:173:PHE:HB2  | 12:sH:187:PHE:CE2  | 2.43                     | 0.54              |
| 15:sC:72:ASP:N     | 15:sC:72:ASP:OD1   | 2.39                     | 0.54              |
| 15:sC:195:LEU:HD23 | 15:sC:195:LEU:H    | 1.72                     | 0.54              |
| 17:sO:31:CYS:HA    | 17:sO:44:VAL:HA    | 1.90                     | 0.54              |
| 24:lC:213:GLU:N    | 24:lC:213:GLU:OE2  | 2.40                     | 0.54              |
| 26:lE:141:ARG:NH2  | 51:lF:108:SER:O    | 2.40                     | 0.54              |
| 26:lE:211:HIS:NE2  | 26:lE:249:ASP:OD2  | 2.39                     | 0.54              |
| 26:lE:270:TYR:OH   | 33:lM:107:PHE:HA   | 2.08                     | 0.54              |
| 27:lF:203:GLU:N    | 27:lF:203:GLU:OE2  | 2.40                     | 0.54              |
| 34:lN:120:TRP:NE1  | 34:lN:122:GLY:N    | 2.50                     | 0.54              |
| 35:lO:85:ARG:NH2   | 85:l5:3887:C:OP2   | 2.26                     | 0.54              |
| 36:lP:101:ASN:OD1  | 85:l5:400:A:O2'    | 2.16                     | 0.54              |
| 37:lQ:88:ASP:OD1   | 37:lQ:89:ASP:N     | 2.40                     | 0.54              |
| 62:lr:61:VAL:HA    | 62:lr:81:THR:HA    | 1.88                     | 0.54              |
| 62:lr:85:ASN:O     | 62:lr:89:THR:HG23  | 2.08                     | 0.54              |
| 64:sR:61:ILE:HG12  | 64:sR:73:LEU:HD21  | 1.90                     | 0.54              |
| 65:sD:163:PRO:HA   | 65:sD:166:TYR:CE2  | 2.42                     | 0.54              |
| 66:sF:188:TYR:OH   | 66:sF:192:LYS:NZ   | 2.41                     | 0.54              |
| 68:sP:90:VAL:HA    | 68:sP:107:ILE:HG22 | 1.88                     | 0.54              |
| 74:sd:14:PHE:CE1   | 79:s2:1617:G:H4'   | 2.41                     | 0.54              |
| 75:sg:107:ASP:OD2  | 75:sg:125:ARG:NH2  | 2.36                     | 0.54              |
| 77:sZ:101:SER:OG   | 77:sZ:102:LYS:N    | 2.39                     | 0.54              |
| 79:s2:148:U:O2     | 79:s2:171:A:N6     | 2.41                     | 0.54              |
| 79:s2:859:G:H2'    | 79:s2:860:G:C8     | 2.42                     | 0.54              |
| 79:s2:1416:C:P     | 79:s2:1416:C:H6    | 2.31                     | 0.54              |
| 80:cB:13:MET:C     | 80:cB:13:MET:HE3   | 2.32                     | 0.54              |
| 80:cB:99:LEU:HD23  | 80:cB:100:ILE:N    | 2.22                     | 0.54              |
| 80:cB:169:LEU:HD12 | 80:cB:170:GLU:H    | 1.72                     | 0.54              |
| 80:cB:361:PRO:O    | 80:cB:365:GLN:HG2  | 2.07                     | 0.54              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 80:cB:829:SER:O    | 80:cB:832:SER:OG  | 2.19                     | 0.54              |
| 85:l5:651:C:H2'    | 85:l5:652:G:C8    | 2.43                     | 0.54              |
| 85:l5:1702:C:H3'   | 85:l5:1703:C:H5'' | 1.90                     | 0.54              |
| 85:l5:2689:C:H2'   | 85:l5:2690:C:C6   | 2.43                     | 0.54              |
| 85:l5:2897:G:H2'   | 85:l5:2898:G:H8   | 1.72                     | 0.54              |
| 85:l5:4411:G:H2'   | 85:l5:4412:C:C6   | 2.42                     | 0.54              |
| 85:l5:4627:U:H2'   | 85:l5:4628:U:O4'  | 2.08                     | 0.54              |
| 85:l5:4913:G:H4'   | 85:l5:4914:C:O5'  | 2.07                     | 0.54              |
| 4:SL:5:GLN:HE22    | 4:SL:11:GLN:HE22  | 1.56                     | 0.54              |
| 6:SG:56:ASN:ND2    | 79:S2:156:G:N3    | 2.56                     | 0.54              |
| 10:SA:18:PHE:CZ    | 10:SA:51:LEU:HD22 | 2.42                     | 0.54              |
| 14:Sa:13:LYS:HZ2   | 79:S2:1132:C:H2'  | 1.66                     | 0.54              |
| 15:SC:115:GLN:HG2  | 15:SC:120:GLN:HG3 | 1.90                     | 0.54              |
| 17:SO:31:CYS:HA    | 17:SO:44:VAL:HA   | 1.88                     | 0.54              |
| 85:L5:10:A:H2'     | 85:L5:11:G:C8     | 2.42                     | 0.54              |
| 85:L5:1420:A:C5'   | 37:LQ:68:ARG:HH21 | 2.21                     | 0.54              |
| 85:L5:1925:G:P     | 33:LM:34:ASN:HD21 | 2.30                     | 0.54              |
| 85:L5:2582:A:N3    | 85:L5:2654:C:H1'  | 2.23                     | 0.54              |
| 85:L5:2756:G:H2'   | 85:L5:2757:A:C8   | 2.42                     | 0.54              |
| 85:L5:3937:C:H1'   | 34:LN:125:SER:CB  | 2.30                     | 0.54              |
| 85:L5:4078:C:OP1   | 34:LN:31:ARG:NH1  | 2.40                     | 0.54              |
| 85:L5:4102:C:C6    | 85:L5:4102:C:C1'  | 2.84                     | 0.54              |
| 85:L5:4111:U:P     | 85:L5:4112:C:C2   | 3.01                     | 0.54              |
| 85:L5:4333:C:H1'   | 40:LT:8:ARG:HH12  | 1.73                     | 0.54              |
| 85:L5:4524:G:C2    | 23:LB:252:ALA:HB1 | 2.43                     | 0.54              |
| 21:L8:96:C:H5''    | 53:Lh:66:LYS:HG2  | 1.90                     | 0.54              |
| 32:LL:55:ILE:HD12  | 32:LL:155:MET:HE3 | 1.89                     | 0.54              |
| 62:Lr:5:LEU:HD22   | 62:Lr:5:LEU:N     | 2.22                     | 0.54              |
| 66:SF:104:THR:HG1  | 66:SF:106:GLU:CD  | 2.15                     | 0.54              |
| 69:SQ:139:ALA:HB2  | 79:S2:1650:A:H5'' | 1.89                     | 0.54              |
| 75:Sg:218:LEU:HD12 | 75:Sg:228:TYR:HB3 | 1.89                     | 0.54              |
| 79:S2:567:C:O2'    | 79:S2:583:A:N6    | 2.34                     | 0.54              |
| 79:S2:677:G:N1     | 79:S2:1027:A:OP2  | 2.20                     | 0.54              |
| 79:S2:947:G:H2'    | 79:S2:948:C:C6    | 2.42                     | 0.54              |
| 79:S2:1472:C:H2'   | 79:S2:1473:G:O4'  | 2.07                     | 0.54              |
| 1:cH:47:GLY:O      | 79:s2:605:A:H4'   | 2.07                     | 0.54              |
| 4:sL:107:LYS:NZ    | 79:s2:355:G:OP2   | 2.34                     | 0.54              |
| 5:sX:77:ASN:O      | 5:sX:79:LYS:N     | 2.39                     | 0.54              |
| 5:sX:100:VAL:HG21  | 5:sX:122:VAL:HG13 | 1.89                     | 0.54              |
| 12:sH:40:LEU:H     | 12:sH:40:LEU:HD12 | 1.72                     | 0.54              |
| 14:sa:88:SER:OG    | 79:s2:1691:U:H4'  | 2.07                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 15:sC:78:LEU:O     | 15:sC:81:ILE:HG22  | 2.08                     | 0.54              |
| 15:sC:81:ILE:CD1   | 15:sC:86:LEU:HB2   | 2.38                     | 0.54              |
| 22:1A:102:LEU:HD11 | 22:1A:107:MET:HG2  | 1.90                     | 0.54              |
| 26:1E:134:SER:N    | 85:l5:1288:G:OP1   | 2.41                     | 0.54              |
| 30:1I:156:LYS:HD3  | 30:1I:165:ILE:HD11 | 1.90                     | 0.54              |
| 31:1J:56:THR:HG22  | 31:1J:63:ARG:HG3   | 1.90                     | 0.54              |
| 35:1O:188:LYS:NZ   | 85:l5:4893:A:OP1   | 2.36                     | 0.54              |
| 45:1Z:113:GLU:OE2  | 45:1Z:117:LYS:HG3  | 2.07                     | 0.54              |
| 56:1k:7:GLU:OE1    | 56:1k:9:LYS:N      | 2.41                     | 0.54              |
| 64:sR:1:MET:SD     | 64:sR:2:GLY:N      | 2.68                     | 0.54              |
| 71:sT:71:GLY:N     | 71:sT:74:SER:OG    | 2.37                     | 0.54              |
| 71:sT:139:ALA:HA   | 71:sT:142:ASN:HD21 | 1.73                     | 0.54              |
| 73:sc:21:THR:HG23  | 73:sc:27:CYS:HB2   | 1.90                     | 0.54              |
| 78:sf:102:VAL:HG12 | 78:sf:103:LEU:N    | 2.22                     | 0.54              |
| 79:s2:433:A:H2'    | 79:s2:434:G:C8     | 2.43                     | 0.54              |
| 79:s2:806:U:H2'    | 79:s2:807:G:C8     | 2.42                     | 0.54              |
| 79:s2:896:U:C4     | 79:s2:897:U:H5     | 2.26                     | 0.54              |
| 79:s2:918:U:H2'    | 79:s2:919:A:C4     | 2.42                     | 0.54              |
| 80:cB:599:HIS:HB3  | 80:cB:710:HIS:HB2  | 1.89                     | 0.54              |
| 80:cB:832:SER:HA   | 80:cB:835:VAL:HG22 | 1.90                     | 0.54              |
| 81:aP:68:G:H2'     | 81:aP:69:A:C8      | 2.43                     | 0.54              |
| 82:pE:36:U:H2'     | 82:pE:37:A:O4'     | 2.08                     | 0.54              |
| 82:pE:76:A:O2'     | 85:l5:4371:G:N2    | 2.41                     | 0.54              |
| 85:l5:657:C:H2'    | 85:l5:658:C:C6     | 2.43                     | 0.54              |
| 85:l5:1297:U:H2'   | 85:l5:1298:C:H6    | 1.72                     | 0.54              |
| 85:l5:2020:U:H2'   | 85:l5:2021:G:H8    | 1.73                     | 0.54              |
| 85:l5:2579:G:N1    | 85:l5:2583:C:N3    | 2.56                     | 0.54              |
| 85:l5:2590:G:N2    | 85:l5:2754:G:N3    | 2.55                     | 0.54              |
| 85:l5:2764:A:H2'   | 85:l5:2765:A:C8    | 2.43                     | 0.54              |
| 85:l5:4049:U:O2    | 85:l5:4051:C:N4    | 2.40                     | 0.54              |
| 85:l5:4092:G:H2'   | 85:l5:4093:G:N3    | 2.23                     | 0.54              |
| 80:CB:13:MET:HA    | 80:CB:19:ILE:HD11  | 1.89                     | 0.54              |
| 80:CB:43:ALA:CB    | 80:CB:79:TYR:CE2   | 2.80                     | 0.54              |
| 80:CB:410:PHE:CZ   | 80:CB:526:ARG:HG2  | 2.40                     | 0.54              |
| 80:CB:730:TYR:HB3  | 80:CB:854:PHE:CD2  | 2.42                     | 0.54              |
| 3:SI:91:VAL:O      | 3:SI:94:LYS:HD2    | 2.07                     | 0.54              |
| 6:SG:142:ARG:HB3   | 6:SG:147:LEU:HB2   | 1.88                     | 0.54              |
| 7:SJ:117:LEU:HD12  | 7:SJ:119:LEU:H     | 1.73                     | 0.54              |
| 10:SA:186:ARG:HB2  | 10:SA:186:ARG:NH1  | 2.23                     | 0.54              |
| 14:Sa:92:ARG:HG3   | 79:S2:1865:C:P     | 2.47                     | 0.54              |
| 85:L5:433:A:H2'    | 85:L5:434:A:O4'    | 2.08                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 85:L5:1271:G:OP2   | 85:L5:1271:G:N2    | 2.24                     | 0.54              |
| 85:L5:1392:A:H2'   | 85:L5:1393:G:C8    | 2.42                     | 0.54              |
| 85:L5:1700:G:C8    | 85:L5:2097:U:H1'   | 2.42                     | 0.54              |
| 85:L5:2389:A:H5'   | 49:Ld:70:LYS:HE3   | 1.89                     | 0.54              |
| 85:L5:2699:C:H2'   | 85:L5:2700:G:C8    | 2.43                     | 0.54              |
| 85:L5:4485:C:H2'   | 85:L5:4486:C:C6    | 2.43                     | 0.54              |
| 20:L7:82:G:H2'     | 20:L7:83:A:C8      | 2.43                     | 0.54              |
| 24:LC:25:PRO:HD2   | 24:LC:28:PHE:CE2   | 2.37                     | 0.54              |
| 24:LC:263:LEU:HG   | 24:LC:264:TYR:CE2  | 2.43                     | 0.54              |
| 25:LD:195:HIS:CE1  | 25:LD:199:ILE:HD11 | 2.43                     | 0.54              |
| 26:LE:120:ASP:OD1  | 26:LE:121:VAL:N    | 2.40                     | 0.54              |
| 27:LF:33:LEU:HA    | 27:LF:36:LYS:HG2   | 1.90                     | 0.54              |
| 29:LH:106:GLN:N    | 29:LH:111:LEU:O    | 2.38                     | 0.54              |
| 29:LH:120:GLU:HG3  | 29:LH:124:ARG:HH12 | 1.72                     | 0.54              |
| 30:LI:170:LYS:HA   | 30:LI:177:ASN:HA   | 1.90                     | 0.54              |
| 36:LP:15:CYS:SG    | 36:LP:150:LEU:HB2  | 2.47                     | 0.54              |
| 41:LU:105:ASN:OD1  | 41:LU:109:SER:HB2  | 2.08                     | 0.54              |
| 52:Lg:46:CYS:HB2   | 52:Lg:86:CYS:SG    | 2.47                     | 0.54              |
| 58:Lm:110:CYS:HB3  | 58:Lm:115:CYS:SG   | 2.48                     | 0.54              |
| 62:Lr:108:MET:HE2  | 62:Lr:108:MET:H    | 1.72                     | 0.54              |
| 65:SD:223:ILE:HD11 | 75:Sg:189:ILE:HD11 | 1.89                     | 0.54              |
| 67:SK:49:MET:HE2   | 67:SK:69:TRP:CG    | 2.43                     | 0.54              |
| 68:SP:30:TYR:O     | 68:SP:33:LEU:HB3   | 2.08                     | 0.54              |
| 72:SU:51:LYS:NZ    | 79:S2:1401:A:O3'   | 2.40                     | 0.54              |
| 79:S2:1817:G:H2'   | 79:S2:1818:A:C8    | 2.43                     | 0.54              |
| 82:PE:9:A:O2'      | 82:PE:45:G:N3      | 2.35                     | 0.54              |
| 83:Ls:160:LEU:HD21 | 83:Ls:175:LEU:HD11 | 1.88                     | 0.54              |
| 84:Lt:64:ILE:O     | 84:Lt:71:ILE:N     | 2.29                     | 0.54              |
| 1:cH:53:SER:HA     | 9:se:59:SER:N      | 2.22                     | 0.54              |
| 13:sV:55:ILE:HG21  | 13:sV:60:ARG:HB2   | 1.90                     | 0.54              |
| 22:lA:9:ARG:NH2    | 85:l5:1629:G:OP2   | 2.28                     | 0.54              |
| 24:lC:289:LEU:HD21 | 37:lQ:31:LEU:HB2   | 1.89                     | 0.54              |
| 25:lD:70:GLU:OE1   | 25:lD:70:GLU:N     | 2.30                     | 0.54              |
| 25:lD:155:THR:OG1  | 25:lD:179:ARG:NH1  | 2.34                     | 0.54              |
| 26:lE:224:LYS:HG2  | 26:lE:227:HIS:HB2  | 1.89                     | 0.54              |
| 28:lG:136:LEU:HB2  | 28:lG:203:ALA:O    | 2.08                     | 0.54              |
| 29:lH:71:ARG:HD3   | 85:l5:4691:A:O3'   | 2.08                     | 0.54              |
| 35:lO:109:PRO:C    | 35:lO:111:PRO:HD2  | 2.32                     | 0.54              |
| 35:lO:118:MET:HE3  | 35:lO:119:VAL:H    | 1.73                     | 0.54              |
| 41:lU:39:PHE:HD2   | 41:lU:43:LEU:HD11  | 1.73                     | 0.54              |
| 41:lU:106:SER:OG   | 41:lU:109:SER:OG   | 2.21                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 50:le:45:VAL:HG11  | 50:le:53:ILE:HG22  | 1.90                     | 0.54              |
| 55:lj:67:LEU:O     | 55:lj:71:TYR:HD2   | 1.90                     | 0.54              |
| 64:sR:5:ARG:HA     | 79:s2:1368:U:C2    | 2.42                     | 0.54              |
| 64:sR:26:ASN:HA    | 64:sR:59:LYS:HE2   | 1.90                     | 0.54              |
| 67:sK:26:ASP:OD1   | 67:sK:29:MET:HE2   | 2.07                     | 0.54              |
| 69:sQ:11:GLN:HE22  | 79:s2:1442:U:H1'   | 1.72                     | 0.54              |
| 71:sT:7:LYS:CE     | 79:s2:1426:U:H5'   | 2.38                     | 0.54              |
| 79:s2:454:U:H2'    | 79:s2:455:A:C8     | 2.40                     | 0.54              |
| 79:s2:511:U:H2'    | 79:s2:512:A:H8     | 1.72                     | 0.54              |
| 79:s2:1452:A:C2    | 79:s2:1475:G:H2'   | 2.43                     | 0.54              |
| 79:s2:1523:C:H2'   | 79:s2:1524:G:H8    | 1.71                     | 0.54              |
| 80:cB:750:GLN:HB2  | 80:cB:809:PHE:HB2  | 1.90                     | 0.54              |
| 80:cB:839:ARG:NH1  | 80:cB:845:LYS:O    | 2.33                     | 0.54              |
| 82:pE:9:A:H2'      | 82:pE:11:C:H41     | 1.72                     | 0.54              |
| 82:pE:22:G:H2'     | 82:pE:23:A:C8      | 2.42                     | 0.54              |
| 85:l5:267:G:H2'    | 85:l5:268:G:C8     | 2.42                     | 0.54              |
| 85:l5:458:C:H2'    | 85:l5:459:C:H6     | 1.73                     | 0.54              |
| 85:l5:1084:C:H2'   | 85:l5:1085:C:C6    | 2.42                     | 0.54              |
| 85:l5:1291:G:H2'   | 85:l5:1292:C:C6    | 2.43                     | 0.54              |
| 85:l5:3910:C:H2'   | 85:l5:3911:C:C6    | 2.43                     | 0.54              |
| 85:l5:4040:C:O2'   | 85:l5:4049:U:OP2   | 2.20                     | 0.54              |
| 2:SE:91:SER:OG     | 2:SE:93:ASP:OD1    | 2.24                     | 0.54              |
| 5:SX:93:PHE:HB3    | 5:SX:133:LEU:HD21  | 1.89                     | 0.54              |
| 6:SG:4:ASN:ND2     | 79:S2:154:U:O2     | 2.29                     | 0.54              |
| 7:SJ:162:ARG:NH2   | 79:S2:583:A:OP1    | 2.37                     | 0.54              |
| 11:SB:157:GLN:HE22 | 11:SB:159:GLN:HG2  | 1.73                     | 0.54              |
| 14:Sa:64:LEU:HD12  | 14:Sa:64:LEU:H     | 1.73                     | 0.54              |
| 15:SC:133:TYR:CE1  | 15:SC:216:MET:HG2  | 2.42                     | 0.54              |
| 16:SN:70:LYS:O     | 16:SN:74:ILE:HD12  | 2.07                     | 0.54              |
| 85:L5:1588:U:H2'   | 85:L5:1589:C:C6    | 2.43                     | 0.54              |
| 85:L5:3606:U:H2'   | 85:L5:3607:U:H6    | 1.69                     | 0.54              |
| 85:L5:4095:G:O2'   | 85:L5:4110:C:O4'   | 2.26                     | 0.54              |
| 21:L8:6:C:H2'      | 21:L8:7:U:C6       | 2.43                     | 0.54              |
| 21:L8:27:U:H2'     | 21:L8:28:C:H6      | 1.72                     | 0.54              |
| 26:LE:164:PHE:HE1  | 26:LE:173:LEU:HB3  | 1.72                     | 0.54              |
| 26:LE:166:LYS:HG2  | 26:LE:208:ILE:HD13 | 1.88                     | 0.54              |
| 34:LN:47:LYS:HD3   | 34:LN:50:ARG:HH11  | 1.73                     | 0.54              |
| 34:LN:80:THR:HG21  | 34:LN:87:HIS:HA    | 1.90                     | 0.54              |
| 39:LS:79:GLY:H     | 39:LS:132:ILE:HG12 | 1.73                     | 0.54              |
| 66:SF:152:TRP:O    | 66:SF:156:THR:HG23 | 2.08                     | 0.54              |
| 76:SM:84:LYS:CD    | 76:SM:88:TRP:HE1   | 2.18                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 79:S2:12:U:H2'     | 79:S2:13:C:H6      | 1.72                     | 0.54              |
| 79:S2:479:C:C2     | 79:S2:480:G:C8     | 2.96                     | 0.54              |
| 79:S2:1093:A:H2'   | 79:S2:1094:C:H6    | 1.71                     | 0.54              |
| 79:S2:1395:C:H2'   | 79:S2:1396:A:O4'   | 2.07                     | 0.54              |
| 79:S2:1396:A:C5    | 79:S2:1449:G:O6    | 2.59                     | 0.54              |
| 6:sG:59:GLN:N      | 6:sG:59:GLN:OE1    | 2.41                     | 0.54              |
| 7:sJ:32:ILE:O      | 7:sJ:36:GLY:N      | 2.41                     | 0.54              |
| 15:sC:195:LEU:HB2  | 15:sC:222:CYS:SG   | 2.47                     | 0.54              |
| 18:sW:105:THR:HG22 | 18:sW:110:ILE:HD12 | 1.89                     | 0.54              |
| 21:l8:102:G:OP2    | 21:l8:104:A:O2'    | 2.23                     | 0.54              |
| 21:l8:141:C:H2'    | 21:l8:142:U:C6     | 2.43                     | 0.54              |
| 22:lA:27:ALA:HB2   | 22:lA:58:LEU:HD21  | 1.89                     | 0.54              |
| 22:lA:180:LEU:HD22 | 61:lp:26:VAL:HG21  | 1.89                     | 0.54              |
| 23:lB:252:ALA:HB1  | 85:l5:4524:G:C2    | 2.42                     | 0.54              |
| 29:lH:19:THR:HG22  | 29:lH:26:ILE:HB    | 1.90                     | 0.54              |
| 37:lQ:61:LEU:HD11  | 37:lQ:65:ARG:HB3   | 1.89                     | 0.54              |
| 37:lQ:124:ASP:OD1  | 37:lQ:125:GLN:N    | 2.39                     | 0.54              |
| 43:lX:123:LYS:NZ   | 85:l5:2532:C:OP1   | 2.28                     | 0.54              |
| 45:lZ:89:ILE:HD12  | 45:lZ:90:PRO:HD3   | 1.90                     | 0.54              |
| 49:ld:63:ARG:HB2   | 49:ld:105:LEU:HD23 | 1.90                     | 0.54              |
| 65:sD:27:ARG:HH22  | 79:s2:1498:A:P     | 2.31                     | 0.54              |
| 65:sD:74:GLN:HA    | 65:sD:79:PHE:CD2   | 2.43                     | 0.54              |
| 73:sc:33:GLU:HG3   | 73:sc:41:SER:HB2   | 1.90                     | 0.54              |
| 75:sg:164:ILE:HD12 | 75:sg:177:TRP:O    | 2.07                     | 0.54              |
| 77:sZ:43:LYS:HD2   | 77:sZ:45:ASN:HB3   | 1.90                     | 0.54              |
| 79:s2:49:C:H2'     | 79:s2:472:C:H41    | 1.71                     | 0.54              |
| 79:s2:458:A:H2'    | 79:s2:459:C:H6     | 1.73                     | 0.54              |
| 80:cB:19:ILE:HG21  | 80:cB:468:ASN:HD21 | 1.72                     | 0.54              |
| 80:cB:225:LEU:HD21 | 80:cB:260:LEU:HD23 | 1.89                     | 0.54              |
| 80:cB:801:ARG:HG3  | 80:cB:806:GLY:HA2  | 1.90                     | 0.54              |
| 85:l5:680:G:H2'    | 85:l5:681:G:C8     | 2.43                     | 0.54              |
| 85:l5:1950:U:H2'   | 85:l5:1951:G:H8    | 1.73                     | 0.54              |
| 85:l5:2832:A:H2'   | 85:l5:2833:A:H8    | 1.72                     | 0.54              |
| 85:l5:4566:U:H2'   | 85:l5:4567:G:O4'   | 2.08                     | 0.54              |
| 85:l5:4679:G:H2'   | 85:l5:4680:G:H8    | 1.73                     | 0.54              |
| 85:l5:4970:C:C2    | 85:l5:4971:A:C8    | 2.96                     | 0.54              |
| 80:CB:156:MET:C    | 80:CB:157:MET:HE2  | 2.33                     | 0.54              |
| 6:SG:176:ILE:HG22  | 6:SG:179:LEU:HD23  | 1.90                     | 0.54              |
| 6:SG:231:ARG:HD2   | 79:S2:786:G:H5''   | 1.90                     | 0.54              |
| 86:Se:35:ARG:NH1   | 79:S2:526:A:OP1    | 2.40                     | 0.54              |
| 14:Sa:28:ARG:HB2   | 17:SO:148:GLY:HA3  | 1.90                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 85:L5:119:G:OP1    | 28:LG:132:ARG:NH1  | 2.35                     | 0.54              |
| 85:L5:364:G:H2'    | 55:Lj:56:ARG:CZ    | 2.38                     | 0.54              |
| 85:L5:1705:G:H21   | 27:LF:46:ARG:NH2   | 2.04                     | 0.54              |
| 85:L5:2034:G:H2'   | 85:L5:2035:C:H6    | 1.73                     | 0.54              |
| 27:LF:172:ASN:ND2  | 27:LF:187:MET:HE1  | 2.23                     | 0.54              |
| 30:LI:188:LYS:C    | 30:LI:188:LYS:HZ2  | 2.15                     | 0.54              |
| 34:LN:58:GLY:HA3   | 34:LN:142:ILE:HD11 | 1.90                     | 0.54              |
| 37:LQ:114:LEU:HD21 | 37:LQ:120:ILE:HG12 | 1.90                     | 0.54              |
| 38:LR:140:GLU:O    | 38:LR:144:LYS:HG3  | 2.08                     | 0.54              |
| 51:Lf:77:ALA:HA    | 51:Lf:84:VAL:HA    | 1.88                     | 0.54              |
| 54:Li:7:MET:HE1    | 54:Li:9:VAL:HG22   | 1.90                     | 0.54              |
| 66:SF:78:MET:SD    | 66:SF:159:ARG:NH2  | 2.81                     | 0.54              |
| 72:SU:98:VAL:HG13  | 72:SU:101:ILE:HD11 | 1.90                     | 0.54              |
| 76:SM:20:GLU:O     | 76:SM:24:THR:HG23  | 2.08                     | 0.54              |
| 76:SM:68:LEU:HD21  | 78:Sf:106:TYR:CE2  | 2.43                     | 0.54              |
| 79:S2:1317:C:H2'   | 79:S2:1318:G:C8    | 2.43                     | 0.54              |
| 79:S2:1396:A:N7    | 79:S2:1449:G:C6    | 2.75                     | 0.54              |
| 2:sE:108:ARG:HH22  | 79:s2:846:G:P      | 2.30                     | 0.54              |
| 2:sE:131:VAL:HG22  | 79:s2:297:A:H4'    | 1.89                     | 0.54              |
| 6:sG:131:ARG:HH21  | 6:sG:132:ARG:HE    | 1.56                     | 0.54              |
| 6:sG:132:ARG:NH1   | 79:s2:151:C:C2     | 2.76                     | 0.54              |
| 7:sJ:12:THR:HG21   | 79:s2:521:A:P      | 2.48                     | 0.54              |
| 7:sJ:133:ARG:HH22  | 79:s2:563:G:P      | 2.31                     | 0.54              |
| 10:sA:164:ASN:OD1  | 10:sA:165:ASN:N    | 2.41                     | 0.54              |
| 11:sB:172:MET:SD   | 11:sB:172:MET:C    | 2.91                     | 0.54              |
| 15:sC:130:ILE:HG12 | 15:sC:158:ALA:HB1  | 1.89                     | 0.54              |
| 23:lB:348:ARG:HH12 | 23:lB:351:LEU:HD22 | 1.73                     | 0.54              |
| 24:lC:197:ARG:NH1  | 85:l5:351:C:OP2    | 2.39                     | 0.54              |
| 25:lD:232:THR:OG1  | 25:lD:234:ASP:O    | 2.25                     | 0.54              |
| 27:lF:90:ALA:HB2   | 27:lF:125:LEU:HD11 | 1.89                     | 0.54              |
| 29:lH:106:GLN:CG   | 29:lH:107:GLU:H    | 2.20                     | 0.54              |
| 31:lJ:94:LEU:HD21  | 31:lJ:98:ASN:CB    | 2.29                     | 0.54              |
| 32:lL:5:ARG:NH2    | 85:l5:1850:A:OP2   | 2.40                     | 0.54              |
| 33:lM:74:ARG:NH2   | 33:lM:75:GLN:HB3   | 2.22                     | 0.54              |
| 33:lM:104:MET:HE3  | 33:lM:104:MET:HA   | 1.90                     | 0.54              |
| 35:lO:49:ARG:NH1   | 85:l5:1930:U:OP2   | 2.41                     | 0.54              |
| 35:lO:149:TYR:O    | 35:lO:153:THR:OG1  | 2.19                     | 0.54              |
| 38:lR:15:LEU:HD13  | 38:lR:52:ARG:HB2   | 1.89                     | 0.54              |
| 41:lU:88:LYS:HA    | 41:lU:97:ARG:NH2   | 2.23                     | 0.54              |
| 42:lV:37:LEU:HD21  | 42:lV:105:ILE:HD11 | 1.90                     | 0.54              |
| 44:lY:23:SER:HA    | 44:lY:26:ARG:HB2   | 1.89                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 46:la:4:ARG:NH2    | 85:l5:2341:A:OP2   | 2.33                     | 0.54              |
| 48:lc:31:TYR:HA    | 48:lc:93:THR:OG1   | 2.08                     | 0.54              |
| 52:lg:63:VAL:HG23  | 52:lg:66:ARG:HH21  | 1.73                     | 0.54              |
| 63:lz:90:LEU:HD21  | 63:lz:120:ILE:HD11 | 1.89                     | 0.54              |
| 67:sK:65:ARG:NH2   | 74:sd:25:SER:HA    | 2.16                     | 0.54              |
| 72:sU:85:HIS:ND1   | 79:s2:1447:G:OP1   | 2.41                     | 0.54              |
| 79:s2:64:A:H8      | 79:s2:83:A:H62     | 1.56                     | 0.54              |
| 79:s2:93:U:H2'     | 79:s2:94:G:O4'     | 2.08                     | 0.54              |
| 79:s2:499:G:N1     | 79:s2:501:C:O2     | 2.40                     | 0.54              |
| 79:s2:656:G:H5'    | 79:s2:662:G:N2     | 2.23                     | 0.54              |
| 79:s2:1134:G:H2'   | 79:s2:1135:C:H6    | 1.73                     | 0.54              |
| 79:s2:1286:G:H22   | 79:s2:1312:G:HO2'  | 1.53                     | 0.54              |
| 79:s2:1540:G:H2'   | 79:s2:1541:G:C8    | 2.43                     | 0.54              |
| 80:cB:135:VAL:HG23 | 80:cB:181:ILE:CD1  | 2.38                     | 0.54              |
| 85:l5:184:U:O2'    | 85:l5:189:G:O4'    | 2.26                     | 0.54              |
| 85:l5:418:A:H4'    | 85:l5:2311:C:H5'   | 1.90                     | 0.54              |
| 85:l5:1100:U:O4    | 85:l5:1194:G:O6    | 2.26                     | 0.54              |
| 85:l5:1759:G:N2    | 85:l5:1773:U:O2    | 2.35                     | 0.54              |
| 85:l5:2257:C:N4    | 85:l5:2260:C:O2    | 2.41                     | 0.54              |
| 85:l5:2705:G:H1    | 85:l5:2710:C:N4    | 2.06                     | 0.54              |
| 85:l5:4277:G:H2'   | 85:l5:4278:C:C6    | 2.43                     | 0.54              |
| 85:l5:4680:G:H2'   | 85:l5:4681:A:C8    | 2.43                     | 0.54              |
| 6:SG:216:ARG:C     | 6:SG:218:LYS:H     | 2.16                     | 0.54              |
| 16:SN:4:MET:SD     | 16:SN:5:HIS:NE2    | 2.80                     | 0.54              |
| 18:SW:65:LEU:HG    | 18:SW:67:GLY:H     | 1.73                     | 0.54              |
| 85:L5:250:C:H2'    | 85:L5:251:C:C6     | 2.42                     | 0.54              |
| 85:L5:739:G:H22    | 85:L5:926:G:H1'    | 1.72                     | 0.54              |
| 85:L5:2019:C:H2'   | 85:L5:2020:U:H6    | 1.71                     | 0.54              |
| 85:L5:2090:U:H4'   | 85:L5:2091:C:H3'   | 1.89                     | 0.54              |
| 85:L5:2335:C:H2'   | 85:L5:2336:G:H8    | 1.72                     | 0.54              |
| 85:L5:2638:G:H22   | 85:L5:2719:C:P     | 2.30                     | 0.54              |
| 85:L5:3610:A:H2'   | 85:L5:3611:A:C8    | 2.42                     | 0.54              |
| 85:L5:3971:G:N2    | 85:L5:3973:G:N3    | 2.55                     | 0.54              |
| 85:L5:4892:A:H2'   | 85:L5:4893:A:O4'   | 2.08                     | 0.54              |
| 21:L8:6:C:H2'      | 21:L8:7:U:H6       | 1.73                     | 0.54              |
| 23:LB:305:THR:OG1  | 23:LB:365:LEU:O    | 2.25                     | 0.54              |
| 25:LD:155:THR:OG1  | 25:LD:179:ARG:NH1  | 2.40                     | 0.54              |
| 26:LE:152:ILE:O    | 26:LE:159:GLY:N    | 2.31                     | 0.54              |
| 31:LJ:105:PHE:C    | 31:LJ:105:PHE:CD1  | 2.86                     | 0.54              |
| 32:LL:10:LEU:HD23  | 32:LL:10:LEU:H     | 1.73                     | 0.54              |
| 32:LL:91:ALA:HB1   | 32:LL:96:ILE:HG21  | 1.90                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 39:LS:95:ARG:HD2   | 39:LS:113:MET:HE2  | 1.90                     | 0.54              |
| 40:LT:88:ARG:C     | 40:LT:89:ILE:HD13  | 2.33                     | 0.54              |
| 41:LU:80:LYS:HE3   | 41:LU:110:TYR:CD2  | 2.42                     | 0.54              |
| 60:Lo:102:GLN:HG2  | 60:Lo:104:ILE:HD11 | 1.89                     | 0.54              |
| 61:Lp:51:ALA:HB3   | 61:Lp:54:ILE:HD13  | 1.89                     | 0.54              |
| 69:SQ:62:ARG:HB2   | 69:SQ:96:TYR:OH    | 2.07                     | 0.54              |
| 74:Sd:36:LEU:CD1   | 74:Sd:38:MET:HB3   | 2.38                     | 0.54              |
| 79:S2:16:G:H2'     | 79:S2:17:C:C6      | 2.42                     | 0.54              |
| 79:S2:1432:U:H4'   | 79:S2:1437:C:O2    | 2.08                     | 0.54              |
| 79:S2:1590:C:H4'   | 79:S2:1653:U:H4'   | 1.88                     | 0.54              |
| 87:IW:71:ARG:HD2   | 87:IW:73:ARG:NH1   | 2.23                     | 0.54              |
| 1:CH:99:ILE:HD11   | 1:CH:127:ALA:HB2   | 1.90                     | 0.54              |
| 1:cH:42:LYS:HA     | 9:se:42:PHE:HA     | 1.89                     | 0.54              |
| 2:sE:126:VAL:HA    | 2:sE:141:THR:HA    | 1.89                     | 0.54              |
| 3:sI:47:ARG:NH2    | 79:s2:446:G:OP2    | 2.37                     | 0.54              |
| 3:sI:132:GLU:HG2   | 3:sI:136:ILE:HD13  | 1.88                     | 0.54              |
| 10:sA:135:THR:O    | 10:sA:138:SER:OG   | 2.23                     | 0.54              |
| 10:sA:142:LEU:HA   | 13:sV:32:ILE:HD11  | 1.90                     | 0.54              |
| 13:sV:47:ASN:OD1   | 13:sV:48:GLY:N     | 2.41                     | 0.54              |
| 20:l7:26:C:O2'     | 31:lJ:147:ARG:NH1  | 2.38                     | 0.54              |
| 23:lB:254:ILE:HD12 | 23:lB:262:VAL:HG11 | 1.90                     | 0.54              |
| 24:lC:140:LYS:NZ   | 24:lC:245:HIS:O    | 2.41                     | 0.54              |
| 29:lH:4:ILE:HD13   | 29:lH:61:TRP:NE1   | 2.21                     | 0.54              |
| 32:lL:63:THR:O     | 32:lL:67:HIS:N     | 2.41                     | 0.54              |
| 35:lO:8:VAL:O      | 35:lO:118:MET:HB2  | 2.07                     | 0.54              |
| 37:lQ:79:THR:O     | 37:lQ:136:THR:OG1  | 2.23                     | 0.54              |
| 39:lS:63:TYR:OH    | 85:l5:729:G:OP1    | 2.18                     | 0.54              |
| 46:la:79:TRP:HB3   | 46:la:87:ARG:CZ    | 2.38                     | 0.54              |
| 51:lf:59:THR:OG1   | 51:lf:65:ASN:OD1   | 2.25                     | 0.54              |
| 52:lg:11:LEU:HD21  | 85:l5:2513:A:P     | 2.48                     | 0.54              |
| 63:lz:147:LYS:HE2  | 63:lz:151:VAL:H    | 1.73                     | 0.54              |
| 65:sD:72:VAL:HG12  | 67:sK:20:VAL:HG21  | 1.89                     | 0.54              |
| 67:sK:82:TYR:HD2   | 67:sK:83:LEU:HD22  | 1.71                     | 0.54              |
| 69:sQ:45:ARG:HA    | 69:sQ:48:GLN:HB3   | 1.89                     | 0.54              |
| 71:sT:76:THR:OG1   | 71:sT:95:GLY:O     | 2.26                     | 0.54              |
| 72:sU:66:ARG:HB2   | 79:s2:1256:G:C8    | 2.43                     | 0.54              |
| 75:sg:59:LEU:HD21  | 75:sg:90:TRP:CG    | 2.43                     | 0.54              |
| 75:sg:114:SER:OG   | 75:sg:118:ARG:N    | 2.36                     | 0.54              |
| 79:s2:103:A:N6     | 79:s2:356:C:O5'    | 2.41                     | 0.54              |
| 79:s2:653:A:H2'    | 79:s2:654:A:O4'    | 2.08                     | 0.54              |
| 79:s2:1273:C:O2    | 79:s2:1508:A:N6    | 2.41                     | 0.54              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 79:s2:1310:U:H2'  | 79:s2:1311:C:C6    | 2.43                     | 0.54              |
| 79:s2:1464:C:H2'  | 79:s2:1465:A:C4    | 2.42                     | 0.54              |
| 80:cB:88:PHE:HZ   | 80:cB:253:VAL:HG21 | 1.72                     | 0.54              |
| 80:cB:186:ASN:ND2 | 80:cB:204:MET:SD   | 2.80                     | 0.54              |
| 80:cB:613:LEU:H   | 80:cB:613:LEU:HD12 | 1.72                     | 0.54              |
| 85:l5:967:C:O3'   | 85:l5:968:C:H3'    | 2.07                     | 0.54              |
| 85:l5:1663:C:H1'  | 85:l5:2320:G:H21   | 1.72                     | 0.54              |
| 85:l5:4452:U:OP2  | 85:l5:4522:G:N1    | 2.28                     | 0.54              |
| 85:l5:4934:A:H2'  | 85:l5:4935:C:C6    | 2.43                     | 0.54              |
| 80:CB:77:LEU:HD13 | 80:CB:78:PHE:N     | 2.23                     | 0.54              |
| 80:CB:365:GLN:OE1 | 80:CB:415:ARG:NH2  | 2.41                     | 0.54              |
| 6:SG:116:LYS:HZ3  | 6:SG:125:THR:HG21  | 1.73                     | 0.54              |
| 7:SJ:113:GLN:HE21 | 7:SJ:149:VAL:HG22  | 1.72                     | 0.54              |
| 12:SH:137:SER:HG  | 12:SH:158:LEU:HD12 | 1.72                     | 0.54              |
| 17:SO:113:GLN:O   | 17:SO:117:ARG:HG2  | 2.07                     | 0.54              |
| 85:L5:139:G:H2'   | 85:L5:140:G:C8     | 2.43                     | 0.54              |
| 85:L5:462:G:H2'   | 85:L5:463:A:C8     | 2.43                     | 0.54              |
| 85:L5:1095:A:H2'  | 85:L5:1096:C:H6    | 1.72                     | 0.54              |
| 85:L5:1577:G:OP1  | 61:Lp:17:ARG:NH2   | 2.41                     | 0.54              |
| 85:L5:1993:C:H4'  | 84:Lt:149:HIS:CE1  | 2.43                     | 0.54              |
| 85:L5:2640:G:H2'  | 85:L5:2641:A:H8    | 1.72                     | 0.54              |
| 85:L5:3861:A:H2'  | 85:L5:3862:A:C8    | 2.43                     | 0.54              |
| 85:L5:4541:G:N2   | 85:L5:4544:A:OP2   | 2.39                     | 0.54              |
| 85:L5:4913:G:H4'  | 85:L5:4914:C:O5'   | 2.07                     | 0.54              |
| 26:LE:283:PRO:HA  | 26:LE:286:LEU:HD12 | 1.90                     | 0.54              |
| 28:LG:232:GLU:O   | 28:LG:236:HIS:N    | 2.41                     | 0.54              |
| 41:LU:44:GLN:HA   | 41:LU:56:LEU:HD13  | 1.89                     | 0.54              |
| 51:Lf:45:LYS:HD3  | 51:Lf:106:TYR:O    | 2.08                     | 0.54              |
| 56:Lk:37:ARG:HA   | 56:Lk:42:LEU:HD23  | 1.90                     | 0.54              |
| 65:SD:190:LEU:HB2 | 65:SD:200:PRO:HD3  | 1.90                     | 0.54              |
| 67:SK:76:ILE:HG22 | 67:SK:80:ARG:NH1   | 2.23                     | 0.54              |
| 69:SQ:130:LYS:HA  | 69:SQ:137:ALA:HA   | 1.90                     | 0.54              |
| 71:ST:88:MET:HE1  | 79:S2:1665:G:C8    | 2.43                     | 0.54              |
| 75:Sg:301:GLY:HA2 | 75:Sg:307:VAL:HG22 | 1.88                     | 0.54              |
| 76:SM:119:GLN:OE1 | 76:SM:119:GLN:HA   | 2.08                     | 0.54              |
| 77:SZ:54:THR:O    | 77:SZ:58:LEU:HG    | 2.08                     | 0.54              |
| 79:S2:91:A:OP1    | 79:S2:446:G:N2     | 2.28                     | 0.54              |
| 79:S2:674:C:H2'   | 79:S2:675:U:C6     | 2.43                     | 0.54              |
| 79:S2:876:C:H2'   | 79:S2:877:C:C6     | 2.43                     | 0.54              |
| 79:S2:1010:G:H2'  | 79:S2:1011:A:C8    | 2.43                     | 0.54              |
| 81:AP:3:C:H2'     | 81:AP:4:U:C6       | 2.43                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:cH:121:LEU:HA    | 1:cH:124:ILE:HD12  | 1.90                     | 0.53              |
| 2:sE:67:GLN:HB3    | 2:sE:69:PHE:CE1    | 2.43                     | 0.53              |
| 11:sB:175:GLU:HG2  | 11:sB:193:ILE:HD13 | 1.88                     | 0.53              |
| 15:sC:138:GLY:HA3  | 15:sC:162:ILE:HD13 | 1.89                     | 0.53              |
| 21:l8:123:U:C4     | 21:l8:125:C:H5''   | 2.43                     | 0.53              |
| 26:lE:279:ASN:OD1  | 85:l5:4754:G:C8    | 2.60                     | 0.53              |
| 27:lF:27:GLU:OE2   | 85:l5:2253:A:N6    | 2.41                     | 0.53              |
| 32:lL:48:PRO:HG3   | 53:lh:118:LYS:HE3  | 1.89                     | 0.53              |
| 32:lL:184:MET:HE1  | 85:l5:1487:G:O4'   | 2.07                     | 0.53              |
| 32:lL:184:MET:N    | 32:lL:184:MET:HE2  | 2.22                     | 0.53              |
| 35:lO:25:LYS:HD3   | 85:l5:1913:C:H5''  | 1.89                     | 0.53              |
| 38:lR:176:ARG:HH22 | 38:lR:180:LYS:CE   | 2.21                     | 0.53              |
| 39:lS:157:ARG:NH1  | 85:l5:4870:G:O6    | 2.41                     | 0.53              |
| 47:lb:103:LYS:HG3  | 47:lb:104:LEU:HD13 | 1.90                     | 0.53              |
| 48:lc:36:LYS:HZ1   | 48:lc:39:ARG:HD2   | 1.73                     | 0.53              |
| 56:lk:40:ARG:HG2   | 56:lk:41:TYR:CD2   | 2.43                     | 0.53              |
| 57:ll:20:ASN:OD1   | 57:ll:41:ARG:NH2   | 2.32                     | 0.53              |
| 69:sQ:71:ARG:NH2   | 79:s2:1407:U:H4'   | 2.23                     | 0.53              |
| 70:sS:63:GLU:HG3   | 70:sS:66:ARG:HH21  | 1.73                     | 0.53              |
| 71:sT:84:ARG:NH1   | 79:s2:1531:A:OP1   | 2.41                     | 0.53              |
| 79:s2:456:C:H2'    | 79:s2:457:C:H6     | 1.71                     | 0.53              |
| 79:s2:613:G:N2     | 79:s2:629:A:OP2    | 2.31                     | 0.53              |
| 79:s2:1395:C:H2'   | 79:s2:1396:A:O4'   | 2.08                     | 0.53              |
| 80:cB:141:THR:HG22 | 80:cB:145:GLN:NE2  | 2.23                     | 0.53              |
| 80:cB:200:MET:HE3  | 80:cB:367:TYR:CG   | 2.43                     | 0.53              |
| 81:aP:67:G:H3'     | 81:aP:68:G:H8      | 1.73                     | 0.53              |
| 85:l5:163:A:H2'    | 85:l5:164:G:H8     | 1.73                     | 0.53              |
| 85:l5:387:G:O2'    | 85:l5:412:G:N1     | 2.41                     | 0.53              |
| 85:l5:966:A:H3'    | 85:l5:967:C:C6     | 2.42                     | 0.53              |
| 85:l5:2699:C:H2'   | 85:l5:2700:G:H8    | 1.71                     | 0.53              |
| 85:l5:3661:G:N2    | 85:l5:3681:G:O2'   | 2.41                     | 0.53              |
| 85:l5:4039:G:N2    | 85:l5:4050:A:HO2'  | 2.06                     | 0.53              |
| 85:l5:4345:C:H2'   | 85:l5:4346:U:C6    | 2.43                     | 0.53              |
| 85:l5:4361:U:H2'   | 85:l5:4362:A:C8    | 2.44                     | 0.53              |
| 85:l5:4906:C:H2'   | 85:l5:4907:G:H8    | 1.73                     | 0.53              |
| 80:CB:265:TYR:HD1  | 80:CB:287:ARG:HA   | 1.71                     | 0.53              |
| 80:CB:852:ASP:OD1  | 80:CB:852:ASP:N    | 2.42                     | 0.53              |
| 85:L5:276:C:H2'    | 54:Li:29:ARG:HH12  | 1.73                     | 0.53              |
| 85:L5:325:U:H5''   | 32:LL:103:ARG:HH21 | 1.71                     | 0.53              |
| 85:L5:675:C:H2'    | 85:L5:676:C:H6     | 1.74                     | 0.53              |
| 85:L5:1727:U:H2'   | 85:L5:1728:U:C6    | 2.43                     | 0.53              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 85:L5:3709:U:H2'   | 85:L5:3710:G:O4'   | 2.08                     | 0.53              |
| 85:L5:3896:C:O2'   | 23:LB:268:ARG:NH2  | 2.38                     | 0.53              |
| 85:L5:4581:G:H5'   | 23:LB:28:LYS:NZ    | 2.23                     | 0.53              |
| 85:L5:4910:G:H4'   | 23:LB:95:THR:HG22  | 1.89                     | 0.53              |
| 26:LE:112:MET:O    | 62:Lr:87:ARG:NE    | 2.41                     | 0.53              |
| 30:LI:169:LYS:HG3  | 30:LI:177:ASN:HB3  | 1.90                     | 0.53              |
| 31:LJ:121:PRO:HD2  | 70:SS:101:ASN:ND2  | 2.23                     | 0.53              |
| 33:LM:11:ARG:O     | 33:LM:27:ILE:HG22  | 2.08                     | 0.53              |
| 33:LM:74:ARG:O     | 33:LM:77:TRP:N     | 2.41                     | 0.53              |
| 36:LP:26:PHE:HD2   | 36:LP:144:CYS:HB3  | 1.72                     | 0.53              |
| 54:Li:66:ASP:OD2   | 54:Li:67:LYS:N     | 2.41                     | 0.53              |
| 67:SK:13:GLU:N     | 67:SK:13:GLU:OE1   | 2.41                     | 0.53              |
| 75:Sg:219:TRP:CD1  | 75:Sg:226:HIS:HA   | 2.43                     | 0.53              |
| 76:SM:25:ALA:HB2   | 76:SM:111:VAL:HG23 | 1.91                     | 0.53              |
| 76:SM:53:ALA:HA    | 76:SM:79:VAL:HG12  | 1.90                     | 0.53              |
| 79:S2:638:C:H2'    | 79:S2:639:C:C6     | 2.43                     | 0.53              |
| 79:S2:1136:U:H2'   | 79:S2:1137:U:H6    | 1.74                     | 0.53              |
| 87:LW:6:CYS:SG     | 87:LW:9:SER:OG     | 2.61                     | 0.53              |
| 1:CH:77:VAL:HG12   | 1:CH:132:LEU:HD11  | 1.89                     | 0.53              |
| 3:sI:45:THR:O      | 79:s2:307:G:N2     | 2.41                     | 0.53              |
| 7:sJ:150:ARG:HG3   | 79:s2:821:G:C6     | 2.43                     | 0.53              |
| 9:se:37:GLN:N      | 9:se:37:GLN:OE1    | 2.41                     | 0.53              |
| 12:sH:76:GLN:HE22  | 12:sH:94:PHE:HB2   | 1.73                     | 0.53              |
| 15:sC:109:ILE:HD11 | 15:sC:124:PHE:HB3  | 1.90                     | 0.53              |
| 15:sC:113:GLN:HB3  | 15:sC:122:THR:HA   | 1.90                     | 0.53              |
| 15:sC:121:ARG:HE   | 15:sC:123:ARG:HH22 | 1.54                     | 0.53              |
| 17:sO:88:LEU:HD22  | 17:sO:90:ILE:HG22  | 1.90                     | 0.53              |
| 17:sO:92:ALA:HA    | 17:sO:125:LYS:HB2  | 1.90                     | 0.53              |
| 21:l8:78:G:H2'     | 21:l8:79:G:C8      | 2.43                     | 0.53              |
| 22:lA:101:VAL:HG22 | 22:lA:165:VAL:HG22 | 1.90                     | 0.53              |
| 25:lD:209:ARG:HA   | 25:lD:212:MET:SD   | 2.49                     | 0.53              |
| 28:lG:94:GLN:O     | 28:lG:98:LEU:HG    | 2.09                     | 0.53              |
| 28:lG:105:GLU:HG3  | 28:lG:110:LYS:HD3  | 1.90                     | 0.53              |
| 35:lO:87:MET:SD    | 85:l5:1912:G:N2    | 2.82                     | 0.53              |
| 36:lP:49:LYS:O     | 36:lP:53:LEU:HD22  | 2.09                     | 0.53              |
| 37:lQ:69:LYS:HD2   | 85:l5:1458:C:H5''  | 1.89                     | 0.53              |
| 40:lT:68:THR:HG23  | 40:lT:71:ALA:H     | 1.74                     | 0.53              |
| 42:lV:98:PHE:CD1   | 87:lW:22:ALA:HB3   | 2.39                     | 0.53              |
| 48:lc:11:LEU:HA    | 48:lc:14:ILE:HG22  | 1.90                     | 0.53              |
| 53:lh:13:LYS:HE2   | 53:lh:15:GLU:HB2   | 1.89                     | 0.53              |
| 64:sR:5:ARG:HE     | 79:s2:1367:U:H2'   | 1.73                     | 0.53              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 65:sD:139:SER:OG   | 79:s2:1334:G:H5''  | 2.08                     | 0.53              |
| 75:sg:109:LEU:HD11 | 75:sg:125:ARG:HD3  | 1.89                     | 0.53              |
| 76:sM:49:LEU:HB2   | 76:sM:127:TYR:CE1  | 2.42                     | 0.53              |
| 79:s2:1103:C:H2'   | 79:s2:1104:G:H8    | 1.73                     | 0.53              |
| 79:s2:1203:G:H2'   | 79:s2:1204:A:H8    | 1.72                     | 0.53              |
| 79:s2:1293:A:H3'   | 79:s2:1294:G:H8    | 1.73                     | 0.53              |
| 79:s2:1426:U:H2'   | 79:s2:1427:C:C6    | 2.43                     | 0.53              |
| 80:cB:294:LEU:HA   | 80:cB:297:ILE:HG12 | 1.90                     | 0.53              |
| 85:l5:518:G:H1     | 85:l5:643:C:H2'    | 1.73                     | 0.53              |
| 85:l5:1811:G:H2'   | 85:l5:1812:C:C6    | 2.44                     | 0.53              |
| 85:l5:1975:G:N2    | 85:l5:1983:A:OP1   | 2.40                     | 0.53              |
| 85:l5:2615:C:H2'   | 85:l5:2616:C:H6    | 1.73                     | 0.53              |
| 85:l5:3814:U:H2'   | 85:l5:3815:G:C8    | 2.44                     | 0.53              |
| 85:l5:4667:C:H2'   | 85:l5:4668:U:O4'   | 2.09                     | 0.53              |
| 85:l5:4754:G:N1    | 85:l5:4880:C:N3    | 2.56                     | 0.53              |
| 12:SH:118:ARG:NH2  | 79:S2:687:C:N3     | 2.56                     | 0.53              |
| 14:Sa:89:ARG:NH1   | 79:S2:1146:C:OP1   | 2.40                     | 0.53              |
| 85:L5:159:C:C5'    | 54:Li:25:ARG:HE    | 2.17                     | 0.53              |
| 85:L5:928:C:H2'    | 85:L5:929:A:H8     | 1.72                     | 0.53              |
| 85:L5:1079:C:H2'   | 85:L5:1080:C:C6    | 2.43                     | 0.53              |
| 85:L5:1243:C:C2    | 85:L5:1244:G:C8    | 2.96                     | 0.53              |
| 85:L5:1589:C:H2'   | 85:L5:1590:C:C6    | 2.43                     | 0.53              |
| 85:L5:1752:G:H2'   | 85:L5:1753:G:H8    | 1.73                     | 0.53              |
| 85:L5:2044:U:H1'   | 35:LO:63:ASN:HD21  | 1.74                     | 0.53              |
| 85:L5:2752:G:H4'   | 52:Lg:78:TYR:HE2   | 1.73                     | 0.53              |
| 85:L5:4736:C:H2'   | 85:L5:4737:G:C8    | 2.44                     | 0.53              |
| 85:L5:4957:C:H2'   | 85:L5:4958:C:C6    | 2.44                     | 0.53              |
| 33:LM:125:ASN:OD1  | 33:LM:126:GLU:N    | 2.41                     | 0.53              |
| 38:LR:39:GLN:H     | 38:LR:42:ARG:HG3   | 1.74                     | 0.53              |
| 38:LR:115:ILE:HB   | 38:LR:119:MET:SD   | 2.48                     | 0.53              |
| 61:Lp:44:LYS:HD2   | 61:Lp:59:SER:HB2   | 1.89                     | 0.53              |
| 63:Lz:33:GLU:HG2   | 63:Lz:168:ALA:HA   | 1.90                     | 0.53              |
| 67:SK:35:LEU:O     | 67:SK:37:ASP:N     | 2.42                     | 0.53              |
| 69:SQ:137:ALA:N    | 79:S2:1650:A:OP1   | 2.41                     | 0.53              |
| 73:Sc:34:PHE:O     | 73:Sc:35:MET:HG2   | 2.07                     | 0.53              |
| 75:Sg:194:TYR:O    | 75:Sg:211:GLY:HA3  | 2.08                     | 0.53              |
| 76:SM:60:MET:HA    | 76:SM:63:LYS:HG3   | 1.89                     | 0.53              |
| 79:S2:373:G:H2'    | 79:S2:374:G:H8     | 1.73                     | 0.53              |
| 79:S2:1438:A:H2'   | 79:S2:1439:A:H8    | 1.74                     | 0.53              |
| 79:S2:1473:G:H5'   | 79:S2:1474:A:OP2   | 2.09                     | 0.53              |
| 79:S2:1548:G:N1    | 79:S2:1586:U:O4    | 2.41                     | 0.53              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 84:Lt:81:ILE:HD13 | 84:Lt:113:ALA:HB1  | 1.90                     | 0.53              |
| 87:LW:4:GLU:HG3   | 87:LW:13:ILE:HB    | 1.89                     | 0.53              |
| 1:CH:81:ILE:HG21  | 1:CH:106:ILE:HD11  | 1.90                     | 0.53              |
| 2:sE:66:MET:HE1   | 79:s2:502:C:O4'    | 2.09                     | 0.53              |
| 6:sG:133:LEU:HB2  | 79:s2:65:C:N3      | 2.23                     | 0.53              |
| 10:sA:23:THR:OG1  | 10:sA:163:CYS:HB2  | 2.08                     | 0.53              |
| 11:sB:122:GLU:OE1 | 11:sB:213:ARG:NH1  | 2.42                     | 0.53              |
| 20:l7:57:C:H2'    | 20:l7:58:A:H8      | 1.73                     | 0.53              |
| 21:l8:61:A:O5'    | 53:lh:51:ARG:NH2   | 2.41                     | 0.53              |
| 22:lA:50:HIS:CD2  | 85:l5:2741:U:H2'   | 2.44                     | 0.53              |
| 22:lA:54:ARG:O    | 22:lA:54:ARG:NH1   | 2.41                     | 0.53              |
| 32:lL:184:MET:HE1 | 85:l5:1487:G:C4'   | 2.39                     | 0.53              |
| 34:lN:127:TYR:HB3 | 34:lN:129:PHE:CE2  | 2.40                     | 0.53              |
| 45:lZ:61:LYS:H    | 45:lZ:61:LYS:HD2   | 1.72                     | 0.53              |
| 48:lc:81:LEU:HD23 | 48:lc:91:VAL:O     | 2.08                     | 0.53              |
| 64:sR:29:HIS:HB2  | 79:s2:1455:A:C4    | 2.42                     | 0.53              |
| 64:sR:67:ARG:NH2  | 79:s2:1376:A:OP1   | 2.40                     | 0.53              |
| 69:sQ:33:LYS:NZ   | 71:sT:8:ASP:OD2    | 2.42                     | 0.53              |
| 70:sS:63:GLU:O    | 70:sS:67:VAL:HG13  | 2.08                     | 0.53              |
| 85:l5:350:C:OP1   | 85:l5:2294:G:O2'   | 2.24                     | 0.53              |
| 85:l5:4522:G:O2'  | 85:l5:4525:C:OP2   | 2.14                     | 0.53              |
| 85:l5:4708:A:C2   | 85:l5:4709:U:H5'   | 2.44                     | 0.53              |
| 80:CB:835:VAL:O   | 80:CB:839:ARG:HG2  | 2.08                     | 0.53              |
| 3:SI:197:PHE:HA   | 3:SI:200:ARG:NH1   | 2.23                     | 0.53              |
| 7:SJ:77:LEU:O     | 7:SJ:80:ARG:HG2    | 2.08                     | 0.53              |
| 7:SJ:93:LYS:HG2   | 7:SJ:95:ASP:H      | 1.73                     | 0.53              |
| 7:SJ:93:LYS:NZ    | 7:SJ:95:ASP:HB3    | 2.24                     | 0.53              |
| 7:SJ:142:VAL:HG22 | 79:S2:823:U:H1'    | 1.90                     | 0.53              |
| 10:SA:89:LYS:HG3  | 10:SA:202:TYR:CE1  | 2.42                     | 0.53              |
| 12:SH:12:ASN:ND2  | 12:SH:16:PRO:O     | 2.41                     | 0.53              |
| 12:SH:160:LYS:HD3 | 12:SH:193:GLN:HE21 | 1.73                     | 0.53              |
| 85:L5:25:A:H2'    | 85:L5:26:C:H6      | 1.73                     | 0.53              |
| 85:L5:311:G:H2'   | 85:L5:312:G:H8     | 1.74                     | 0.53              |
| 85:L5:497:G:N2    | 85:L5:658:C:H42    | 2.05                     | 0.53              |
| 85:L5:734:G:C2    | 85:L5:735:G:C8     | 2.97                     | 0.53              |
| 85:L5:1535:C:H2'  | 85:L5:1536:U:O4'   | 2.07                     | 0.53              |
| 85:L5:3795:A:H2'  | 85:L5:3796:U:C6    | 2.43                     | 0.53              |
| 85:L5:4103:C:H5'  | 85:L5:4107:G:OP2   | 2.08                     | 0.53              |
| 85:L5:4312:U:O2   | 40:LT:90:ASN:ND2   | 2.41                     | 0.53              |
| 85:L5:4431:U:O3'  | 30:LI:160:PRO:HB3  | 2.08                     | 0.53              |
| 34:LN:34:SER:OG   | 34:LN:35:ALA:N     | 2.41                     | 0.53              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 38:LR:173:ARG:NH1  | 79:S2:910:G:OP1    | 2.41                     | 0.53              |
| 39:LS:95:ARG:NE    | 39:LS:97:TYR:OH    | 2.34                     | 0.53              |
| 39:LS:137:CYS:O    | 39:LS:143:LYS:NZ   | 2.41                     | 0.53              |
| 43:LX:125:ASN:O    | 43:LX:137:TYR:N    | 2.41                     | 0.53              |
| 52:Lg:85:LYS:HE2   | 52:Lg:88:ARG:HH11  | 1.72                     | 0.53              |
| 63:Lz:73:HIS:NE2   | 63:Lz:111:LEU:HD11 | 2.22                     | 0.53              |
| 67:SK:57:TYR:HB3   | 67:SK:75:GLY:HA3   | 1.91                     | 0.53              |
| 69:SQ:104:SER:HA   | 69:SQ:107:GLU:HG3  | 1.89                     | 0.53              |
| 73:Sc:29:GLN:NE2   | 73:Sc:45:ASN:HB3   | 2.23                     | 0.53              |
| 75:Sg:39:THR:HG23  | 75:Sg:41:ILE:HD11  | 1.91                     | 0.53              |
| 77:SZ:97:ILE:HG22  | 77:SZ:109:TYR:CD2  | 2.43                     | 0.53              |
| 79:S2:1222:G:H2'   | 79:S2:1223:A:C8    | 2.43                     | 0.53              |
| 79:S2:1317:C:H2'   | 79:S2:1318:G:H8    | 1.73                     | 0.53              |
| 79:S2:1468:C:H2'   | 79:S2:1469:A:C8    | 2.41                     | 0.53              |
| 81:AP:18:G:O6      | 81:AP:55:U:C2      | 2.62                     | 0.53              |
| 2:sE:69:PHE:HE2    | 8:sY:17:LEU:HD21   | 1.72                     | 0.53              |
| 4:sL:32:LYS:NZ     | 4:sL:33:LEU:O      | 2.35                     | 0.53              |
| 6:sG:7:PHE:O       | 6:sG:11:GLY:N      | 2.41                     | 0.53              |
| 8:sY:54:VAL:HG22   | 8:sY:76:TYR:HB2    | 1.91                     | 0.53              |
| 11:sB:85:LYS:HB2   | 11:sB:101:HIS:HB3  | 1.89                     | 0.53              |
| 16:sN:142:GLU:OE2  | 16:sN:143:SER:N    | 2.40                     | 0.53              |
| 26:lE:262:LYS:NZ   | 85:l5:4933:C:OP2   | 2.42                     | 0.53              |
| 33:lM:119:ARG:O    | 33:lM:123:ILE:HG12 | 2.08                     | 0.53              |
| 34:lN:77:LYS:HE2   | 85:l5:4184:G:H21   | 1.74                     | 0.53              |
| 34:lN:90:ASN:ND2   | 85:l5:3929:G:OP2   | 2.38                     | 0.53              |
| 36:lP:126:ARG:HA   | 36:lP:140:MET:CE   | 2.37                     | 0.53              |
| 37:lQ:98:LEU:HB2   | 37:lQ:113:ILE:HD11 | 1.90                     | 0.53              |
| 38:lR:117:ARG:HD3  | 85:l5:2663:G:H4'   | 1.89                     | 0.53              |
| 39:lS:29:ARG:HE    | 40:lT:150:LEU:CG   | 2.21                     | 0.53              |
| 41:lU:34:MET:SD    | 41:lU:35:ASP:N     | 2.80                     | 0.53              |
| 41:lU:65:ARG:HE    | 41:lU:67:LYS:H     | 1.56                     | 0.53              |
| 45:lZ:83:THR:HG23  | 52:lg:95:PHE:CZ    | 2.44                     | 0.53              |
| 45:lZ:89:ILE:HD13  | 45:lZ:121:ARG:HG3  | 1.90                     | 0.53              |
| 63:lz:186:ALA:HA   | 63:lz:189:PHE:CE1  | 2.44                     | 0.53              |
| 65:sD:185:LYS:HE2  | 79:s2:1335:G:H5''  | 1.90                     | 0.53              |
| 68:sP:126:VAL:HG11 | 79:s2:1520:G:H21   | 1.72                     | 0.53              |
| 70:sS:54:LYS:HD3   | 70:sS:58:GLU:HG2   | 1.91                     | 0.53              |
| 71:sT:18:LEU:CD2   | 71:sT:58:ALA:HA    | 2.38                     | 0.53              |
| 79:s2:610:G:C4     | 79:s2:611:G:C8     | 2.96                     | 0.53              |
| 79:s2:1162:C:H2'   | 79:s2:1163:C:C6    | 2.43                     | 0.53              |
| 79:s2:1215:C:O2'   | 79:s2:1645:C:OP2   | 2.26                     | 0.53              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 79:s2:1224:G:H1    | 79:s2:1642:U:H3    | 1.55                     | 0.53              |
| 79:s2:1297:U:O2'   | 79:s2:1299:A:N7    | 2.36                     | 0.53              |
| 79:s2:1806:A:H2'   | 79:s2:1807:C:C6    | 2.43                     | 0.53              |
| 83:ls:77:LYS:HD2   | 83:ls:198:ILE:HD11 | 1.91                     | 0.53              |
| 85:l5:457:G:H2'    | 85:l5:458:C:C6     | 2.43                     | 0.53              |
| 85:l5:513:U:O2     | 85:l5:515:C:H3'    | 2.08                     | 0.53              |
| 85:l5:2654:C:H2'   | 85:l5:2655:C:H6    | 1.73                     | 0.53              |
| 85:l5:4364:G:H2'   | 85:l5:4365:C:C6    | 2.44                     | 0.53              |
| 80:CB:13:MET:HE1   | 80:CB:465:PRO:HD2  | 1.89                     | 0.53              |
| 80:CB:428:ARG:O    | 80:CB:485:ILE:HD12 | 2.07                     | 0.53              |
| 80:CB:529:LYS:HE2  | 80:CB:529:LYS:HA   | 1.90                     | 0.53              |
| 80:CB:584:SER:OG   | 80:CB:585:GLU:OE1  | 2.24                     | 0.53              |
| 2:SE:128:LYS:HG2   | 2:SE:140:VAL:HG11  | 1.88                     | 0.53              |
| 5:SX:35:ALA:O      | 5:SX:39:ASN:N      | 2.42                     | 0.53              |
| 8:SY:47:MET:HE1    | 8:SY:48:TYR:CE1    | 2.44                     | 0.53              |
| 16:SN:39:LYS:O     | 16:SN:42:LYS:HG2   | 2.08                     | 0.53              |
| 85:L5:417:G:OP1    | 85:L5:2329:U:O2'   | 2.25                     | 0.53              |
| 85:L5:458:C:OP1    | 62:Lr:87:ARG:NH2   | 2.41                     | 0.53              |
| 85:L5:1199:G:H2'   | 85:L5:1200:G:C8    | 2.42                     | 0.53              |
| 85:L5:1475:G:H2'   | 85:L5:1476:C:C6    | 2.44                     | 0.53              |
| 85:L5:1873:A:OP2   | 47:Lb:5:LYS:NZ     | 2.27                     | 0.53              |
| 85:L5:2616:C:H5''  | 38:LR:64:ARG:HD3   | 1.91                     | 0.53              |
| 85:L5:2758:G:O2'   | 85:L5:2765:A:N3    | 2.33                     | 0.53              |
| 85:L5:3848:U:H4'   | 85:L5:4634:U:C4    | 2.43                     | 0.53              |
| 21:L8:130:C:H2'    | 21:L8:131:G:C8     | 2.43                     | 0.53              |
| 22:LA:41:ILE:HG12  | 22:LA:63:PHE:CE2   | 2.44                     | 0.53              |
| 23:LB:10:ARG:NH2   | 23:LB:11:HIS:O     | 2.41                     | 0.53              |
| 24:LC:210:ILE:HG13 | 24:LC:230:LEU:HB2  | 1.90                     | 0.53              |
| 24:LC:292:ILE:O    | 24:LC:298:ILE:HD11 | 2.09                     | 0.53              |
| 25:LD:133:GLU:N    | 25:LD:133:GLU:OE2  | 2.42                     | 0.53              |
| 25:LD:181:PRO:HD2  | 25:LD:195:HIS:CE1  | 2.44                     | 0.53              |
| 27:LF:236:ARG:HD3  | 27:LF:239:GLN:HB2  | 1.91                     | 0.53              |
| 33:LM:70:GLN:O     | 33:LM:73:VAL:HG12  | 2.08                     | 0.53              |
| 40:LT:157:GLU:N    | 40:LT:157:GLU:OE1  | 2.41                     | 0.53              |
| 46:La:75:LEU:HD11  | 46:La:113:GLY:HA2  | 1.89                     | 0.53              |
| 49:Ld:22:THR:HG23  | 49:Ld:89:SER:HB2   | 1.89                     | 0.53              |
| 63:Lz:172:VAL:HG12 | 63:Lz:174:MET:H    | 1.72                     | 0.53              |
| 66:SF:146:ARG:HH12 | 73:Sc:57:THR:HG21  | 1.74                     | 0.53              |
| 66:SF:204:ARG:CZ   | 73:Sc:63:ARG:HG3   | 2.38                     | 0.53              |
| 69:SQ:146:ARG:HH12 | 82:PE:33:U:H6      | 1.56                     | 0.53              |
| 70:SS:12:ILE:HD11  | 70:SS:19:ASN:ND2   | 2.24                     | 0.53              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 70:SS:82:TRP:CD2  | 79:S2:1567:G:C6    | 2.96                     | 0.53              |
| 71:ST:132:ASP:OD2 | 79:S2:1415:C:O2'   | 2.20                     | 0.53              |
| 78:Sf:90:LYS:HA   | 79:S2:1507:G:C6    | 2.43                     | 0.53              |
| 79:S2:35:C:H5''   | 79:S2:579:C:H5''   | 1.90                     | 0.53              |
| 79:S2:96:C:H2'    | 79:S2:97:U:H6      | 1.74                     | 0.53              |
| 79:S2:455:A:H2'   | 79:S2:456:C:C6     | 2.42                     | 0.53              |
| 79:S2:656:G:H5'   | 79:S2:662:G:N2     | 2.24                     | 0.53              |
| 79:S2:907:G:H2'   | 79:S2:908:A:C8     | 2.43                     | 0.53              |
| 79:S2:941:C:H2'   | 79:S2:942:G:C8     | 2.44                     | 0.53              |
| 82:PE:27:U:H2'    | 82:PE:28:C:C6      | 2.44                     | 0.53              |
| 87:IW:60:LYS:NZ   | 87:IW:62:GLY:O     | 2.30                     | 0.53              |
| 10:sA:17:LYS:HE2  | 64:sR:91:LEU:HG    | 1.90                     | 0.53              |
| 16:sN:146:ALA:O   | 16:sN:150:VAL:HG12 | 2.09                     | 0.53              |
| 17:sO:141:ARG:NH2 | 79:s2:1856:C:OP1   | 2.40                     | 0.53              |
| 20:l7:15:C:H2'    | 20:l7:16:A:C8      | 2.44                     | 0.53              |
| 26:lE:202:ASP:O   | 26:lE:260:LYS:HD3  | 2.08                     | 0.53              |
| 27:lF:164:LYS:NZ  | 85:l5:1842:G:O5'   | 2.37                     | 0.53              |
| 28:lG:232:GLU:OE1 | 28:lG:235:ARG:HD2  | 2.08                     | 0.53              |
| 28:lG:251:ALA:O   | 28:lG:255:LYS:HG2  | 2.08                     | 0.53              |
| 30:lI:146:GLU:N   | 30:lI:146:GLU:OE1  | 2.42                     | 0.53              |
| 41:lU:28:PRO:HG3  | 41:lU:112:LEU:HD22 | 1.90                     | 0.53              |
| 54:li:88:GLU:O    | 54:li:92:ASN:ND2   | 2.42                     | 0.53              |
| 63:lz:204:LEU:O   | 63:lz:215:ARG:NH1  | 2.41                     | 0.53              |
| 64:sR:12:ALA:HB1  | 64:sR:50:ILE:HD13  | 1.90                     | 0.53              |
| 65:sD:47:GLU:OE1  | 65:sD:87:TYR:CE2   | 2.62                     | 0.53              |
| 76:sM:78:LYS:HD3  | 76:sM:79:VAL:N     | 2.22                     | 0.53              |
| 79:s2:845:G:H2'   | 79:s2:846:G:O4'    | 2.08                     | 0.53              |
| 79:s2:1244:U:H2'  | 79:s2:1245:G:C8    | 2.40                     | 0.53              |
| 80:cB:171:PRO:HB3 | 80:cB:294:LEU:HB2  | 1.89                     | 0.53              |
| 80:cB:594:LYS:O   | 80:cB:727:ARG:NH2  | 2.41                     | 0.53              |
| 80:cB:750:GLN:HB3 | 80:cB:781:MET:HE1  | 1.91                     | 0.53              |
| 81:aP:22:U:H2'    | 81:aP:23:C:C6      | 2.43                     | 0.53              |
| 85:l5:1515:A:H2'  | 85:l5:1516:G:O4'   | 2.08                     | 0.53              |
| 85:l5:3633:C:H2'  | 85:l5:3634:G:C8    | 2.43                     | 0.53              |
| 85:l5:4186:A:H2'  | 85:l5:4187:G:H8    | 1.72                     | 0.53              |
| 85:l5:4239:A:H2'  | 85:l5:4240:G:H8    | 1.73                     | 0.53              |
| 2:SE:44:LEU:H     | 2:SE:44:LEU:HD12   | 1.74                     | 0.53              |
| 2:SE:45:ILE:HA    | 2:SE:61:VAL:HG21   | 1.90                     | 0.53              |
| 6:SG:156:TYR:CE1  | 87:LW:101:ARG:CZ   | 2.91                     | 0.53              |
| 11:SB:24:PRO:O    | 11:SB:28:LYS:NZ    | 2.41                     | 0.53              |
| 13:SV:39:VAL:HA   | 13:SV:45:ARG:O     | 2.08                     | 0.53              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 15:SC:86:LEU:HD13  | 15:SC:87:PRO:HD2   | 1.91                     | 0.53              |
| 85:L5:48:G:O5'     | 34:LN:192:TRP:NE1  | 2.41                     | 0.53              |
| 85:L5:216:C:OP2    | 85:L5:219:G:O2'    | 2.26                     | 0.53              |
| 85:L5:223:G:OP1    | 24:LC:163:LYS:NZ   | 2.39                     | 0.53              |
| 85:L5:291:U:N3     | 85:L5:294:G:OP1    | 2.33                     | 0.53              |
| 85:L5:978:G:H2'    | 85:L5:979:C:C6     | 2.44                     | 0.53              |
| 85:L5:1464:C:H2'   | 85:L5:1465:G:O4'   | 2.09                     | 0.53              |
| 85:L5:1535:C:H42   | 85:L5:1636:U:H4'   | 1.74                     | 0.53              |
| 85:L5:2387:G:H2'   | 85:L5:2388:A:H8    | 1.73                     | 0.53              |
| 85:L5:2869:U:H3    | 85:L5:2881:A:P     | 2.30                     | 0.53              |
| 85:L5:3701:C:N4    | 85:L5:3745:U:H2'   | 2.24                     | 0.53              |
| 85:L5:3783:A:N7    | 85:L5:3792:G:C8    | 2.77                     | 0.53              |
| 85:L5:4084:G:O6    | 22:LA:72:ARG:NH2   | 2.42                     | 0.53              |
| 85:L5:4122:G:H4'   | 52:Lg:90:ARG:NE    | 2.23                     | 0.53              |
| 85:L5:4127:A:C2    | 28:LG:37:LYS:HG2   | 2.43                     | 0.53              |
| 85:L5:4729:A:OP2   | 85:L5:5068:G:N1    | 2.30                     | 0.53              |
| 85:L5:4868:G:H5''  | 33:LM:90:ARG:CZ    | 2.39                     | 0.53              |
| 21:L8:151:G:OP2    | 28:LG:65:ARG:NE    | 2.40                     | 0.53              |
| 24:LC:10:VAL:O     | 24:LC:18:SER:OG    | 2.21                     | 0.53              |
| 24:LC:326:LEU:HD22 | 24:LC:333:LYS:HB2  | 1.90                     | 0.53              |
| 29:LH:117:PHE:O    | 29:LH:120:GLU:HG2  | 2.08                     | 0.53              |
| 32:LL:63:THR:O     | 32:LL:67:HIS:N     | 2.38                     | 0.53              |
| 32:LL:123:LYS:O    | 53:Lh:122:LYS:NZ   | 2.41                     | 0.53              |
| 33:LM:13:ALA:O     | 33:LM:25:VAL:HB    | 2.08                     | 0.53              |
| 42:LV:84:GLN:HA    | 42:LV:101:ASN:ND2  | 2.24                     | 0.53              |
| 46:La:83:SER:O     | 46:La:86:THR:OG1   | 2.19                     | 0.53              |
| 65:SD:122:VAL:O    | 65:SD:126:ILE:HG12 | 2.08                     | 0.53              |
| 70:SS:121:ARG:NH2  | 79:S2:1610:G:OP1   | 2.39                     | 0.53              |
| 75:Sg:70:VAL:HG21  | 75:Sg:112:ALA:HA   | 1.91                     | 0.53              |
| 75:Sg:225:LYS:NZ   | 75:Sg:226:HIS:H    | 2.07                     | 0.53              |
| 79:S2:106:C:H2'    | 79:S2:107:A:H8     | 1.73                     | 0.53              |
| 79:S2:1214:A:H2'   | 79:S2:1217:A:N7    | 2.24                     | 0.53              |
| 79:S2:1501:C:H2'   | 79:S2:1502:C:C6    | 2.43                     | 0.53              |
| 1:CH:99:ILE:HG23   | 1:CH:123:LYS:HB3   | 1.91                     | 0.53              |
| 1:cH:50:LYS:NZ     | 79:s2:607:U:OP1    | 2.23                     | 0.53              |
| 2:sE:69:PHE:N      | 2:sE:69:PHE:CD1    | 2.77                     | 0.53              |
| 4:sL:128:VAL:HG22  | 4:sL:140:PHE:HD1   | 1.73                     | 0.53              |
| 8:sY:41:ARG:NH1    | 8:sY:55:ILE:O      | 2.41                     | 0.53              |
| 14:sa:38:LYS:O     | 14:sa:71:LEU:HB3   | 2.09                     | 0.53              |
| 16:sN:55:ARG:HE    | 79:s2:1017:U:H5'   | 1.74                     | 0.53              |
| 24:IC:65:GLU:HB2   | 24:IC:80:ARG:HD3   | 1.91                     | 0.53              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 26:IE:188:ARG:NH1 | 26:IE:214:ASP:O    | 2.41                     | 0.53              |
| 27:IF:226:HIS:CE1 | 27:IF:228:VAL:HG23 | 2.43                     | 0.53              |
| 28:IG:177:MET:SD  | 28:IG:179:VAL:HG12 | 2.48                     | 0.53              |
| 31:IJ:20:LEU:HD12 | 31:IJ:79:ALA:HA    | 1.90                     | 0.53              |
| 32:IL:110:LEU:O   | 32:IL:114:VAL:HG13 | 2.08                     | 0.53              |
| 32:IL:138:ASP:HB3 | 32:IL:143:GLU:OE1  | 2.08                     | 0.53              |
| 34:IN:31:ARG:HD2  | 34:IN:124:ASP:OD2  | 2.09                     | 0.53              |
| 41:IU:64:GLU:N    | 41:IU:64:GLU:OE1   | 2.41                     | 0.53              |
| 54:li:50:PHE:HD1  | 54:li:54:GLU:HB3   | 1.73                     | 0.53              |
| 56:lk:3:ARG:NH1   | 85:l5:2643:G:O2'   | 2.41                     | 0.53              |
| 71:sT:101:ARG:O   | 71:sT:105:GLN:HG2  | 2.09                     | 0.53              |
| 77:sZ:69:THR:O    | 77:sZ:72:VAL:HG12  | 2.09                     | 0.53              |
| 79:s2:212:C:H2'   | 79:s2:213:G:C8     | 2.44                     | 0.53              |
| 79:s2:651:U:H2'   | 79:s2:652:U:C6     | 2.44                     | 0.53              |
| 79:s2:1174:U:H2'  | 79:s2:1175:G:H8    | 1.74                     | 0.53              |
| 79:s2:1230:C:H2'  | 79:s2:1231:C:C6    | 2.43                     | 0.53              |
| 79:s2:1414:A:H3'  | 79:s2:1415:C:H5''  | 1.91                     | 0.53              |
| 80:cB:111:PHE:HE2 | 80:cB:500:SER:H    | 1.57                     | 0.53              |
| 80:cB:158:ASN:HA  | 80:cB:215:GLY:O    | 2.08                     | 0.53              |
| 80:cB:178:PHE:HD2 | 80:cB:214:PHE:CZ   | 2.26                     | 0.53              |
| 80:cB:645:GLU:HG3 | 80:cB:648:LYS:HB2  | 1.90                     | 0.53              |
| 85:l5:267:G:H2'   | 85:l5:268:G:H8     | 1.73                     | 0.53              |
| 85:l5:270:U:H2'   | 85:l5:271:C:C6     | 2.44                     | 0.53              |
| 85:l5:1070:G:O2'  | 85:l5:1071:C:O5'   | 2.26                     | 0.53              |
| 85:l5:1199:G:H2'  | 85:l5:1200:G:H8    | 1.72                     | 0.53              |
| 85:l5:2323:C:H2'  | 85:l5:2324:C:H6    | 1.72                     | 0.53              |
| 4:SL:5:GLN:HG2    | 4:SL:10:TYR:CE2    | 2.44                     | 0.53              |
| 5:SX:139:GLU:HG2  | 5:SX:140:ARG:H     | 1.73                     | 0.53              |
| 6:SG:17:GLU:N     | 6:SG:17:GLU:OE1    | 2.42                     | 0.53              |
| 10:SA:42:LYS:HG3  | 10:SA:44:ASP:H     | 1.73                     | 0.53              |
| 10:SA:51:LEU:O    | 10:SA:54:THR:OG1   | 2.19                     | 0.53              |
| 10:SA:151:ASP:OD1 | 10:SA:151:ASP:N    | 2.40                     | 0.53              |
| 12:SH:12:ASN:HB3  | 12:SH:16:PRO:HD2   | 1.90                     | 0.53              |
| 15:SC:223:TYR:HD1 | 79:S2:2:A:H2'      | 1.73                     | 0.53              |
| 85:L5:1360:G:H2'  | 85:L5:1361:G:C8    | 2.43                     | 0.53              |
| 85:L5:1534:A:O3'  | 55:Lj:11:ARG:CZ    | 2.57                     | 0.53              |
| 85:L5:1662:C:H2'  | 85:L5:1663:C:H6    | 1.72                     | 0.53              |
| 85:L5:1669:A:H4'  | 85:L5:1685:G:N2    | 2.24                     | 0.53              |
| 85:L5:2078:C:H2'  | 85:L5:2079:G:C8    | 2.44                     | 0.53              |
| 85:L5:2568:C:H2'  | 85:L5:2569:G:C8    | 2.43                     | 0.53              |
| 85:L5:2770:C:H2'  | 85:L5:2771:G:H8    | 1.73                     | 0.53              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 85:L5:3710:G:N2    | 85:L5:3713:U:H3   | 2.06                     | 0.53              |
| 85:L5:4101:C:H5'   | 85:L5:4107:G:C3'  | 2.38                     | 0.53              |
| 85:L5:4220:A:H2'   | 85:L5:4222:G:H5'' | 1.90                     | 0.53              |
| 85:L5:4524:G:H2'   | 85:L5:4525:C:H6   | 1.74                     | 0.53              |
| 85:L5:4585:U:OP1   | 35:LO:74:ARG:N    | 2.41                     | 0.53              |
| 33:LM:50:MET:N     | 33:LM:50:MET:SD   | 2.81                     | 0.53              |
| 36:LP:10:ASN:HD21  | 36:LP:13:LYS:HB2  | 1.74                     | 0.53              |
| 41:LU:44:GLN:N     | 41:LU:44:GLN:OE1  | 2.41                     | 0.53              |
| 47:Lb:62:ALA:O     | 47:Lb:65:MET:SD   | 2.66                     | 0.53              |
| 64:SR:72:LYS:HZ2   | 64:SR:76:GLU:HG2  | 1.74                     | 0.53              |
| 66:SF:23:TRP:HE1   | 66:SF:101:HIS:CE1 | 2.26                     | 0.53              |
| 66:SF:28:VAL:HG21  | 66:SF:109:LEU:HB2 | 1.91                     | 0.53              |
| 79:S2:532:C:N4     | 79:S2:552:G:H21   | 2.07                     | 0.53              |
| 79:S2:804:U:H2'    | 79:S2:805:U:C6    | 2.44                     | 0.53              |
| 79:S2:1146:C:H2'   | 79:S2:1147:C:C6   | 2.44                     | 0.53              |
| 79:S2:1221:G:H2'   | 79:S2:1222:G:H8   | 1.73                     | 0.53              |
| 87:IW:97:LYS:O     | 87:IW:99:GLU:N    | 2.41                     | 0.53              |
| 1:CH:36:GLU:O      | 1:CH:37:ASP:HB3   | 2.07                     | 0.53              |
| 1:cH:128:ILE:HG22  | 1:cH:130:LEU:H    | 1.73                     | 0.53              |
| 2:sE:247:THR:OG1   | 2:sE:250:GLU:OE1  | 2.16                     | 0.53              |
| 6:sG:48:TYR:OH     | 6:sG:119:LYS:O    | 2.25                     | 0.53              |
| 10:sA:132:GLN:NE2  | 79:s2:1378:A:OP1  | 2.42                     | 0.53              |
| 14:sa:86:ASN:OD1   | 14:sa:86:ASN:N    | 2.39                     | 0.53              |
| 14:sa:95:ARG:NH1   | 79:s2:1865:C:O2'  | 2.41                     | 0.53              |
| 15:sC:174:ILE:HG13 | 15:sC:175:GLY:H   | 1.72                     | 0.53              |
| 20:l7:114:U:C4'    | 25:ID:73:MET:HE1  | 2.37                     | 0.53              |
| 22:lA:61:VAL:HG13  | 22:lA:74:GLU:HB2  | 1.89                     | 0.53              |
| 24:lC:182:LYS:NZ   | 85:l5:2300:A:H5'  | 2.24                     | 0.53              |
| 31:lJ:35:ARG:HH22  | 31:lJ:124:GLY:HA3 | 1.74                     | 0.53              |
| 31:lJ:119:TYR:HD1  | 31:lJ:120:ASP:N   | 2.06                     | 0.53              |
| 37:lQ:68:ARG:HH22  | 85:l5:1420:A:H2'  | 1.73                     | 0.53              |
| 55:lJ:48:ASN:ND2   | 85:l5:52:G:OP2    | 2.32                     | 0.53              |
| 64:sR:14:ARG:HD3   | 64:sR:14:ARG:N    | 2.24                     | 0.53              |
| 64:sR:71:ILE:HD12  | 64:sR:74:GLN:NE2  | 2.23                     | 0.53              |
| 66:sF:139:VAL:CA   | 73:sc:63:ARG:HH12 | 2.21                     | 0.53              |
| 67:sK:96:ARG:HD2   | 67:sK:97:SER:N    | 2.24                     | 0.53              |
| 75:sg:279:SER:HB2  | 75:sg:280:LYS:HE3 | 1.89                     | 0.53              |
| 79:s2:72:C:H2'     | 79:s2:73:C:C2     | 2.44                     | 0.53              |
| 79:s2:1202:U:H2'   | 79:s2:1203:G:C8   | 2.44                     | 0.53              |
| 79:s2:1255:G:OP1   | 79:s2:1256:G:O2'  | 2.18                     | 0.53              |
| 79:s2:1373:C:H2'   | 79:s2:1374:C:C6   | 2.41                     | 0.53              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 79:s2:1829:G:H1'   | 79:s2:1850:A:C2    | 2.44                     | 0.53              |
| 80:cB:214:PHE:O    | 80:cB:223:PHE:N    | 2.27                     | 0.53              |
| 80:cB:228:PHE:HD1  | 80:cB:293:ILE:HD13 | 1.74                     | 0.53              |
| 81:aP:4:U:H2'      | 81:aP:5:C:C6       | 2.44                     | 0.53              |
| 83:ls:62:ARG:NH2   | 83:ls:83:ARG:HD2   | 2.24                     | 0.53              |
| 85:l5:60:G:C4      | 85:l5:61:A:C8      | 2.97                     | 0.53              |
| 85:l5:1079:C:H2'   | 85:l5:1080:C:H6    | 1.74                     | 0.53              |
| 85:l5:1514:U:H2'   | 85:l5:1515:A:C8    | 2.44                     | 0.53              |
| 85:l5:1749:A:H2'   | 85:l5:1750:G:C8    | 2.44                     | 0.53              |
| 85:l5:4178:A:H2'   | 85:l5:4179:G:C8    | 2.44                     | 0.53              |
| 85:l5:4444:C:H2'   | 85:l5:4445:U:H6    | 1.72                     | 0.53              |
| 85:l5:4708:A:N3    | 85:l5:4709:U:H5'   | 2.23                     | 0.53              |
| 85:l5:4895:C:H3'   | 85:l5:4895:C:OP2   | 2.09                     | 0.53              |
| 80:CB:284:LYS:HZ2  | 80:CB:285:LEU:C    | 2.14                     | 0.53              |
| 80:CB:420:LEU:HD21 | 80:CB:463:ASP:HB2  | 1.91                     | 0.53              |
| 2:SE:108:ARG:NH2   | 79:S2:847:A:OP1    | 2.41                     | 0.53              |
| 2:SE:252:ARG:O     | 2:SE:256:LEU:HG    | 2.08                     | 0.53              |
| 3:SI:124:LYS:HE2   | 3:SI:128:LYS:NZ    | 2.24                     | 0.53              |
| 5:SX:57:VAL:O      | 5:SX:67:ARG:N      | 2.36                     | 0.53              |
| 6:SG:21:GLU:CD     | 6:SG:21:GLU:H      | 2.17                     | 0.53              |
| 7:SJ:101:LYS:NZ    | 7:SJ:102:ILE:HG22  | 2.24                     | 0.53              |
| 11:SB:180:ASP:OD1  | 11:SB:181:LEU:N    | 2.42                     | 0.53              |
| 12:SH:122:LEU:HA   | 12:SH:125:VAL:HG22 | 1.91                     | 0.53              |
| 14:Sa:10:ARG:HH11  | 14:Sa:12:LYS:HE3   | 1.74                     | 0.53              |
| 14:Sa:98:PRO:O     | 79:S2:1868:U:N3    | 2.32                     | 0.53              |
| 15:SC:224:THR:O    | 79:S2:2:A:O2'      | 2.25                     | 0.53              |
| 19:Sb:20:LYS:HB3   | 19:Sb:29:ASN:ND2   | 2.24                     | 0.53              |
| 85:L5:266:C:HO2'   | 85:L5:267:G:H8     | 1.55                     | 0.53              |
| 85:L5:424:U:OP1    | 36:LP:30:ARG:NH2   | 2.33                     | 0.53              |
| 85:L5:513:U:O2     | 85:L5:515:C:H3'    | 2.08                     | 0.53              |
| 85:L5:996:G:N2     | 85:L5:1048:G:OP1   | 2.29                     | 0.53              |
| 85:L5:1326:A:H2'   | 85:L5:1327:C:C6    | 2.44                     | 0.53              |
| 85:L5:1573:G:OP1   | 38:LR:92:LYS:NZ    | 2.36                     | 0.53              |
| 85:L5:2654:C:H2'   | 85:L5:2655:C:H6    | 1.74                     | 0.53              |
| 85:L5:2812:A:OP1   | 38:LR:83:GLY:N     | 2.25                     | 0.53              |
| 85:L5:3717:A:H2'   | 85:L5:3718:A:C8    | 2.43                     | 0.53              |
| 85:L5:3777:G:H22   | 85:L5:3816:A:P     | 2.32                     | 0.53              |
| 85:L5:4460:U:H2'   | 85:L5:4461:C:H6    | 1.72                     | 0.53              |
| 85:L5:4481:U:H2'   | 85:L5:4482:U:H6    | 1.74                     | 0.53              |
| 85:L5:4764:A:N1    | 29:LH:60:TRP:HB2   | 2.23                     | 0.53              |
| 21:L8:18:U:H2'     | 21:L8:19:C:C6      | 2.44                     | 0.53              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 45:LZ:57:MET:SD    | 45:LZ:57:MET:N     | 2.82                     | 0.53              |
| 46:La:46:ASP:OD1   | 46:La:46:ASP:N     | 2.37                     | 0.53              |
| 51:Lf:42:TYR:HA    | 51:Lf:45:LYS:HG3   | 1.90                     | 0.53              |
| 65:SD:135:GLU:HG3  | 65:SD:153:VAL:HG23 | 1.90                     | 0.53              |
| 65:SD:183:GLY:HA3  | 79:S2:1334:G:O3'   | 2.09                     | 0.53              |
| 66:SF:121:PRO:CD   | 66:SF:193:LYS:HG3  | 2.39                     | 0.53              |
| 70:SS:139:THR:OG1  | 70:SS:140:GLY:N    | 2.41                     | 0.53              |
| 71:ST:62:ARG:HH12  | 79:S2:1542:C:C5'   | 2.17                     | 0.53              |
| 79:S2:185:G:N1     | 79:S2:214:U:N3     | 2.56                     | 0.53              |
| 79:S2:688:U:O2'    | 79:S2:689:U:OP2    | 2.19                     | 0.53              |
| 79:S2:918:U:H2'    | 79:S2:919:A:C4     | 2.43                     | 0.53              |
| 79:S2:1741:U:H2'   | 79:S2:1742:C:O4'   | 2.09                     | 0.53              |
| 6:sG:1:MET:HG2     | 6:sG:24:LEU:HD21   | 1.91                     | 0.53              |
| 7:sJ:136:ARG:NH1   | 28:LG:266:GLY:H    | 2.06                     | 0.53              |
| 12:sH:98:ARG:NH1   | 12:sH:128:ALA:HB3  | 2.23                     | 0.53              |
| 12:sH:144:ILE:O    | 12:sH:145:ARG:NH1  | 2.41                     | 0.53              |
| 15:sC:188:CYS:SG   | 15:sC:238:LYS:HB2  | 2.49                     | 0.53              |
| 18:sW:20:ARG:NH2   | 79:s2:1096:G:O4'   | 2.42                     | 0.53              |
| 20:l7:5:A:OP2      | 25:ID:27:LYS:NZ    | 2.39                     | 0.53              |
| 20:l7:45:U:H2'     | 20:l7:46:C:H6      | 1.74                     | 0.53              |
| 21:l8:45:C:OP1     | 57:ll:15:LYS:HD2   | 2.09                     | 0.53              |
| 24:lC:12:SER:HB3   | 24:lC:18:SER:HB3   | 1.89                     | 0.53              |
| 27:lF:27:GLU:O     | 27:lF:30:ILE:HG13  | 2.08                     | 0.53              |
| 35:lO:93:LYS:HG2   | 35:lO:94:ARG:N     | 2.24                     | 0.53              |
| 38:lR:62:ARG:NH1   | 85:l5:4645:C:OP2   | 2.42                     | 0.53              |
| 39:lS:60:GLU:CD    | 40:lT:136:ARG:NH2  | 2.67                     | 0.53              |
| 44:lY:1:MET:N      | 85:l5:226:G:OP2    | 2.42                     | 0.53              |
| 47:lb:111:ARG:HA   | 47:lb:114:LYS:HG2  | 1.91                     | 0.53              |
| 72:sU:116:ILE:HG13 | 72:sU:119:ALA:H    | 1.74                     | 0.53              |
| 77:sZ:52:LYS:NZ    | 77:sZ:56:ASP:HB3   | 2.23                     | 0.53              |
| 79:s2:530:U:H2'    | 79:s2:531:A:N9     | 2.23                     | 0.53              |
| 79:s2:603:C:N4     | 79:s2:620:G:O6     | 2.31                     | 0.53              |
| 79:s2:1269:G:H2'   | 79:s2:1270:G:H8    | 1.74                     | 0.53              |
| 79:s2:1518:C:H5''  | 79:s2:1519:U:H5''  | 1.90                     | 0.53              |
| 85:l5:1092:G:H2'   | 85:l5:1093:C:H6    | 1.73                     | 0.53              |
| 85:l5:2384:U:H2'   | 85:l5:2385:U:C6    | 2.44                     | 0.53              |
| 85:l5:2811:G:N1    | 85:l5:2814:C:OP2   | 2.29                     | 0.53              |
| 85:l5:3727:A:H2'   | 85:l5:3728:A:C8    | 2.44                     | 0.53              |
| 85:l5:4186:A:H2'   | 85:l5:4187:G:C8    | 2.44                     | 0.53              |
| 3:SI:12:ARG:NE     | 79:S2:104:A:OP1    | 2.34                     | 0.53              |
| 3:SI:141:ARG:HD3   | 3:SI:145:ILE:HG21  | 1.90                     | 0.53              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:SJ:111:GLN:HA    | 7:SJ:130:ILE:HD11  | 1.91                     | 0.53              |
| 12:SH:143:ARG:NE   | 12:SH:157:HIS:HE1  | 2.06                     | 0.53              |
| 18:SW:120:HIS:HE2  | 79:S2:806:U:P      | 2.31                     | 0.53              |
| 85:L5:17:A:OP2     | 43:LX:60:TYR:OH    | 2.16                     | 0.53              |
| 85:L5:75:G:H1      | 32:LL:103:ARG:HH12 | 1.55                     | 0.53              |
| 85:L5:726:G:H2'    | 85:L5:727:C:C6     | 2.44                     | 0.53              |
| 85:L5:1171:G:N7    | 85:L5:1172:C:N4    | 2.57                     | 0.53              |
| 85:L5:1176:C:H42   | 85:L5:1184:A:H61   | 0.67                     | 0.53              |
| 85:L5:1259:G:H2'   | 85:L5:1260:G:H8    | 1.72                     | 0.53              |
| 85:L5:1309:C:H2'   | 85:L5:1310:C:H6    | 1.73                     | 0.53              |
| 85:L5:1586:G:H2'   | 85:L5:1587:G:C8    | 2.43                     | 0.53              |
| 85:L5:1759:G:H1    | 85:L5:1773:U:H3    | 1.55                     | 0.53              |
| 85:L5:2107:C:H2'   | 85:L5:2108:G:H8    | 1.73                     | 0.53              |
| 85:L5:2495:U:H2'   | 85:L5:2496:G:C8    | 2.43                     | 0.53              |
| 85:L5:2503:G:O4'   | 85:L5:4084:G:N2    | 2.42                     | 0.53              |
| 85:L5:2624:G:H2'   | 85:L5:2625:U:H6    | 1.73                     | 0.53              |
| 85:L5:4513:A:H2'   | 85:L5:4514:G:C8    | 2.44                     | 0.53              |
| 63:Lz:207:LYS:HG2  | 63:Lz:211:GLY:HA3  | 1.90                     | 0.53              |
| 65:SD:24:PHE:CE2   | 67:SK:63:ALA:HB2   | 2.44                     | 0.53              |
| 68:SP:59:ARG:O     | 68:SP:62:LYS:HG3   | 2.08                     | 0.53              |
| 69:SQ:9:SER:HB2    | 69:SQ:26:LYS:HD2   | 1.91                     | 0.53              |
| 70:SS:10:GLN:N     | 70:SS:10:GLN:OE1   | 2.42                     | 0.53              |
| 75:Sg:8:ARG:N      | 75:Sg:309:VAL:O    | 2.41                     | 0.53              |
| 75:Sg:131:LEU:HD11 | 75:Sg:139:LYS:HD2  | 1.89                     | 0.53              |
| 75:Sg:191:HIS:CE1  | 75:Sg:210:GLY:HA2  | 2.44                     | 0.53              |
| 79:S2:880:G:H3'    | 79:S2:881:G:H8     | 1.74                     | 0.53              |
| 79:S2:910:G:H2'    | 79:S2:911:C:C6     | 2.43                     | 0.53              |
| 79:S2:976:G:H2'    | 79:S2:977:C:C6     | 2.44                     | 0.53              |
| 79:S2:1249:C:OP2   | 79:S2:1250:A:O2'   | 2.25                     | 0.53              |
| 79:S2:1667:U:H2'   | 79:S2:1668:U:C6    | 2.43                     | 0.53              |
| 79:S2:1687:C:H2'   | 79:S2:1688:C:C6    | 2.43                     | 0.53              |
| 81:AP:50:U:H2'     | 81:AP:51:C:C6      | 2.43                     | 0.53              |
| 82:PE:26:A:N1      | 82:PE:44:G:O6      | 2.42                     | 0.53              |
| 2:sE:98:ASN:O      | 2:sE:114:ILE:HG12  | 2.09                     | 0.53              |
| 10:sA:45:GLY:HA3   | 64:sR:128:PHE:CE2  | 2.43                     | 0.53              |
| 14:sa:4:LYS:HE3    | 14:sa:5:ARG:HH12   | 1.74                     | 0.53              |
| 15:sC:191:VAL:HG11 | 15:sC:236:PHE:HA   | 1.89                     | 0.53              |
| 21:l8:22:U:O4      | 85:l5:352:G:O2'    | 2.26                     | 0.53              |
| 21:l8:102:G:H4'    | 55:lj:21:ARG:HB2   | 1.91                     | 0.53              |
| 22:lA:71:LYS:NZ    | 85:l5:2594:C:O3'   | 2.42                     | 0.53              |
| 23:lB:10:ARG:HH12  | 23:lB:265:SER:HB2  | 1.74                     | 0.53              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:lB:220:ILE:HG23 | 23:lB:278:THR:HG22 | 1.90                     | 0.53              |
| 26:lE:117:PRO:O    | 62:lR:112:ARG:NH1  | 2.40                     | 0.53              |
| 28:lG:177:MET:HE1  | 28:lG:179:VAL:H    | 1.74                     | 0.53              |
| 33:lM:27:ILE:HA    | 33:lM:38:VAL:HA    | 1.91                     | 0.53              |
| 34:lN:190:ALA:HA   | 34:lN:193:ARG:NE   | 2.24                     | 0.53              |
| 37:lQ:35:LEU:HB3   | 37:lQ:44:ASN:ND2   | 2.24                     | 0.53              |
| 62:lR:11:ARG:NH2   | 85:l5:2269:C:N3    | 2.57                     | 0.53              |
| 63:lZ:53:VAL:HG22  | 63:lZ:157:PHE:CZ   | 2.44                     | 0.53              |
| 63:lZ:92:LYS:HA    | 63:lZ:97:LYS:HG3   | 1.91                     | 0.53              |
| 63:lZ:174:MET:HE3  | 63:lZ:175:THR:H    | 1.73                     | 0.53              |
| 66:sF:68:ILE:HA    | 66:sF:71:ARG:HG3   | 1.90                     | 0.53              |
| 66:sF:85:LYS:O     | 66:sF:88:MET:HB2   | 2.09                     | 0.53              |
| 66:sF:122:ARG:HB3  | 66:sF:146:ARG:NH2  | 2.24                     | 0.53              |
| 67:sK:32:HIS:CE1   | 67:sK:34:GLU:OE1   | 2.62                     | 0.53              |
| 70:sS:11:HIS:CD2   | 70:sS:12:ILE:HG23  | 2.44                     | 0.53              |
| 75:sg:154:VAL:O    | 75:sg:155:ARG:NE   | 2.41                     | 0.53              |
| 79:s2:442:C:H2'    | 79:s2:443:U:H6     | 1.74                     | 0.53              |
| 79:s2:525:A:H2'    | 79:s2:526:A:C8     | 2.37                     | 0.53              |
| 79:s2:832:G:H2'    | 79:s2:833:C:H6     | 1.73                     | 0.53              |
| 79:s2:1337:C:H2'   | 79:s2:1338:G:C8    | 2.44                     | 0.53              |
| 79:s2:1384:C:H2'   | 79:s2:1385:G:C8    | 2.39                     | 0.53              |
| 79:s2:1474:A:H2'   | 79:s2:1475:G:C8    | 2.44                     | 0.53              |
| 79:s2:1748:G:H2'   | 79:s2:1749:G:C8    | 2.44                     | 0.53              |
| 80:cB:337:LYS:C    | 80:cB:341:ARG:NH1  | 2.66                     | 0.53              |
| 80:cB:480:VAL:O    | 80:cB:482:THR:N    | 2.41                     | 0.53              |
| 80:cB:827:ASN:O    | 80:cB:832:SER:OG   | 2.26                     | 0.53              |
| 84:lt:134:GLY:O    | 84:lt:137:GLN:NE2  | 2.30                     | 0.53              |
| 85:l5:210:C:H5'    | 85:l5:235:A:C2     | 2.44                     | 0.53              |
| 85:l5:678:C:H2'    | 85:l5:679:C:H6     | 1.72                     | 0.53              |
| 85:l5:1588:U:H2'   | 85:l5:1589:C:C6    | 2.44                     | 0.53              |
| 85:l5:1949:U:H3    | 85:l5:2034:G:H1    | 1.56                     | 0.53              |
| 85:l5:3606:U:H2'   | 85:l5:3607:U:C6    | 2.44                     | 0.53              |
| 85:l5:4153:C:H2'   | 85:l5:4154:G:H8    | 1.74                     | 0.53              |
| 85:l5:4563:U:C2    | 85:l5:4564:A:C8    | 2.97                     | 0.53              |
| 2:SE:92:ILE:HG22   | 2:SE:94:LYS:HG2    | 1.91                     | 0.53              |
| 7:SJ:132:GLN:HB3   | 7:SJ:134:HIS:CE1   | 2.44                     | 0.53              |
| 10:SA:27:GLY:HA3   | 10:SA:46:ILE:HA    | 1.89                     | 0.53              |
| 85:L5:714:G:H2'    | 85:L5:715:G:C8     | 2.44                     | 0.53              |
| 85:L5:1089:G:H2'   | 85:L5:1090:G:C8    | 2.43                     | 0.53              |
| 85:L5:1095:A:H2'   | 85:L5:1096:C:C6    | 2.44                     | 0.53              |
| 85:L5:1662:C:H2'   | 85:L5:1663:C:C6    | 2.43                     | 0.53              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 85:L5:2378:G:N2    | 85:L5:2381:A:OP2   | 2.42                     | 0.53              |
| 85:L5:2776:G:H2'   | 85:L5:2777:G:C8    | 2.44                     | 0.53              |
| 85:L5:2819:U:O2'   | 38:LR:58:HIS:ND1   | 2.36                     | 0.53              |
| 85:L5:3844:U:H2'   | 85:L5:3845:A:H8    | 1.73                     | 0.53              |
| 85:L5:3900:G:OP1   | 85:L5:3901:A:O2'   | 2.14                     | 0.53              |
| 85:L5:4102:C:C6    | 85:L5:4105:A:O4'   | 2.61                     | 0.53              |
| 85:L5:4453:C:H2'   | 85:L5:4454:G:O4'   | 2.08                     | 0.53              |
| 85:L5:4989:U:C6    | 85:L5:4991:U:H1'   | 2.44                     | 0.53              |
| 22:LA:83:HIS:O     | 22:LA:86:GLN:NE2   | 2.23                     | 0.53              |
| 22:LA:83:HIS:ND1   | 22:LA:84:THR:O     | 2.41                     | 0.53              |
| 23:LB:53:MET:HB3   | 23:LB:77:THR:HG23  | 1.91                     | 0.53              |
| 30:LI:63:GLU:OE2   | 30:LI:63:GLU:N     | 2.34                     | 0.53              |
| 31:LJ:13:ARG:O     | 31:LJ:136:ARG:NH1  | 2.41                     | 0.53              |
| 52:Lg:106:VAL:HG13 | 52:Lg:107:LEU:HD23 | 1.91                     | 0.53              |
| 55:Lj:18:LEU:HD21  | 57:Ll:51:LEU:HD22  | 1.91                     | 0.53              |
| 56:Lk:5:ILE:CD1    | 56:Lk:43:TYR:HB3   | 2.32                     | 0.53              |
| 61:Lp:38:THR:HA    | 61:Lp:45:THR:HA    | 1.91                     | 0.53              |
| 66:SF:32:ASP:O     | 66:SF:35:LEU:HD23  | 2.09                     | 0.53              |
| 75:Sg:87:LEU:HD12  | 75:Sg:111:VAL:HG11 | 1.90                     | 0.53              |
| 79:S2:323:C:H4'    | 79:S2:324:C:C5     | 2.44                     | 0.53              |
| 79:S2:638:C:H2'    | 79:S2:639:C:H6     | 1.73                     | 0.53              |
| 79:S2:1181:A:H2'   | 79:S2:1182:A:C8    | 2.44                     | 0.53              |
| 81:AP:19:G:H4'     | 81:AP:20(A):U:H5'  | 1.91                     | 0.53              |
| 82:PE:6:G:H2'      | 82:PE:7:A:C8       | 2.44                     | 0.53              |
| 83:Ls:20:LEU:HG    | 83:Ls:90:PHE:HD2   | 1.74                     | 0.53              |
| 2:sE:18:TRP:HD1    | 2:sE:46:ILE:HD11   | 1.73                     | 0.53              |
| 2:sE:94:LYS:HE2    | 8:sY:17:LEU:HG     | 1.91                     | 0.53              |
| 6:sG:137:ARG:HD2   | 6:sG:178:ARG:HD3   | 1.91                     | 0.53              |
| 10:sA:174:MET:HA   | 10:sA:177:MET:HG2  | 1.90                     | 0.53              |
| 15:sC:272:HIS:CE1  | 15:sC:276:THR:HG21 | 2.44                     | 0.53              |
| 17:sO:95:ILE:HB    | 17:sO:129:ILE:CD1  | 2.39                     | 0.53              |
| 21:lh:96:C:OP1     | 53:lh:70:ARG:NH1   | 2.41                     | 0.53              |
| 23:IB:83:PRO:O     | 23:IB:167:GLN:NE2  | 2.42                     | 0.53              |
| 27:IF:68:GLU:OE2   | 27:IF:82:TYR:HE2   | 1.92                     | 0.53              |
| 30:II:153:ARG:HA   | 30:II:156:LYS:HZ3  | 1.74                     | 0.53              |
| 30:II:170:LYS:HA   | 30:II:177:ASN:HA   | 1.91                     | 0.53              |
| 36:IP:111:SER:OG   | 36:IP:111:SER:O    | 2.27                     | 0.53              |
| 38:IR:60:ARG:HH12  | 85:l5:2809:G:P     | 2.32                     | 0.53              |
| 40:IT:13:TYR:OH    | 85:l5:1790:U:OP2   | 2.20                     | 0.53              |
| 45:IZ:3:LYS:HZ3    | 48:lc:40:GLN:HA    | 1.74                     | 0.53              |
| 45:IZ:25:ILE:HD11  | 45:lZ:28:ASN:HB3   | 1.89                     | 0.53              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 46:la:8:THR:HG21  | 85:l5:1339:U:OP1   | 2.09                     | 0.53              |
| 47:lb:57:MET:CE   | 85:l5:1828:C:H1'   | 2.38                     | 0.53              |
| 49:ld:38:PHE:HB3  | 49:ld:78:ARG:HB3   | 1.90                     | 0.53              |
| 51:lf:76:ARG:O    | 51:lf:84:VAL:HG13  | 2.09                     | 0.53              |
| 53:lh:98:HIS:CD2  | 85:l5:137:G:H4'    | 2.44                     | 0.53              |
| 56:lk:68:GLU:N    | 56:lk:68:GLU:OE1   | 2.41                     | 0.53              |
| 62:lr:65:LYS:O    | 62:lr:102:TYR:OH   | 2.26                     | 0.53              |
| 64:sR:14:ARG:NH2  | 79:s2:1373:C:O2    | 2.42                     | 0.53              |
| 66:sF:83:ASN:CG   | 79:s2:1651:A:HO2'  | 2.16                     | 0.53              |
| 67:sK:10:ALA:HB1  | 67:sK:38:LYS:HD2   | 1.91                     | 0.53              |
| 79:s2:58:C:N4     | 79:s2:62:G:O6      | 2.20                     | 0.53              |
| 79:s2:130:G:O2'   | 79:s2:131:C:O3'    | 2.26                     | 0.53              |
| 79:s2:1792:G:H2'  | 79:s2:1793:A:H8    | 1.74                     | 0.53              |
| 79:s2:1828:C:H2'  | 79:s2:1829:G:H8    | 1.74                     | 0.53              |
| 80:cB:152:LYS:NZ  | 80:cB:359:PRO:HG3  | 2.24                     | 0.53              |
| 80:cB:742:GLU:OE2 | 80:cB:790:VAL:N    | 2.41                     | 0.53              |
| 80:cB:759:ILE:HA  | 80:cB:762:VAL:HG22 | 1.89                     | 0.53              |
| 81:aP:29:C:H2'    | 81:aP:30:G:C8      | 2.43                     | 0.53              |
| 84:lt:105:THR:OG1 | 84:lt:143:VAL:HG13 | 2.08                     | 0.53              |
| 85:l5:2732:G:H2'  | 85:l5:2733:C:C6    | 2.44                     | 0.53              |
| 85:l5:5002:U:H2'  | 85:l5:5003:U:C6    | 2.44                     | 0.53              |
| 80:CB:221:TRP:HE3 | 80:CB:344:LEU:HD12 | 1.74                     | 0.53              |
| 5:SX:32:LEU:HD22  | 5:SX:34:THR:HB     | 1.91                     | 0.53              |
| 10:SA:108:PHE:CE2 | 10:SA:119:PRO:CD   | 2.92                     | 0.53              |
| 13:SV:50:PHE:HE2  | 13:SV:52:THR:HB    | 1.73                     | 0.53              |
| 16:SN:55:ARG:NH1  | 79:S2:1015:U:O2'   | 2.42                     | 0.53              |
| 19:Sb:72:ARG:NH1  | 79:S2:1119:A:O2'   | 2.42                     | 0.53              |
| 85:L5:273:U:H2'   | 85:L5:274:C:H6     | 1.74                     | 0.53              |
| 85:L5:966:A:OP1   | 85:L5:967:C:N4     | 2.42                     | 0.53              |
| 85:L5:1577:G:O4'  | 22:LA:181:LYS:NZ   | 2.42                     | 0.53              |
| 85:L5:2038:U:H2'  | 85:L5:2039:G:O4'   | 2.08                     | 0.53              |
| 85:L5:2055:G:O5'  | 35:LO:130:LYS:NZ   | 2.42                     | 0.53              |
| 85:L5:2605:G:H2'  | 85:L5:2606:G:H8    | 1.74                     | 0.53              |
| 85:L5:2776:G:H2'  | 85:L5:2777:G:H8    | 1.75                     | 0.53              |
| 85:L5:3911:C:H2'  | 85:L5:3912:U:H6    | 1.74                     | 0.53              |
| 85:L5:4485:C:H2'  | 85:L5:4486:C:H6    | 1.73                     | 0.53              |
| 85:L5:5055:G:H2'  | 85:L5:5056:A:C8    | 2.44                     | 0.53              |
| 23:LB:241:PRO:O   | 23:LB:244:THR:OG1  | 2.24                     | 0.53              |
| 24:LC:10:VAL:HG23 | 24:LC:153:VAL:CG1  | 2.37                     | 0.53              |
| 27:LF:88:LYS:O    | 27:LF:125:LEU:N    | 2.40                     | 0.53              |
| 27:LF:102:SER:OG  | 27:LF:105:VAL:HG12 | 2.09                     | 0.53              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 32:LL:195:ARG:HA   | 32:LL:198:ARG:HH11 | 1.73                     | 0.53              |
| 33:LM:86:TRP:HA    | 33:LM:89:THR:HB    | 1.90                     | 0.53              |
| 43:LX:96:LEU:HB2   | 43:LX:138:VAL:HG13 | 1.91                     | 0.53              |
| 51:Lf:78:HIS:ND1   | 51:Lf:78:HIS:O     | 2.42                     | 0.53              |
| 52:Lg:8:ARG:HB2    | 52:Lg:34:TYR:HE1   | 1.74                     | 0.53              |
| 59:Ln:15:ARG:O     | 59:Ln:18:ARG:HG2   | 2.09                     | 0.53              |
| 61:Lp:33:GLN:OE1   | 61:Lp:49:ARG:NH2   | 2.41                     | 0.53              |
| 65:SD:95:GLY:HA2   | 65:SD:101:GLN:NE2  | 2.24                     | 0.53              |
| 66:SF:55:ARG:HB3   | 66:SF:58:ALA:HB2   | 1.91                     | 0.53              |
| 68:SP:28:MET:CE    | 68:SP:33:LEU:HB2   | 2.39                     | 0.53              |
| 71:ST:33:TRP:NE1   | 79:S2:1567:G:OP2   | 2.42                     | 0.53              |
| 71:ST:143:LYS:O    | 71:ST:144:LYS:NZ   | 2.30                     | 0.53              |
| 75:Sg:149:GLU:OE2  | 75:Sg:150:TRP:N    | 2.41                     | 0.53              |
| 76:SM:12:MET:HG2   | 76:SM:16:THR:HG21  | 1.91                     | 0.53              |
| 76:SM:47:ALA:HB1   | 76:SM:110:VAL:HG21 | 1.92                     | 0.53              |
| 79:S2:43:U:H2'     | 79:S2:44:U:H5      | 1.73                     | 0.53              |
| 79:S2:79:A:H2'     | 79:S2:80:G:O4'     | 2.09                     | 0.53              |
| 79:S2:218:U:H2'    | 79:S2:219:U:C6     | 2.44                     | 0.53              |
| 79:S2:221:A:H2'    | 79:S2:222:U:C6     | 2.44                     | 0.53              |
| 79:S2:1676:U:H2'   | 79:S2:1677:U:O4'   | 2.08                     | 0.53              |
| 84:Lt:112:ILE:O    | 84:Lt:115:GLN:N    | 2.42                     | 0.53              |
| 1:cH:43:LYS:HG2    | 9:se:44:ASN:ND2    | 2.23                     | 0.52              |
| 1:cH:47:GLY:H      | 9:se:55:PRO:CG     | 2.22                     | 0.52              |
| 2:sE:36:HIS:CE1    | 2:sE:85:GLY:HA3    | 2.44                     | 0.52              |
| 3:sI:72:CYS:HG     | 3:sI:112:TRP:CG    | 2.26                     | 0.52              |
| 3:sI:148:LYS:HG2   | 3:sI:152:ARG:HD2   | 1.90                     | 0.52              |
| 15:sC:183:LYS:HG2  | 18:sW:95:PRO:HA    | 1.90                     | 0.52              |
| 20:l7:15:C:H1'     | 25:lD:13:PHE:HE1   | 1.73                     | 0.52              |
| 23:lB:133:TYR:O    | 23:lB:136:LYS:HG2  | 2.09                     | 0.52              |
| 34:lN:31:ARG:NH2   | 85:l5:4077:A:O3'   | 2.42                     | 0.52              |
| 36:lP:22:LEU:HB3   | 36:lP:90:PHE:HE2   | 1.72                     | 0.52              |
| 54:li:51:ALA:N     | 54:li:54:GLU:OE1   | 2.41                     | 0.52              |
| 54:li:52:PRO:HA    | 54:li:55:ARG:HG2   | 1.91                     | 0.52              |
| 56:lk:9:LYS:NZ     | 56:lk:13:LEU:HB3   | 2.23                     | 0.52              |
| 61:lp:28:LYS:NZ    | 79:s2:1040:G:O2'   | 2.39                     | 0.52              |
| 64:sR:17:ILE:HG12  | 64:sR:54:VAL:HG13  | 1.90                     | 0.52              |
| 67:sK:12:TYR:OH    | 67:sK:52:LEU:HD21  | 2.09                     | 0.52              |
| 68:sP:28:MET:HE1   | 68:sP:33:LEU:N     | 2.23                     | 0.52              |
| 75:sg:186:THR:HG22 | 75:sg:188:HIS:HB2  | 1.91                     | 0.52              |
| 75:sg:269:GLU:OE1  | 75:sg:269:GLU:N    | 2.33                     | 0.52              |
| 79:s2:511:U:H2'    | 79:s2:512:A:C8     | 2.44                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 80:cB:420:LEU:HD12 | 80:cB:465:PRO:HB3  | 1.90                     | 0.52              |
| 80:cB:852:ASP:OD1  | 80:cB:853:ASN:N    | 2.42                     | 0.52              |
| 81:aP:49:C:H2'     | 81:aP:50:U:C6      | 2.44                     | 0.52              |
| 85:l5:181:C:H3'    | 85:l5:182:G:C8     | 2.42                     | 0.52              |
| 85:l5:1563:A:H2'   | 85:l5:1564:A:C8    | 2.44                     | 0.52              |
| 85:l5:1998:A:H2'   | 85:l5:1999:A:C8    | 2.43                     | 0.52              |
| 85:l5:2259:G:H5'   | 85:l5:2260:C:C5    | 2.42                     | 0.52              |
| 85:l5:4089:G:H2'   | 85:l5:4090:G:H8    | 1.74                     | 0.52              |
| 85:l5:4666:G:H2'   | 85:l5:4667:C:C6    | 2.44                     | 0.52              |
| 6:SG:31:ARG:NH2    | 79:S2:1745:A:O3'   | 2.42                     | 0.52              |
| 6:SG:149:LYS:N     | 6:SG:151:ASP:OD2   | 2.42                     | 0.52              |
| 7:SJ:17:ARG:NH2    | 7:SJ:18:ARG:HB2    | 2.24                     | 0.52              |
| 10:SA:198:MET:HE1  | 64:SR:86:PRO:O     | 2.10                     | 0.52              |
| 11:SB:225:LEU:O    | 11:SB:229:MET:HG2  | 2.09                     | 0.52              |
| 13:SV:34:MET:O     | 13:SV:52:THR:OG1   | 2.21                     | 0.52              |
| 85:L5:286:U:H2'    | 85:L5:287:U:C6     | 2.44                     | 0.52              |
| 85:L5:1308:C:H2'   | 85:L5:1309:C:C6    | 2.44                     | 0.52              |
| 85:L5:1673:U:H2'   | 85:L5:1674:C:C6    | 2.44                     | 0.52              |
| 85:L5:2648:G:H2'   | 85:L5:2649:G:C8    | 2.44                     | 0.52              |
| 85:L5:2657:G:H2'   | 85:L5:2658:G:C8    | 2.44                     | 0.52              |
| 85:L5:4101:C:C2'   | 85:L5:4106:G:C8    | 2.91                     | 0.52              |
| 85:L5:4102:C:C4    | 85:L5:4105:A:N7    | 2.76                     | 0.52              |
| 85:L5:4373:G:N7    | 60:Lo:61:LYS:NZ    | 2.56                     | 0.52              |
| 85:L5:4989:U:H1'   | 85:L5:4990:C:C5    | 2.43                     | 0.52              |
| 23:LB:36:ASP:OD1   | 23:LB:36:ASP:N     | 2.42                     | 0.52              |
| 24:LC:284:MET:HE2  | 24:LC:284:MET:HA   | 1.90                     | 0.52              |
| 30:LI:52:MET:HG2   | 30:LI:152:LEU:HD13 | 1.91                     | 0.52              |
| 32:LL:90:VAL:HA    | 32:LL:93:THR:HG22  | 1.90                     | 0.52              |
| 35:LO:31:ARG:O     | 35:LO:33:VAL:HG23  | 2.08                     | 0.52              |
| 37:LQ:146:ARG:HB3  | 37:LQ:148:VAL:HG22 | 1.90                     | 0.52              |
| 65:SD:27:ARG:HH22  | 79:S2:1498:A:P     | 2.32                     | 0.52              |
| 69:SQ:39:LEU:HB2   | 69:SQ:51:LEU:HD11  | 1.90                     | 0.52              |
| 77:SZ:87:ALA:HA    | 77:SZ:90:GLU:OE1   | 2.09                     | 0.52              |
| 79:S2:380:G:N1     | 79:S2:383:G:OP2    | 2.24                     | 0.52              |
| 79:S2:511:U:H2'    | 79:S2:512:A:H8     | 1.73                     | 0.52              |
| 79:S2:696:G:H2'    | 79:S2:734:C:C2     | 2.44                     | 0.52              |
| 79:S2:1324:G:O6    | 79:S2:1504:U:O4    | 2.27                     | 0.52              |
| 79:S2:1779:G:C2    | 79:S2:1780:G:C5    | 2.97                     | 0.52              |
| 81:AP:29:C:H2'     | 81:AP:30:G:C8      | 2.44                     | 0.52              |
| 84:Lt:126:SER:CB   | 84:Lt:130:LYS:HE2  | 2.39                     | 0.52              |
| 2:sE:3:ARG:NH2     | 79:s2:92:A:O5'     | 2.42                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:sE:171:ASP:HB3   | 2:sE:235:TRP:HZ3   | 1.74                     | 0.52              |
| 5:sX:107:ARG:HG2   | 5:sX:112:VAL:HG22  | 1.90                     | 0.52              |
| 6:sG:136:LYS:NZ    | 6:sG:174:PRO:HB2   | 2.19                     | 0.52              |
| 11:sB:203:SER:HA   | 79:s2:1113:A:H1'   | 1.91                     | 0.52              |
| 14:sa:51:ARG:O     | 14:sa:54:SER:OG    | 2.26                     | 0.52              |
| 18:sW:109:GLY:C    | 18:sW:111:MET:HE1  | 2.35                     | 0.52              |
| 24:lC:10:VAL:HG12  | 24:lC:20:LYS:HB2   | 1.89                     | 0.52              |
| 24:lC:31:PRO:HB3   | 37:lQ:24:TYR:HE1   | 1.74                     | 0.52              |
| 24:lC:182:LYS:HZ2  | 85:l5:2300:A:H5'   | 1.74                     | 0.52              |
| 24:lC:223:ASN:ND2  | 85:l5:226:G:H2'    | 2.24                     | 0.52              |
| 25:lD:85:LYS:HE3   | 25:lD:86:TYR:HD1   | 1.74                     | 0.52              |
| 27:lF:180:GLY:HA3  | 85:l5:1705:G:N7    | 2.24                     | 0.52              |
| 28:lG:230:TYR:HA   | 28:lG:233:ILE:HB   | 1.92                     | 0.52              |
| 31:lJ:21:CYS:HB3   | 31:lJ:131:TYR:O    | 2.08                     | 0.52              |
| 31:lJ:95:ARG:HG2   | 31:lJ:96:LYS:N     | 2.24                     | 0.52              |
| 31:lJ:107:PHE:O    | 31:lJ:130:PHE:N    | 2.42                     | 0.52              |
| 32:lL:36:ARG:HH22  | 85:l5:1363:C:H3'   | 1.74                     | 0.52              |
| 32:lL:108:GLU:OE2  | 32:lL:108:GLU:N    | 2.41                     | 0.52              |
| 33:lM:46:ARG:O     | 33:lM:48:GLN:NE2   | 2.23                     | 0.52              |
| 33:lM:98:ARG:NH2   | 85:l5:4876:U:O2    | 2.43                     | 0.52              |
| 37:lQ:180:ARG:HH11 | 46:la:50:PRO:HG2   | 1.73                     | 0.52              |
| 41:lU:76:VAL:HG23  | 41:lU:78:PHE:H     | 1.74                     | 0.52              |
| 48:lc:35:LEU:HD22  | 48:lc:39:ARG:HH21  | 1.74                     | 0.52              |
| 52:lg:103:VAL:O    | 52:lg:106:VAL:HG22 | 2.09                     | 0.52              |
| 55:lj:25:LYS:HD3   | 57:ll:51:LEU:HA    | 1.92                     | 0.52              |
| 59:ln:1:MET:HB3    | 59:ln:6:ARG:NH1    | 2.25                     | 0.52              |
| 63:lz:53:VAL:HG22  | 63:lz:157:PHE:HZ   | 1.75                     | 0.52              |
| 65:sD:177:LEU:HG   | 65:sD:179:GLN:H    | 1.74                     | 0.52              |
| 66:sF:128:ILE:CD1  | 73:sc:23:SER:HB3   | 2.39                     | 0.52              |
| 74:sd:3:HIS:HE1    | 74:sd:5:GLN:HB3    | 1.73                     | 0.52              |
| 75:sg:237:ASN:ND2  | 75:sg:287:THR:HA   | 2.25                     | 0.52              |
| 79:s2:59:U:H5''    | 79:s2:503:C:H41    | 1.73                     | 0.52              |
| 79:s2:573:U:O2'    | 79:s2:575:A:N7     | 2.36                     | 0.52              |
| 79:s2:655:A:H4'    | 79:s2:656:G:H3'    | 1.90                     | 0.52              |
| 79:s2:958:G:H2'    | 79:s2:959:G:C8     | 2.44                     | 0.52              |
| 79:s2:1360:U:C4    | 79:s2:1361:G:C6    | 2.97                     | 0.52              |
| 80:cB:452:LEU:HD12 | 80:cB:453:MET:H    | 1.74                     | 0.52              |
| 81:aP:34:A:H2'     | 81:aP:35:A:C8      | 2.44                     | 0.52              |
| 85:l5:663:G:H2'    | 85:l5:664:G:H8     | 1.70                     | 0.52              |
| 85:l5:1504:G:H2'   | 85:l5:1505:C:C6    | 2.44                     | 0.52              |
| 85:l5:1837:A:H2'   | 85:l5:1838:A:H8    | 1.73                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 85:L5:2019:C:H2'   | 85:L5:2020:U:C6    | 2.44                     | 0.52              |
| 85:L5:3921:U:H1'   | 85:L5:4543:G:N2    | 2.24                     | 0.52              |
| 85:L5:4653:C:H2'   | 85:L5:4654:C:C6    | 2.45                     | 0.52              |
| 85:L5:4879:C:H2'   | 85:L5:4880:C:C6    | 2.43                     | 0.52              |
| 80:CB:72:SER:OG    | 80:CB:400:LYS:NZ   | 2.36                     | 0.52              |
| 80:CB:650:TRP:N    | 80:CB:662:LEU:O    | 2.34                     | 0.52              |
| 80:CB:661:ILE:HD11 | 80:CB:701:ARG:HG3  | 1.90                     | 0.52              |
| 6:SG:67:VAL:HG11   | 6:SG:99:GLY:HA2    | 1.91                     | 0.52              |
| 8:SY:55:ILE:HD13   | 8:SY:75:ILE:HG22   | 1.91                     | 0.52              |
| 11:SB:115:LYS:H    | 11:SB:118:GLN:HE22 | 1.58                     | 0.52              |
| 15:SC:63:VAL:O     | 15:SC:64:THR:OG1   | 2.23                     | 0.52              |
| 16:SN:55:ARG:HD3   | 79:S2:1017:U:H5'   | 1.91                     | 0.52              |
| 16:SN:120:SER:OG   | 79:S2:677:G:OP1    | 2.27                     | 0.52              |
| 85:L5:326:C:H2'    | 85:L5:327:U:C6     | 2.45                     | 0.52              |
| 85:L5:399:G:H4'    | 36:LP:18:ARG:HG2   | 1.90                     | 0.52              |
| 85:L5:1252:C:N4    | 85:L5:1253:G:N3    | 2.57                     | 0.52              |
| 85:L5:1666:C:H2'   | 85:L5:1667:G:O4'   | 2.09                     | 0.52              |
| 85:L5:1870:C:H2'   | 85:L5:1871:A:H8    | 1.74                     | 0.52              |
| 85:L5:2686:G:O2'   | 85:L5:2688:G:N7    | 2.35                     | 0.52              |
| 85:L5:3642:A:C4    | 55:Lj:3:LYS:HB3    | 2.44                     | 0.52              |
| 85:L5:3770:U:H2'   | 85:L5:3771:C:H6    | 1.73                     | 0.52              |
| 85:L5:4345:C:H2'   | 85:L5:4346:U:C6    | 2.44                     | 0.52              |
| 85:L5:4551:U:H2'   | 85:L5:4552:U:C6    | 2.45                     | 0.52              |
| 85:L5:4577:U:H2'   | 85:L5:4578:G:C8    | 2.44                     | 0.52              |
| 85:L5:4677:U:O2    | 85:L5:4713:G:N2    | 2.42                     | 0.52              |
| 85:L5:4941:G:H2'   | 85:L5:4942:C:C6    | 2.44                     | 0.52              |
| 24:LC:331:TYR:CZ   | 27:LF:55:LYS:HA    | 2.43                     | 0.52              |
| 31:LJ:169:LYS:HG3  | 31:LJ:170:TYR:CD2  | 2.44                     | 0.52              |
| 44:LY:80:ILE:HD12  | 44:LY:99:ILE:O     | 2.09                     | 0.52              |
| 48:Lc:37:MET:SD    | 48:Lc:37:MET:N     | 2.82                     | 0.52              |
| 48:Lc:45:LEU:HB3   | 48:Lc:96:ILE:HD11  | 1.90                     | 0.52              |
| 54:Li:58:MET:O     | 54:Li:61:LEU:HD12  | 2.09                     | 0.52              |
| 54:Li:59:GLU:HA    | 54:Li:62:LYS:HD2   | 1.91                     | 0.52              |
| 77:SZ:61:GLU:OE1   | 77:SZ:64:ASN:ND2   | 2.42                     | 0.52              |
| 77:SZ:102:LYS:NZ   | 79:S2:1595:U:OP1   | 2.42                     | 0.52              |
| 79:S2:96:C:H2'     | 79:S2:97:U:C6      | 2.44                     | 0.52              |
| 79:S2:1228:A:H2'   | 79:S2:1229:G:H8    | 1.73                     | 0.52              |
| 79:S2:1392:U:H2'   | 79:S2:1393:G:H8    | 1.75                     | 0.52              |
| 1:cH:133:ARG:NH2   | 79:s2:534:G:O2'    | 2.42                     | 0.52              |
| 1:cH:133:ARG:HH12  | 79:s2:535:G:P      | 2.31                     | 0.52              |
| 2:sE:87:MET:HA     | 2:sE:101:LEU:O     | 2.08                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:sJ:107:GLU:O     | 7:sJ:112:THR:OG1   | 2.28                     | 0.52              |
| 9:se:34:ARG:NH2    | 79:s2:642:U:OP2    | 2.43                     | 0.52              |
| 11:sB:148:ASN:C    | 64:sR:131:PRO:HB3  | 2.35                     | 0.52              |
| 18:sW:16:ASN:OD1   | 79:s2:1152:U:O2'   | 2.21                     | 0.52              |
| 18:sW:76:SER:OG    | 79:s2:1159:G:OP1   | 2.20                     | 0.52              |
| 20:l7:4:U:H2'      | 20:l7:5:A:H8       | 1.74                     | 0.52              |
| 23:lB:55:HIS:NE2   | 23:lB:369:ASP:OD2  | 2.42                     | 0.52              |
| 23:lB:119:TYR:OH   | 23:lB:128:LYS:N    | 2.43                     | 0.52              |
| 32:lL:92:ARG:NH2   | 32:lL:98:VAL:O     | 2.41                     | 0.52              |
| 38:lR:25:ASP:OD2   | 38:lR:28:GLU:N     | 2.31                     | 0.52              |
| 42:IV:43:LYS:HB2   | 42:IV:60:MET:O     | 2.10                     | 0.52              |
| 52:lg:97:ILE:HD11  | 85:l5:4122:G:N7    | 2.24                     | 0.52              |
| 55:lj:17:THR:OG1   | 55:lj:18:LEU:N     | 2.41                     | 0.52              |
| 63:lz:24:LYS:NZ    | 63:lz:30:GLU:O     | 2.42                     | 0.52              |
| 75:sg:112:ALA:HB3  | 75:sg:121:VAL:HG22 | 1.91                     | 0.52              |
| 76:sM:41:ALA:HA    | 76:sM:44:LYS:NZ    | 2.24                     | 0.52              |
| 79:s2:458:A:H2'    | 79:s2:459:C:C6     | 2.44                     | 0.52              |
| 79:s2:1337:C:H2'   | 79:s2:1338:G:H8    | 1.74                     | 0.52              |
| 79:s2:1495:G:O2'   | 79:s2:1496:U:O4'   | 2.15                     | 0.52              |
| 80:cB:127:VAL:HG13 | 80:cB:155:LEU:HA   | 1.92                     | 0.52              |
| 80:cB:738:PRO:O    | 80:cB:739:ARG:NE   | 2.43                     | 0.52              |
| 81:aP:5:C:H2'      | 81:aP:6:C:C6       | 2.44                     | 0.52              |
| 85:l5:25:A:H2'     | 85:l5:26:C:H6      | 1.74                     | 0.52              |
| 85:l5:325:U:H2'    | 85:l5:326:C:H6     | 1.73                     | 0.52              |
| 85:l5:3848:U:H2'   | 85:l5:3849:A:C8    | 2.43                     | 0.52              |
| 85:l5:3954:A:O2'   | 85:l5:3955:G:O5'   | 2.26                     | 0.52              |
| 80:CB:64:GLN:CD    | 80:CB:64:GLN:H     | 2.18                     | 0.52              |
| 80:CB:364:ALA:HA   | 80:CB:367:TYR:CZ   | 2.44                     | 0.52              |
| 11:SB:35:ALA:O     | 11:SB:42:ARG:NE    | 2.31                     | 0.52              |
| 11:SB:65:ARG:HB3   | 11:SB:67:PHE:HE1   | 1.73                     | 0.52              |
| 13:SV:22:ARG:NH2   | 18:SW:18:GLU:O     | 2.42                     | 0.52              |
| 15:SC:60:TRP:CH2   | 15:SC:93:ILE:HG22  | 2.43                     | 0.52              |
| 17:SO:38:ASN:ND2   | 79:S2:960:U:O4     | 2.37                     | 0.52              |
| 85:L5:231:U:O2     | 44:LY:103:LYS:NZ   | 2.41                     | 0.52              |
| 85:L5:450:G:O6     | 85:L5:1297:U:O4    | 2.27                     | 0.52              |
| 85:L5:928:C:H2'    | 85:L5:929:A:C8     | 2.45                     | 0.52              |
| 85:L5:1559:G:H5'   | 38:LR:126:LYS:HZ1  | 1.74                     | 0.52              |
| 85:L5:1567:U:H2'   | 85:L5:1568:C:H6    | 1.74                     | 0.52              |
| 85:L5:1998:A:H2'   | 85:L5:1999:A:C8    | 2.44                     | 0.52              |
| 85:L5:2289:C:O2    | 62:Lr:22:LYS:N     | 2.31                     | 0.52              |
| 85:L5:2448:G:OP2   | 85:L5:2510:G:N1    | 2.29                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 85:L5:2545:U:N3    | 85:L5:2547:G:OP1   | 2.41                     | 0.52              |
| 85:L5:3611:A:H2'   | 85:L5:3612:C:H6    | 1.74                     | 0.52              |
| 85:L5:4139:G:H1'   | 85:L5:4146:G:N1    | 2.24                     | 0.52              |
| 85:L5:4340:U:OP1   | 37:LQ:185:GLY:N    | 2.43                     | 0.52              |
| 85:L5:4761:G:P     | 35:LO:37:ARG:HH12  | 2.32                     | 0.52              |
| 20:L7:7:G:OP2      | 25:LD:28:THR:OG1   | 2.17                     | 0.52              |
| 25:LD:197:LYS:HB3  | 25:LD:202:GLN:HB2  | 1.92                     | 0.52              |
| 38:LR:105:LEU:HD23 | 38:LR:138:LEU:HD23 | 1.92                     | 0.52              |
| 40:LT:102:ARG:HD3  | 40:LT:106:LEU:CD2  | 2.39                     | 0.52              |
| 59:Ln:17:ARG:HA    | 59:Ln:20:MET:CE    | 2.37                     | 0.52              |
| 64:SR:47:ARG:HH21  | 64:SR:48:ASN:HB3   | 1.75                     | 0.52              |
| 79:S2:140:C:O2'    | 79:S2:143:U:OP1    | 2.27                     | 0.52              |
| 79:S2:564:A:C2     | 79:S2:565:G:H1'    | 2.43                     | 0.52              |
| 79:S2:906:U:H2'    | 79:S2:907:G:H8     | 1.73                     | 0.52              |
| 79:S2:1725:U:N3    | 79:S2:1726:G:N7    | 2.58                     | 0.52              |
| 83:Ls:18:ILE:HD13  | 83:Ls:21:LEU:HD21  | 1.90                     | 0.52              |
| 6:sG:21:GLU:CD     | 6:sG:21:GLU:H      | 2.15                     | 0.52              |
| 6:sG:183:ARG:HH12  | 79:s2:317:C:H5     | 1.57                     | 0.52              |
| 10:sA:3:GLY:N      | 10:sA:9:GLN:HE22   | 2.07                     | 0.52              |
| 16:sN:120:SER:OG   | 79:s2:677:G:OP1    | 2.23                     | 0.52              |
| 18:sW:98:GLN:OE1   | 18:sW:98:GLN:N     | 2.28                     | 0.52              |
| 20:l7:118:C:H2'    | 20:l7:119:U:C6     | 2.43                     | 0.52              |
| 22:lA:40:TYR:CE2   | 22:lA:89:TYR:CD1   | 2.97                     | 0.52              |
| 23:lB:161:ARG:HG2  | 23:lB:184:GLN:HA   | 1.90                     | 0.52              |
| 25:lD:48:LYS:NZ    | 85:l5:4325:A:O3'   | 2.43                     | 0.52              |
| 28:lG:249:ARG:HH12 | 85:l5:4075:U:P     | 2.31                     | 0.52              |
| 34:lN:50:ARG:NH2   | 85:l5:278:G:O3'    | 2.42                     | 0.52              |
| 53:lh:89:ARG:NH2   | 85:l5:20:U:OP2     | 2.41                     | 0.52              |
| 55:lj:29:LEU:H     | 55:lj:29:LEU:HD12  | 1.74                     | 0.52              |
| 69:sQ:78:VAL:HG21  | 79:s2:1674:G:OP2   | 2.10                     | 0.52              |
| 72:sU:56:MET:HE2   | 79:s2:1580:A:H5'   | 1.89                     | 0.52              |
| 75:sg:110:SER:CB   | 75:sg:153:CYS:HA   | 2.39                     | 0.52              |
| 79:s2:21:U:H2'     | 79:s2:22:A:H8      | 1.73                     | 0.52              |
| 79:s2:35:C:H5''    | 79:s2:579:C:H5''   | 1.92                     | 0.52              |
| 79:s2:376:A:H2'    | 79:s2:377:G:O4'    | 2.08                     | 0.52              |
| 79:s2:420:G:O2'    | 79:s2:421:G:OP1    | 2.25                     | 0.52              |
| 79:s2:955:A:N3     | 79:s2:956:G:H1'    | 2.24                     | 0.52              |
| 79:s2:1278:A:H2'   | 79:s2:1279:C:C6    | 2.45                     | 0.52              |
| 79:s2:1446:A:O2'   | 79:s2:1447:G:H8    | 1.91                     | 0.52              |
| 79:s2:1531:A:H2'   | 79:s2:1532:C:C6    | 2.45                     | 0.52              |
| 79:s2:1729:U:O4    | 79:s2:1805:G:O6    | 2.27                     | 0.52              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 80:cB:13:MET:SD   | 80:cB:468:ASN:CG   | 2.92                     | 0.52              |
| 80:cB:138:GLN:O   | 80:cB:142:VAL:HG13 | 2.09                     | 0.52              |
| 85:l5:280:G:H4'   | 85:l5:281:U:H6     | 1.75                     | 0.52              |
| 85:l5:1089:G:H2'  | 85:l5:1090:G:C8    | 2.44                     | 0.52              |
| 85:l5:1351:G:H2'  | 85:l5:1352:C:C6    | 2.44                     | 0.52              |
| 85:l5:1778:C:H2'  | 85:l5:1779:U:C6    | 2.44                     | 0.52              |
| 85:l5:2558:C:H2'  | 85:l5:2559:G:C8    | 2.44                     | 0.52              |
| 85:l5:3771:C:H2'  | 85:l5:3772:U:C6    | 2.44                     | 0.52              |
| 85:l5:3893:C:H2'  | 85:l5:3894:A:C8    | 2.45                     | 0.52              |
| 85:l5:3910:C:H2'  | 85:l5:3911:C:H6    | 1.74                     | 0.52              |
| 85:l5:3965:A:O2'  | 85:l5:4050:A:OP2   | 2.25                     | 0.52              |
| 85:l5:4336:A:H5'' | 85:l5:4337:C:H5'   | 1.92                     | 0.52              |
| 7:SJ:50:LEU:O     | 7:SJ:54:ARG:HG3    | 2.10                     | 0.52              |
| 10:SA:85:ARG:HG2  | 10:SA:89:LYS:HZ3   | 1.74                     | 0.52              |
| 11:SB:219:LYS:NZ  | 61:Lp:91:ASP:O     | 2.42                     | 0.52              |
| 14:Sa:7:ASN:ND2   | 14:Sa:10:ARG:O     | 2.42                     | 0.52              |
| 15:SC:78:LEU:O    | 15:SC:81:ILE:HG12  | 2.08                     | 0.52              |
| 16:SN:48:SER:O    | 16:SN:52:VAL:HG13  | 2.08                     | 0.52              |
| 16:SN:115:LEU:O   | 16:SN:119:GLU:HG2  | 2.09                     | 0.52              |
| 85:L5:254:G:H2'   | 85:L5:255:C:O4'    | 2.09                     | 0.52              |
| 85:L5:263:G:N7    | 85:L5:264:C:N4     | 2.57                     | 0.52              |
| 85:L5:735:G:H4'   | 33:LM:74:ARG:HH22  | 1.74                     | 0.52              |
| 85:L5:1079:C:H2'  | 85:L5:1080:C:H6    | 1.74                     | 0.52              |
| 85:L5:1275:G:H2'  | 85:L5:1276:C:H6    | 1.73                     | 0.52              |
| 85:L5:1907:A:H4'  | 27:LF:223:LYS:HD3  | 1.92                     | 0.52              |
| 85:L5:1973:G:O2'  | 84:Lt:78:SER:HB3   | 2.09                     | 0.52              |
| 85:L5:2293:U:H2'  | 85:L5:2294:G:C8    | 2.45                     | 0.52              |
| 85:L5:2671:C:H2'  | 85:L5:2672:C:C6    | 2.44                     | 0.52              |
| 85:L5:2902:G:N7   | 85:L5:2903:G:N2    | 2.58                     | 0.52              |
| 85:L5:4063:U:H2'  | 85:L5:4064:C:N1    | 2.25                     | 0.52              |
| 85:L5:4359:U:OP1  | 32:LL:197:LYS:NZ   | 2.42                     | 0.52              |
| 85:L5:4372:U:OP2  | 60:Lo:61:LYS:HG2   | 2.09                     | 0.52              |
| 85:L5:4604:G:P    | 29:LH:174:LYS:HZ1  | 2.32                     | 0.52              |
| 85:L5:5055:G:H2'  | 85:L5:5056:A:H8    | 1.74                     | 0.52              |
| 21:L8:111:U:H5'   | 21:L8:112:G:H5'    | 1.91                     | 0.52              |
| 23:LB:115:LYS:NZ  | 23:LB:129:ALA:O    | 2.42                     | 0.52              |
| 26:LE:67:ALA:HA   | 26:LE:69:TYR:CE2   | 2.45                     | 0.52              |
| 26:LE:141:ARG:H   | 26:LE:191:GLN:HE22 | 1.56                     | 0.52              |
| 27:LF:226:HIS:HD2 | 27:LF:228:VAL:H    | 1.58                     | 0.52              |
| 28:LG:85:GLN:OE1  | 28:LG:85:GLN:N     | 2.38                     | 0.52              |
| 29:LH:26:ILE:HG22 | 29:LH:35:ARG:HB3   | 1.91                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 33:LM:55:MET:N     | 33:LM:55:MET:SD    | 2.81                     | 0.52              |
| 35:LO:62:MET:HE1   | 35:LO:65:ASN:O     | 2.09                     | 0.52              |
| 38:LR:15:LEU:HD21  | 38:LR:52:ARG:HB2   | 1.91                     | 0.52              |
| 43:LX:80:PRO:HG2   | 43:LX:155:ILE:HG21 | 1.91                     | 0.52              |
| 46:La:36:GLY:HA3   | 46:La:40:HIS:CD2   | 2.44                     | 0.52              |
| 52:Lg:78:TYR:HB3   | 52:Lg:82:MET:HB2   | 1.90                     | 0.52              |
| 55:Lj:74:PHE:HA    | 55:Lj:78:PHE:HE2   | 1.74                     | 0.52              |
| 70:SS:86:ARG:HB3   | 70:SS:89:ASP:OD1   | 2.08                     | 0.52              |
| 72:SU:18:HIS:ND1   | 72:SU:94:PRO:HA    | 2.23                     | 0.52              |
| 75:Sg:153:CYS:O    | 75:Sg:168:CYS:HB3  | 2.09                     | 0.52              |
| 76:SM:54:SER:OG    | 76:SM:80:ASP:O     | 2.28                     | 0.52              |
| 79:S2:1806:A:H2'   | 79:S2:1807:C:C6    | 2.45                     | 0.52              |
| 4:sL:97:ARG:NH2    | 79:s2:420:G:O3'    | 2.42                     | 0.52              |
| 4:sL:132:ARG:HE    | 79:s2:383:G:H4'    | 1.73                     | 0.52              |
| 5:sX:121:LYS:NZ    | 79:s2:647:U:O2'    | 2.39                     | 0.52              |
| 7:sJ:86:VAL:HG11   | 7:sJ:105:PHE:CD2   | 2.45                     | 0.52              |
| 10:sA:65:ILE:HG22  | 10:sA:74:VAL:HG21  | 1.91                     | 0.52              |
| 11:sB:179:ASN:HB2  | 11:sB:183:GLU:HB2  | 1.92                     | 0.52              |
| 14:sa:13:LYS:HE2   | 79:s2:1133:A:C4'   | 2.40                     | 0.52              |
| 14:sa:97:PRO:HB2   | 79:s2:1868:U:C2    | 2.43                     | 0.52              |
| 17:sO:143:LYS:HB2  | 79:s2:1047:C:H5'   | 1.90                     | 0.52              |
| 24:lC:205:ARG:NH1  | 85:l5:2297:G:OP1   | 2.41                     | 0.52              |
| 25:lD:39:GLN:OE1   | 25:lD:40:ASP:N     | 2.38                     | 0.52              |
| 26:lE:218:LYS:NZ   | 85:l5:1289:C:OP1   | 2.31                     | 0.52              |
| 35:lO:3:GLU:OE1    | 35:lO:31:ARG:NH2   | 2.42                     | 0.52              |
| 37:lQ:6:ARG:NH2    | 37:lQ:8:ASN:HD21   | 2.08                     | 0.52              |
| 40:lT:81:LYS:HB2   | 47:lb:16:TRP:CZ3   | 2.44                     | 0.52              |
| 46:la:100:ILE:HD11 | 46:la:123:ILE:HD12 | 1.90                     | 0.52              |
| 47:lb:13:SER:O     | 47:lb:17:HIS:HB2   | 2.10                     | 0.52              |
| 49:ld:96:GLU:OE2   | 49:ld:98:SER:OG    | 2.28                     | 0.52              |
| 53:lh:27:GLU:OE1   | 53:lh:31:LEU:HD22  | 2.10                     | 0.52              |
| 55:lj:12:ARG:NH2   | 85:l5:1617:G:O3'   | 2.42                     | 0.52              |
| 63:lz:47:LYS:O     | 63:lz:48:ARG:NH1   | 2.43                     | 0.52              |
| 67:sK:80:ARG:NH2   | 67:sK:90:VAL:HA    | 2.23                     | 0.52              |
| 69:sQ:94:ALA:O     | 69:sQ:97:GLN:HG3   | 2.10                     | 0.52              |
| 72:sU:35:VAL:HG11  | 72:sU:107:GLU:HG2  | 1.91                     | 0.52              |
| 72:sU:37:ALA:O     | 72:sU:41:ARG:HG2   | 2.09                     | 0.52              |
| 78:sf:120:GLU:HG2  | 78:sf:128:ALA:HA   | 1.90                     | 0.52              |
| 79:s2:1121:G:C6    | 79:s2:1122:A:C5    | 2.98                     | 0.52              |
| 79:s2:1511:U:H2'   | 79:s2:1512:C:C6    | 2.44                     | 0.52              |
| 79:s2:1639:G:N3    | 82:pE:41:U:O2'     | 2.42                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 80:cB:451:ILE:HD11 | 80:cB:473:VAL:HG12 | 1.91                     | 0.52              |
| 82:pE:19:G:N2      | 82:pE:57:A:H1'     | 2.24                     | 0.52              |
| 85:l5:268:G:H2'    | 85:l5:269:G:C8     | 2.45                     | 0.52              |
| 85:l5:1194:G:H2'   | 85:l5:1195:G:H8    | 1.73                     | 0.52              |
| 85:l5:1507:C:H2'   | 85:l5:1508:A:H8    | 1.75                     | 0.52              |
| 85:l5:1541:C:H1'   | 85:l5:2448:G:H21   | 1.73                     | 0.52              |
| 85:l5:2019:C:H2'   | 85:l5:2020:U:H6    | 1.74                     | 0.52              |
| 85:l5:2786:C:O2'   | 85:l5:2787:A:OP2   | 2.24                     | 0.52              |
| 85:l5:4481:U:H2'   | 85:l5:4482:U:C6    | 2.44                     | 0.52              |
| 80:CB:117:ALA:HA   | 80:CB:497:MET:HE1  | 1.91                     | 0.52              |
| 2:SE:63:LYS:O      | 2:SE:67:GLN:HG3    | 2.10                     | 0.52              |
| 8:SY:112:ASN:HA    | 8:SY:115:LYS:HG2   | 1.91                     | 0.52              |
| 15:SC:69:LEU:HD22  | 15:SC:269:PHE:HD1  | 1.75                     | 0.52              |
| 17:SO:84:ARG:HD3   | 17:SO:88:LEU:HD23  | 1.92                     | 0.52              |
| 17:SO:147:ARG:HB2  | 17:SO:150:ARG:HH21 | 1.75                     | 0.52              |
| 19:Sb:53:VAL:HG22  | 19:Sb:64:CYS:O     | 2.10                     | 0.52              |
| 85:L5:271:C:H2'    | 85:L5:272:U:C6     | 2.43                     | 0.52              |
| 85:L5:351:C:H2'    | 85:L5:352:G:C8     | 2.44                     | 0.52              |
| 85:L5:1786:A:O2'   | 85:L5:1788:A:OP2   | 2.23                     | 0.52              |
| 85:L5:1807:C:O3'   | 40:LT:110:LYS:NZ   | 2.38                     | 0.52              |
| 85:L5:2610:G:H2'   | 85:L5:2611:A:C8    | 2.44                     | 0.52              |
| 85:L5:3594:C:H2'   | 85:L5:3597:G:N3    | 2.25                     | 0.52              |
| 85:L5:3684:G:H2'   | 85:L5:3685:C:C6    | 2.44                     | 0.52              |
| 85:L5:3954:A:O2'   | 85:L5:3955:G:O5'   | 2.27                     | 0.52              |
| 85:L5:4101:C:O5'   | 85:L5:4107:G:P     | 2.68                     | 0.52              |
| 85:L5:4261:C:H2'   | 85:L5:4262:C:H6    | 1.74                     | 0.52              |
| 85:L5:4578:G:H2'   | 85:L5:4579:U:C6    | 2.45                     | 0.52              |
| 85:L5:4723:A:H2'   | 85:L5:4724:A:C8    | 2.44                     | 0.52              |
| 85:L5:5051:C:H2'   | 85:L5:5052:C:C6    | 2.45                     | 0.52              |
| 20:L7:4:U:H2'      | 20:L7:5:A:C8       | 2.45                     | 0.52              |
| 21:L8:94:G:H21     | 55:Lj:82:THR:HB    | 1.75                     | 0.52              |
| 21:L8:141:C:H2'    | 21:L8:142:U:H6     | 1.72                     | 0.52              |
| 22:LA:63:PHE:N     | 22:LA:72:ARG:O     | 2.43                     | 0.52              |
| 23:LB:285:TYR:CZ   | 23:LB:334:LYS:HB2  | 2.45                     | 0.52              |
| 25:LD:53:VAL:O     | 25:LD:54:ARG:NH1   | 2.42                     | 0.52              |
| 30:LI:76:MET:SD    | 30:LI:151:ALA:HB2  | 2.49                     | 0.52              |
| 34:LN:53:TYR:HE2   | 34:LN:55:ALA:HA    | 1.75                     | 0.52              |
| 45:LZ:7:PRO:HA     | 45:LZ:25:ILE:HG23  | 1.92                     | 0.52              |
| 56:Lk:25:ILE:HB    | 56:Lk:68:GLU:HG2   | 1.91                     | 0.52              |
| 65:SD:225:GLU:HB2  | 75:Sg:187:ASN:HB3  | 1.92                     | 0.52              |
| 69:SQ:31:LEU:HD21  | 69:SQ:69:ARG:NH2   | 2.25                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 71:ST:27:LYS:HZ1   | 71:ST:110:LEU:HD23 | 1.74                     | 0.52              |
| 75:Sg:12:LYS:NZ    | 75:Sg:13:GLY:O     | 2.42                     | 0.52              |
| 75:Sg:149:GLU:CD   | 75:Sg:150:TRP:H    | 2.18                     | 0.52              |
| 79:S2:1103:C:H2'   | 79:S2:1104:G:C8    | 2.45                     | 0.52              |
| 79:S2:1198:G:H2'   | 79:S2:1199:A:H8    | 1.72                     | 0.52              |
| 79:S2:1533:A:H2    | 79:S2:1536:G:N3    | 2.08                     | 0.52              |
| 1:CH:99:ILE:HG22   | 1:CH:101:GLU:HG2   | 1.91                     | 0.52              |
| 6:sG:32:MET:HE2    | 6:sG:100:CYS:HB2   | 1.92                     | 0.52              |
| 6:sG:126:ASP:OD1   | 6:sG:126:ASP:N     | 2.43                     | 0.52              |
| 7:sJ:41:ARG:NH2    | 79:s2:642:U:O3'    | 2.42                     | 0.52              |
| 10:sA:85:ARG:HA    | 10:sA:88:LEU:HG    | 1.90                     | 0.52              |
| 10:sA:176:TRP:CZ2  | 10:sA:199:PRO:HD3  | 2.44                     | 0.52              |
| 11:sB:133:TYR:CD2  | 11:sB:181:LEU:HD22 | 2.45                     | 0.52              |
| 12:sH:83:LEU:HD22  | 12:sH:92:VAL:HG11  | 1.91                     | 0.52              |
| 29:IH:28:LYS:NZ    | 29:IH:33:THR:HB    | 2.25                     | 0.52              |
| 29:IH:146:LEU:HD23 | 29:IH:146:LEU:H    | 1.75                     | 0.52              |
| 31:IJ:35:ARG:O     | 31:IJ:39:VAL:HG13  | 2.10                     | 0.52              |
| 32:IL:176:PHE:HZ   | 46:la:146:LEU:HD12 | 1.74                     | 0.52              |
| 37:IQ:53:MET:SD    | 37:IQ:53:MET:N     | 2.70                     | 0.52              |
| 38:IR:103:ARG:HG2  | 38:IR:124:TYR:CE2  | 2.43                     | 0.52              |
| 39:IS:170:LYS:NZ   | 85:l5:4875:G:OP1   | 2.41                     | 0.52              |
| 43:IX:78:LYS:HG3   | 43:IX:100:VAL:HA   | 1.92                     | 0.52              |
| 43:IX:79:PHE:CE2   | 43:IX:99:ILE:HG21  | 2.45                     | 0.52              |
| 50:le:53:ILE:HD12  | 50:le:54:LEU:H     | 1.74                     | 0.52              |
| 52:lg:43:LYS:NZ    | 85:l5:2597:G:H5''  | 2.25                     | 0.52              |
| 60:lo:82:MET:HE1   | 85:l5:4345:C:O2'   | 2.09                     | 0.52              |
| 63:lz:84:HIS:O     | 63:lz:85:MET:HE2   | 2.10                     | 0.52              |
| 64:sR:5:ARG:HG2    | 64:sR:9:VAL:CG2    | 2.39                     | 0.52              |
| 68:sP:93:MET:HE1   | 68:sP:104:GLN:OE1  | 2.08                     | 0.52              |
| 79:s2:811:A:H2'    | 79:s2:812:A:H8     | 1.75                     | 0.52              |
| 79:s2:911:C:H2'    | 79:s2:912:C:C6     | 2.44                     | 0.52              |
| 79:s2:977:C:H2'    | 79:s2:978:G:O4'    | 2.09                     | 0.52              |
| 79:s2:1033:G:H22   | 79:s2:1080:A:HO2'  | 1.58                     | 0.52              |
| 79:s2:1452:A:O4'   | 79:s2:1453:C:C2    | 2.62                     | 0.52              |
| 80:cB:192:TYR:CZ   | 80:cB:780:PRO:HG2  | 2.45                     | 0.52              |
| 82:pE:15:G:H22     | 82:pE:21:A:H1'     | 1.74                     | 0.52              |
| 85:l5:138:G:H2'    | 85:l5:139:G:H8     | 1.75                     | 0.52              |
| 85:l5:287:U:H2'    | 85:l5:288:G:C8     | 2.45                     | 0.52              |
| 85:l5:458:C:H2'    | 85:l5:459:C:C6     | 2.45                     | 0.52              |
| 85:l5:1481:C:O2'   | 85:l5:1482:G:O5'   | 2.28                     | 0.52              |
| 85:l5:1643:A:H2'   | 85:l5:1644:C:H6    | 1.75                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 85:L5:3771:C:O2'   | 85:L5:3772:U:H5'   | 2.10                     | 0.52              |
| 80:CB:263:ASP:OD1  | 80:CB:287:ARG:NH1  | 2.42                     | 0.52              |
| 80:CB:396:MET:HG3  | 80:CB:415:ARG:O    | 2.09                     | 0.52              |
| 2:SE:18:TRP:CH2    | 2:SE:31:PRO:HD3    | 2.43                     | 0.52              |
| 2:SE:87:MET:HE1    | 2:SE:123:LEU:H     | 1.75                     | 0.52              |
| 3:SI:98:LYS:HB3    | 79:S2:377:G:H5'    | 1.89                     | 0.52              |
| 8:SY:62:THR:HA     | 8:SY:69:THR:HA     | 1.90                     | 0.52              |
| 11:SB:87:ILE:HB    | 11:SB:101:HIS:CG   | 2.45                     | 0.52              |
| 16:SN:29:THR:OG1   | 16:SN:32:ASP:OD2   | 2.22                     | 0.52              |
| 85:L5:162:A:H2'    | 85:L5:163:A:H8     | 1.73                     | 0.52              |
| 85:L5:210:C:H5'    | 85:L5:235:A:C2     | 2.45                     | 0.52              |
| 85:L5:423:G:H2'    | 85:L5:424:U:C6     | 2.44                     | 0.52              |
| 85:L5:921:C:H2'    | 85:L5:922:C:C6     | 2.44                     | 0.52              |
| 85:L5:1426:G:N1    | 85:L5:1458:C:OP2   | 2.43                     | 0.52              |
| 85:L5:1631:A:C4    | 22:LA:204:MET:HE1  | 2.44                     | 0.52              |
| 85:L5:1919:G:N2    | 39:LS:166:ARG:HB2  | 2.24                     | 0.52              |
| 85:L5:2630:U:H5''  | 41:LU:48:LYS:HZ3   | 1.75                     | 0.52              |
| 85:L5:4096:C:O3'   | 85:L5:4111:U:O2    | 2.27                     | 0.52              |
| 85:L5:4689:U:H2'   | 85:L5:4690:G:O4'   | 2.10                     | 0.52              |
| 85:L5:4736:C:H4'   | 85:L5:5068:G:C4    | 2.44                     | 0.52              |
| 85:L5:4891:G:H3'   | 85:L5:4892:A:H2    | 1.73                     | 0.52              |
| 25:LD:200:MET:HE3  | 25:LD:240:TYR:HD2  | 1.74                     | 0.52              |
| 30:LI:89:VAL:HG12  | 30:LI:136:MET:HG2  | 1.91                     | 0.52              |
| 30:LI:169:LYS:HZ3  | 30:LI:179:ASP:HB3  | 1.75                     | 0.52              |
| 34:LN:149:GLN:O    | 34:LN:152:THR:OG1  | 2.26                     | 0.52              |
| 36:LP:36:ILE:O     | 36:LP:39:MET:HE3   | 2.09                     | 0.52              |
| 39:LS:127:MET:SD   | 40:LT:153:PRO:HG2  | 2.50                     | 0.52              |
| 43:LX:150:ALA:HA   | 43:LX:153:ILE:HG12 | 1.92                     | 0.52              |
| 48:Lc:40:GLN:HB2   | 48:Lc:42:LYS:HZ2   | 1.73                     | 0.52              |
| 79:S2:1125:C:H2'   | 79:S2:1126:G:O4'   | 2.10                     | 0.52              |
| 79:S2:1651:A:H2'   | 79:S2:1652:G:H8    | 1.75                     | 0.52              |
| 83:Ls:40:MET:SD    | 83:Ls:41:GLN:N     | 2.83                     | 0.52              |
| 87:LW:101:ARG:HD3  | 87:LW:104:GLN:OE1  | 2.10                     | 0.52              |
| 1:cH:64:GLU:OE2    | 1:cH:66:GLU:N      | 2.42                     | 0.52              |
| 4:sL:47:PRO:HG2    | 4:sL:50:ALA:HB2    | 1.92                     | 0.52              |
| 4:sL:71:ARG:NH1    | 79:s2:855:G:O2'    | 2.43                     | 0.52              |
| 10:sA:118:GLU:HB3  | 15:sC:65:LYS:HD2   | 1.92                     | 0.52              |
| 10:sA:144:THR:HG23 | 10:sA:157:VAL:HA   | 1.91                     | 0.52              |
| 11:sB:70:SER:OG    | 11:sB:73:ASP:OD1   | 2.22                     | 0.52              |
| 12:sH:52:GLU:N     | 12:sH:52:GLU:OE2   | 2.43                     | 0.52              |
| 13:sV:10:ASP:OD1   | 13:sV:10:ASP:N     | 2.39                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 18:sW:5:ASN:OD1    | 18:sW:7:LEU:HG     | 2.09                     | 0.52              |
| 20:l7:89:G:H8      | 20:l7:89:G:OP2     | 1.92                     | 0.52              |
| 24:lC:209:ILE:HG21 | 24:lC:221:PHE:HE2  | 1.75                     | 0.52              |
| 26:lE:48:PRO:HD2   | 26:lE:56:ARG:HB2   | 1.90                     | 0.52              |
| 28:lG:177:MET:HE1  | 28:lG:179:VAL:N    | 2.24                     | 0.52              |
| 34:lN:77:LYS:NZ    | 85:l5:4185:G:O2'   | 2.42                     | 0.52              |
| 34:lN:190:ALA:HA   | 34:lN:193:ARG:HE   | 1.74                     | 0.52              |
| 35:lO:62:MET:HE3   | 35:lO:70:PRO:CD    | 2.34                     | 0.52              |
| 37:lQ:33:ARG:HA    | 37:lQ:48:LEU:HD22  | 1.92                     | 0.52              |
| 38:lR:177:LEU:O    | 38:lR:181:LYS:HG3  | 2.10                     | 0.52              |
| 39:lS:14:GLY:HA2   | 39:lS:62:VAL:HG22  | 1.91                     | 0.52              |
| 39:lS:95:ARG:NH2   | 39:lS:113:MET:SD   | 2.83                     | 0.52              |
| 49:ld:90:ARG:HD2   | 49:ld:102:LEU:HD21 | 1.91                     | 0.52              |
| 49:ld:96:GLU:N     | 49:ld:96:GLU:OE1   | 2.42                     | 0.52              |
| 54:li:52:PRO:HA    | 54:li:55:ARG:CG    | 2.39                     | 0.52              |
| 60:lo:37:GLY:HA3   | 85:l5:4342:C:O3'   | 2.09                     | 0.52              |
| 63:lz:32:VAL:HG11  | 63:lz:172:VAL:HG23 | 1.92                     | 0.52              |
| 63:lz:104:ALA:O    | 63:lz:133:LYS:NZ   | 2.23                     | 0.52              |
| 68:sP:18:ARG:NH1   | 70:sS:88:LYS:O     | 2.42                     | 0.52              |
| 69:sQ:23:ALA:HB2   | 69:sQ:70:VAL:HB    | 1.92                     | 0.52              |
| 70:sS:22:GLY:HA2   | 70:sS:56:ALA:HB3   | 1.92                     | 0.52              |
| 73:sc:17:VAL:HG13  | 73:sc:29:GLN:O     | 2.08                     | 0.52              |
| 74:sd:26:ASN:ND2   | 79:s2:1495:G:H4'   | 2.25                     | 0.52              |
| 75:sg:241:PHE:CG   | 75:sg:248:LEU:HD13 | 2.45                     | 0.52              |
| 76:sM:59:PRO:HD2   | 76:sM:60:MET:SD    | 2.50                     | 0.52              |
| 79:s2:15:U:O2'     | 79:s2:669:A:N6     | 2.43                     | 0.52              |
| 79:s2:1811:C:H3'   | 79:s2:1812:U:H4'   | 1.92                     | 0.52              |
| 85:l5:492:U:H2'    | 85:l5:493:G:C8     | 2.45                     | 0.52              |
| 85:l5:1244:G:H2'   | 85:l5:1245:C:C6    | 2.45                     | 0.52              |
| 85:l5:1442:C:H42   | 85:l5:2104:G:H2'   | 1.73                     | 0.52              |
| 85:l5:1976:G:O6    | 85:l5:1991:A:N6    | 2.43                     | 0.52              |
| 85:l5:2505:C:N4    | 85:l5:4084:G:H4'   | 2.24                     | 0.52              |
| 85:l5:4039:G:H21   | 85:l5:4050:A:HO2'  | 1.57                     | 0.52              |
| 85:l5:4141:G:O2'   | 85:l5:4143:G:O6    | 2.27                     | 0.52              |
| 85:l5:4173:G:H2'   | 85:l5:4174:U:C6    | 2.45                     | 0.52              |
| 6:SG:3:LEU:N       | 6:SG:16:ILE:O      | 2.39                     | 0.52              |
| 6:SG:6:SER:HA      | 6:SG:13:GLN:HB3    | 1.91                     | 0.52              |
| 14:Sa:6:ARG:NE     | 79:S2:1147:C:OP1   | 2.35                     | 0.52              |
| 15:SC:263:LYS:HB3  | 15:SC:268:GLU:OE1  | 2.10                     | 0.52              |
| 16:SN:45:LEU:HB2   | 16:SN:50:ILE:HG23  | 1.91                     | 0.52              |
| 16:SN:142:GLU:HG3  | 16:SN:145:THR:H    | 1.75                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 18:SW:4:MET:HE2    | 79:S2:683:G:H4'    | 1.85                     | 0.52              |
| 85:L5:716:C:OP1    | 24:LC:317:ASN:HB2  | 2.10                     | 0.52              |
| 85:L5:1316:G:OP1   | 50:Le:43:ASN:HB2   | 2.10                     | 0.52              |
| 85:L5:2569:G:H2'   | 85:L5:2570:U:C6    | 2.43                     | 0.52              |
| 85:L5:2571:C:H2'   | 85:L5:2572:C:C6    | 2.44                     | 0.52              |
| 85:L5:2667:C:OP1   | 38:LR:100:ARG:NH2  | 2.42                     | 0.52              |
| 85:L5:4096:C:C2    | 85:L5:4110:C:H2'   | 2.45                     | 0.52              |
| 85:L5:4188:U:H2'   | 85:L5:4189:U:H6    | 1.75                     | 0.52              |
| 85:L5:4219:A:H2'   | 85:L5:4220:A:C8    | 2.44                     | 0.52              |
| 85:L5:4263:C:H2'   | 85:L5:4264:G:O4'   | 2.10                     | 0.52              |
| 85:L5:5025:C:N4    | 85:L5:5027:C:N3    | 2.58                     | 0.52              |
| 22:LA:62:VAL:HG23  | 22:LA:73:THR:HG22  | 1.92                     | 0.52              |
| 24:LC:25:PRO:HD2   | 24:LC:257:PHE:HE2  | 1.75                     | 0.52              |
| 24:LC:110:ARG:HA   | 34:LN:204:ARG:HH21 | 1.75                     | 0.52              |
| 24:LC:325:MET:HE2  | 24:LC:328:LEU:HD12 | 1.92                     | 0.52              |
| 54:Li:40:VAL:O     | 54:Li:44:ILE:HG22  | 2.09                     | 0.52              |
| 65:SD:76:ARG:HB2   | 67:SK:22:VAL:HG21  | 1.91                     | 0.52              |
| 65:SD:101:GLN:HG2  | 65:SD:126:ILE:HD11 | 1.91                     | 0.52              |
| 67:SK:3:MET:SD     | 67:SK:7:ASN:HB2    | 2.50                     | 0.52              |
| 69:SQ:51:LEU:HD22  | 69:SQ:84:ILE:HD11  | 1.90                     | 0.52              |
| 74:Sd:19:ARG:HD3   | 74:Sd:32:ARG:CD    | 2.37                     | 0.52              |
| 79:S2:57:U:H1'     | 79:S2:499:G:H1'    | 1.92                     | 0.52              |
| 79:S2:647:U:H2'    | 79:S2:648:A:H8     | 1.75                     | 0.52              |
| 79:S2:996:A:H2'    | 79:S2:997:A:C8     | 2.44                     | 0.52              |
| 81:AP:58:A:O2'     | 81:AP:60:A:OP2     | 2.22                     | 0.52              |
| 83:Ls:160:LEU:HD23 | 83:Ls:161:ILE:HB   | 1.92                     | 0.52              |
| 84:Lt:106:PHE:O    | 84:Lt:110:VAL:HG13 | 2.10                     | 0.52              |
| 9:se:34:ARG:HA     | 9:se:37:GLN:NE2    | 2.24                     | 0.52              |
| 11:sB:38:MET:HE3   | 11:sB:186:ASN:HB3  | 1.92                     | 0.52              |
| 12:sH:10:LYS:HE2   | 12:sH:17:ASP:HB3   | 1.91                     | 0.52              |
| 22:IA:44:ILE:O     | 22:IA:44:ILE:HG13  | 2.10                     | 0.52              |
| 24:IC:128:LEU:O    | 24:IC:131:SER:OG   | 2.25                     | 0.52              |
| 24:IC:140:LYS:NZ   | 24:IC:242:PRO:HD2  | 2.25                     | 0.52              |
| 25:ID:14:LYS:O     | 40:IT:20:ARG:NH2   | 2.43                     | 0.52              |
| 25:ID:279:ARG:NH2  | 85:I5:1177:U:OP1   | 2.43                     | 0.52              |
| 26:IE:180:VAL:HG23 | 85:I5:4935:C:H5    | 1.74                     | 0.52              |
| 31:IJ:37:ALA:O     | 31:IJ:40:LEU:HB2   | 2.10                     | 0.52              |
| 34:IN:120:TRP:CZ3  | 85:I5:280:G:H5'    | 2.43                     | 0.52              |
| 34:IN:204:ARG:HD2  | 85:I5:1342:A:OP1   | 2.10                     | 0.52              |
| 35:IO:21:ALA:HA    | 35:IO:87:MET:HE3   | 1.92                     | 0.52              |
| 37:IQ:66:MET:O     | 37:IQ:70:MET:HG2   | 2.10                     | 0.52              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 38:IR:172:ARG:O    | 38:IR:175:GLU:HG3 | 2.10                     | 0.52              |
| 43:IX:87:MET:HA    | 43:IX:90:ILE:HB   | 1.91                     | 0.52              |
| 43:IX:107:HIS:O    | 43:IX:111:GLN:HG2 | 2.10                     | 0.52              |
| 45:IZ:51:ARG:NH1   | 85:I5:2755:A:OP2  | 2.38                     | 0.52              |
| 55:Ij:28:HIS:ND1   | 55:Ij:31:LYS:HG3  | 2.24                     | 0.52              |
| 57:Il:5:LYS:NZ     | 85:I5:2781:G:O3'  | 2.42                     | 0.52              |
| 68:sP:89:MET:O     | 68:sP:92:SER:OG   | 2.22                     | 0.52              |
| 68:sP:111:MET:HG2  | 68:sP:119:PHE:HZ  | 1.75                     | 0.52              |
| 70:sS:70:ILE:HD12  | 70:sS:77:TYR:CZ   | 2.44                     | 0.52              |
| 71:sT:33:TRP:C     | 71:sT:33:TRP:CD1  | 2.88                     | 0.52              |
| 77:sZ:82:SER:OG    | 79:s2:1598:G:OP2  | 2.26                     | 0.52              |
| 79:s2:91:A:OP1     | 79:s2:446:G:N2    | 2.39                     | 0.52              |
| 79:s2:1512:C:H2'   | 79:s2:1513:C:H6   | 1.75                     | 0.52              |
| 79:s2:1687:C:H2'   | 79:s2:1688:C:C6   | 2.45                     | 0.52              |
| 79:s2:1713:C:H2'   | 79:s2:1714:U:C6   | 2.45                     | 0.52              |
| 80:cB:349:ALA:HA   | 80:cB:352:GLN:OE1 | 2.10                     | 0.52              |
| 80:cB:404:THR:OG1  | 80:cB:406:ASP:OD1 | 2.22                     | 0.52              |
| 84:lt:125:LEU:O    | 84:lt:128:THR:OG1 | 2.21                     | 0.52              |
| 85:I5:162:A:H2'    | 85:I5:163:A:C8    | 2.44                     | 0.52              |
| 85:I5:2318:G:N1    | 85:I5:2322:G:C6   | 2.78                     | 0.52              |
| 85:I5:2784:C:H2'   | 85:I5:2785:C:H6   | 1.74                     | 0.52              |
| 85:I5:4140:C:N3    | 85:I5:4145:C:O2'  | 2.42                     | 0.52              |
| 85:I5:4968:A:H2'   | 85:I5:4969:C:H6   | 1.73                     | 0.52              |
| 80:CB:222:ALA:O    | 80:CB:344:LEU:HB3 | 2.09                     | 0.52              |
| 80:CB:409:ARG:HH22 | 79:S2:478:G:H5'   | 1.74                     | 0.52              |
| 4:SL:106:HIS:NE2   | 79:S2:397:G:OP1   | 2.43                     | 0.52              |
| 5:SX:134:TYR:OH    | 86:Se:13:ARG:NE   | 2.42                     | 0.52              |
| 6:SG:194:LEU:O     | 6:SG:197:GLN:NE2  | 2.42                     | 0.52              |
| 15:SC:272:HIS:CG   | 15:SC:275:LYS:NZ  | 2.78                     | 0.52              |
| 17:SO:75:MET:HE1   | 66:SF:204:ARG:NH1 | 2.25                     | 0.52              |
| 85:L5:83:C:O2'     | 85:L5:100:C:N4    | 2.43                     | 0.52              |
| 85:L5:123:C:H2'    | 85:L5:124:C:C6    | 2.45                     | 0.52              |
| 85:L5:133:C:H2'    | 85:L5:134:G:H4'   | 1.91                     | 0.52              |
| 85:L5:419:A:H61    | 21:L8:15:G:H1'    | 1.74                     | 0.52              |
| 85:L5:1354:A:N6    | 85:L5:1503:A:O4'  | 2.43                     | 0.52              |
| 85:L5:1397:A:C8    | 46:La:114:LYS:HB2 | 2.44                     | 0.52              |
| 85:L5:1482:G:N7    | 54:Li:4:ARG:NH2   | 2.49                     | 0.52              |
| 85:L5:2413:U:H2'   | 85:L5:2414:G:H8   | 1.75                     | 0.52              |
| 85:L5:2638:G:N1    | 85:L5:2718:U:H2'  | 2.24                     | 0.52              |
| 85:L5:2673:G:C8    | 48:Lc:29:LEU:HD11 | 2.45                     | 0.52              |
| 85:L5:4121:G:N2    | 22:LA:46:LYS:HD3  | 2.25                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 85:L5:4581:G:H5'   | 23:LB:28:LYS:HZ3   | 1.75                     | 0.52              |
| 21:L8:27:U:H2'     | 21:L8:28:C:C6      | 2.44                     | 0.52              |
| 25:LD:108:ARG:CZ   | 25:LD:253:TYR:HB2  | 2.39                     | 0.52              |
| 29:LH:132:VAL:HG13 | 29:LH:154:VAL:HG12 | 1.92                     | 0.52              |
| 30:LI:52:MET:O     | 30:LI:135:ILE:N    | 2.24                     | 0.52              |
| 33:LM:28:VAL:CG1   | 33:LM:37:LEU:HD22  | 2.39                     | 0.52              |
| 36:LP:36:ILE:O     | 36:LP:114:ILE:HD11 | 2.10                     | 0.52              |
| 37:LQ:21:GLN:OE1   | 37:LQ:26:ARG:NH2   | 2.43                     | 0.52              |
| 53:Lh:91:MET:HA    | 53:Lh:94:ARG:HG2   | 1.92                     | 0.52              |
| 58:Lm:96:CYS:HB2   | 58:Lm:110:CYS:SG   | 2.48                     | 0.52              |
| 64:SR:23:ARG:O     | 64:SR:23:ARG:NH1   | 2.43                     | 0.52              |
| 66:SF:40:ALA:HB1   | 66:SF:67:PRO:HA    | 1.90                     | 0.52              |
| 66:SF:112:LEU:HD13 | 66:SF:177:LEU:HD11 | 1.90                     | 0.52              |
| 68:SP:54:HIS:O     | 68:SP:57:LEU:HG    | 2.10                     | 0.52              |
| 76:SM:79:VAL:HG22  | 76:SM:80:ASP:H     | 1.75                     | 0.52              |
| 77:SZ:99:LEU:HD12  | 77:SZ:100:VAL:H    | 1.74                     | 0.52              |
| 79:S2:509:G:H2'    | 79:S2:510:G:H8     | 1.75                     | 0.52              |
| 79:S2:959:G:H2'    | 79:S2:960:U:C6     | 2.45                     | 0.52              |
| 79:S2:1324:G:N2    | 79:S2:1504:U:O2    | 2.26                     | 0.52              |
| 82:PE:22:G:H2'     | 82:PE:23:A:C8      | 2.45                     | 0.52              |
| 2:sE:43:PRO:HB2    | 2:sE:45:ILE:HG22   | 1.92                     | 0.52              |
| 2:sE:52:LEU:HG     | 2:sE:54:TYR:HB2    | 1.91                     | 0.52              |
| 6:sG:32:MET:HE3    | 6:sG:65:GLN:NE2    | 2.25                     | 0.52              |
| 6:sG:116:LYS:HE2   | 6:sG:125:THR:HG21  | 1.91                     | 0.52              |
| 10:sA:88:LEU:HD21  | 10:sA:100:ALA:HB2  | 1.92                     | 0.52              |
| 10:sA:145:ILE:HG13 | 10:sA:159:ILE:HB   | 1.92                     | 0.52              |
| 12:sH:129:ILE:HD11 | 12:sH:177:TYR:CE1  | 2.45                     | 0.52              |
| 12:sH:166:VAL:HA   | 12:sH:169:LYS:NZ   | 2.24                     | 0.52              |
| 17:sO:103:ASN:ND2  | 17:sO:142:ARG:HA   | 2.24                     | 0.52              |
| 20:l7:12:U:O3'     | 20:l7:109:U:O2'    | 2.21                     | 0.52              |
| 21:l8:65:A:C4      | 21:l8:66:A:C8      | 2.97                     | 0.52              |
| 26:lE:94:LYS:HD3   | 26:lE:107:VAL:CG2  | 2.36                     | 0.52              |
| 26:lE:168:LEU:HD21 | 26:lE:174:LEU:HD12 | 1.92                     | 0.52              |
| 26:lE:178:PRO:O    | 26:lE:181:LEU:N    | 2.34                     | 0.52              |
| 27:lF:41:MET:SD    | 27:lF:41:MET:C     | 2.93                     | 0.52              |
| 33:lM:83:ASN:OD1   | 33:lM:83:ASN:N     | 2.39                     | 0.52              |
| 57:ll:10:LYS:NZ    | 85:l5:2782:U:OP2   | 2.43                     | 0.52              |
| 62:lr:90:LEU:CD1   | 62:lr:111:ILE:HG23 | 2.39                     | 0.52              |
| 63:lz:208:SER:N    | 63:lz:211:GLY:HA3  | 2.24                     | 0.52              |
| 64:sR:8:THR:O      | 64:sR:11:LYS:HB3   | 2.10                     | 0.52              |
| 65:sD:76:ARG:C     | 65:sD:76:ARG:HH11  | 2.18                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 66:sF:60:ARG:HG2   | 79:s2:1679:A:C2    | 2.45                     | 0.52              |
| 69:sQ:9:SER:N      | 69:sQ:99:TYR:OH    | 2.42                     | 0.52              |
| 71:sT:138:VAL:O    | 71:sT:142:ASN:ND2  | 2.42                     | 0.52              |
| 76:sM:37:GLU:OE1   | 76:sM:37:GLU:N     | 2.26                     | 0.52              |
| 76:sM:41:ALA:C     | 76:sM:44:LYS:HZ2   | 2.18                     | 0.52              |
| 77:sZ:66:LYS:HB2   | 77:sZ:110:THR:HG23 | 1.92                     | 0.52              |
| 79:s2:853:C:C2     | 79:s2:854:A:C8     | 2.98                     | 0.52              |
| 80:cB:434:TYR:HB2  | 80:cB:441:ASP:HB3  | 1.92                     | 0.52              |
| 80:cB:596:PRO:O    | 80:cB:598:LYS:NZ   | 2.34                     | 0.52              |
| 80:cB:770:VAL:HG22 | 80:cB:786:ALA:HB2  | 1.92                     | 0.52              |
| 85:l5:272:U:H2'    | 85:l5:273:U:C6     | 2.44                     | 0.52              |
| 85:l5:288:G:H2'    | 85:l5:289:C:H6     | 1.75                     | 0.52              |
| 85:l5:419:A:H2'    | 85:l5:420:A:C8     | 2.44                     | 0.52              |
| 85:l5:1187:G:H2'   | 85:l5:1188:C:C6    | 2.44                     | 0.52              |
| 85:l5:1468:C:H2'   | 85:l5:1469:C:C6    | 2.45                     | 0.52              |
| 85:l5:1473:U:H2'   | 85:l5:1474:C:C6    | 2.45                     | 0.52              |
| 85:l5:2045:G:O2'   | 85:l5:2046:G:H5''  | 2.10                     | 0.52              |
| 85:l5:2539:C:H2'   | 85:l5:2540:C:C6    | 2.44                     | 0.52              |
| 85:l5:4585:U:H2'   | 85:l5:4586:G:C8    | 2.45                     | 0.52              |
| 85:l5:4688:C:H2'   | 85:l5:4689:U:C6    | 2.45                     | 0.52              |
| 85:l5:4968:A:H2'   | 85:l5:4969:C:C6    | 2.45                     | 0.52              |
| 85:l5:5037:U:H2'   | 85:l5:5038:A:C8    | 2.44                     | 0.52              |
| 80:CB:208:VAL:HG13 | 80:CB:258:LYS:HA   | 1.91                     | 0.52              |
| 80:CB:328:LYS:HD2  | 6:SG:19:ASP:OD2    | 2.10                     | 0.52              |
| 80:CB:801:ARG:HB3  | 85:L5:4605:A:C4    | 2.44                     | 0.52              |
| 2:SE:38:LEU:HD22   | 79:S2:346:C:H5''   | 1.92                     | 0.52              |
| 5:SX:76:LYS:NZ     | 79:S2:481:C:O3'    | 2.42                     | 0.52              |
| 17:SO:42:VAL:CG1   | 17:SO:81:VAL:HG11  | 2.40                     | 0.52              |
| 19:Sb:19:HIS:O     | 19:Sb:23:ARG:NE    | 2.43                     | 0.52              |
| 19:Sb:83:GLN:NE2   | 19:Sb:84:HIS:O     | 2.43                     | 0.52              |
| 85:L5:114:G:H22    | 85:L5:158:A:H61    | 1.56                     | 0.52              |
| 85:L5:239:C:H5'    | 44:LY:33:PRO:HD3   | 1.91                     | 0.52              |
| 85:L5:494:U:H2'    | 85:L5:495:C:C6     | 2.44                     | 0.52              |
| 85:L5:1092:G:H2'   | 85:L5:1093:C:H6    | 1.72                     | 0.52              |
| 85:L5:1681:G:H2'   | 85:L5:1682:A:C8    | 2.45                     | 0.52              |
| 85:L5:2514:G:OP1   | 52:Lg:17:SER:OG    | 2.27                     | 0.52              |
| 85:L5:2605:G:H2'   | 85:L5:2606:G:C8    | 2.45                     | 0.52              |
| 85:L5:4603:C:O3'   | 29:LH:174:LYS:NZ   | 2.43                     | 0.52              |
| 85:L5:4716:C:H2'   | 85:L5:4717:A:C8    | 2.44                     | 0.52              |
| 24:LC:138:MET:HE2  | 24:LC:138:MET:HA   | 1.92                     | 0.52              |
| 24:LC:335:MET:SD   | 24:LC:335:MET:N    | 2.77                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:LD:63:GLN:HE21 | 25:LD:74:ILE:HD12 | 1.75                     | 0.52              |
| 28:LG:77:PRO:HD2  | 28:LG:80:ILE:HD12 | 1.92                     | 0.52              |
| 28:LG:181:TYR:CE2 | 28:LG:226:TYR:HB3 | 2.45                     | 0.52              |
| 30:LI:180:GLU:OE1 | 30:LI:180:GLU:N   | 2.35                     | 0.52              |
| 34:LN:120:TRP:CZ2 | 34:LN:122:GLY:HA2 | 2.45                     | 0.52              |
| 39:LS:80:ILE:HD11 | 39:LS:109:CYS:SG  | 2.50                     | 0.52              |
| 42:LV:99:GLU:OE2  | 42:LV:99:GLU:N    | 2.40                     | 0.52              |
| 62:Lr:108:MET:SD  | 62:Lr:108:MET:N   | 2.82                     | 0.52              |
| 69:SQ:23:ALA:HB1  | 69:SQ:68:ILE:HD11 | 1.91                     | 0.52              |
| 79:S2:296:U:C2    | 79:S2:297:A:C8    | 2.98                     | 0.52              |
| 79:S2:601:G:H2'   | 79:S2:602:G:C8    | 2.45                     | 0.52              |
| 79:S2:615:C:H2'   | 79:S2:616:A:O4'   | 2.10                     | 0.52              |
| 79:S2:692:G:N7    | 79:S2:693:A:N6    | 2.58                     | 0.52              |
| 79:S2:941:C:H2'   | 79:S2:942:G:H8    | 1.74                     | 0.52              |
| 79:S2:1379:A:H2'  | 79:S2:1380:C:C6   | 2.45                     | 0.52              |
| 82:PE:33:U:H4'    | 82:PE:34:U:OP1    | 2.09                     | 0.52              |
| 84:Lt:127:GLY:HA2 | 84:Lt:130:LYS:HG2 | 1.92                     | 0.52              |
| 5:sX:109:GLY:C    | 5:sX:119:ARG:HD3  | 2.34                     | 0.52              |
| 15:sC:60:TRP:CZ2  | 15:sC:62:PRO:HB3  | 2.45                     | 0.52              |
| 21:l8:90:C:H2'    | 21:l8:91:A:C8     | 2.45                     | 0.52              |
| 24:lC:20:LYS:HD2  | 24:lC:20:LYS:H    | 1.75                     | 0.52              |
| 25:lD:284:LYS:CE  | 25:lD:284:LYS:HA  | 2.40                     | 0.52              |
| 28:lG:81:ASN:O    | 28:lG:84:THR:OG1  | 2.28                     | 0.52              |
| 35:lO:118:MET:HE1 | 39:lS:168:THR:C   | 2.34                     | 0.52              |
| 35:lO:179:LYS:HA  | 35:lO:182:GLU:OE1 | 2.10                     | 0.52              |
| 38:lR:38:ARG:C    | 38:lR:40:GLN:H    | 2.18                     | 0.52              |
| 48:lc:35:LEU:O    | 48:lc:39:ARG:HG2  | 2.10                     | 0.52              |
| 64:sR:29:HIS:H    | 79:s2:1455:A:C5'  | 2.23                     | 0.52              |
| 65:sD:29:LEU:HD12 | 65:sD:29:LEU:N    | 2.24                     | 0.52              |
| 71:sT:24:LYS:HD3  | 71:sT:24:LYS:C    | 2.36                     | 0.52              |
| 79:s2:152:U:C2    | 79:s2:167:G:C2    | 2.98                     | 0.52              |
| 79:s2:925:G:H1    | 79:s2:1017:U:H3   | 0.70                     | 0.52              |
| 79:s2:1098:C:H2'  | 79:s2:1099:G:C8   | 2.45                     | 0.52              |
| 79:s2:1332:A:C2   | 79:s2:1500:G:C4   | 2.98                     | 0.52              |
| 79:s2:1389:C:H2'  | 79:s2:1390:U:C6   | 2.44                     | 0.52              |
| 79:s2:1397:U:H3'  | 79:s2:1397:U:OP2  | 2.10                     | 0.52              |
| 80:cB:160:MET:O   | 80:cB:164:LEU:HG  | 2.10                     | 0.52              |
| 83:ls:34:ASN:HA   | 85:l5:1968:G:O2'  | 2.09                     | 0.52              |
| 83:ls:135:THR:HA  | 83:ls:138:PHE:CD2 | 2.45                     | 0.52              |
| 85:l5:693:C:H2'   | 85:l5:694:C:C6    | 2.44                     | 0.52              |
| 85:l5:921:C:H2'   | 85:l5:922:C:C6    | 2.45                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 85:L5:1308:C:H2'  | 85:L5:1309:C:C5   | 2.45                     | 0.52              |
| 85:L5:2022:C:H2'  | 85:L5:2023:C:O4'  | 2.09                     | 0.52              |
| 85:L5:2102:G:H1'  | 85:L5:2103:G:C8   | 2.45                     | 0.52              |
| 85:L5:2571:C:H2'  | 85:L5:2572:C:C6   | 2.45                     | 0.52              |
| 85:L5:3911:C:H2'  | 85:L5:3912:U:H6   | 1.73                     | 0.52              |
| 85:L5:4220:A:H2'  | 85:L5:4222:G:H5'' | 1.91                     | 0.52              |
| 80:CB:651:CYS:SG  | 80:CB:662:LEU:HB3 | 2.50                     | 0.52              |
| 80:CB:663:THR:OG1 | 80:CB:703:ASP:OD1 | 2.20                     | 0.52              |
| 2:SE:164:LEU:HD12 | 2:SE:165:GLU:OE2  | 2.09                     | 0.52              |
| 4:SL:99:TYR:CE2   | 5:SX:13:LEU:HD13  | 2.44                     | 0.52              |
| 6:SG:15:LEU:HD22  | 79:S2:155:G:H4'   | 1.90                     | 0.52              |
| 6:SG:162:LEU:HD11 | 6:SG:172:LYS:HB2  | 1.91                     | 0.52              |
| 8:SY:16:ARG:HA    | 8:SY:19:GLN:HA    | 1.92                     | 0.52              |
| 10:SA:14:ASP:OD2  | 10:SA:15:VAL:N    | 2.42                     | 0.52              |
| 15:SC:60:TRP:CZ2  | 15:SC:62:PRO:HB3  | 2.44                     | 0.52              |
| 15:SC:203:GLY:N   | 15:SC:221:ASP:OD1 | 2.43                     | 0.52              |
| 16:SN:86:GLU:OE1  | 79:S2:925:G:O2'   | 2.25                     | 0.52              |
| 17:SO:42:VAL:HB   | 17:SO:56:VAL:O    | 2.10                     | 0.52              |
| 85:L5:947:C:H2'   | 85:L5:948:C:H6    | 1.75                     | 0.52              |
| 85:L5:1824:G:H2'  | 85:L5:1825:A:H8   | 1.73                     | 0.52              |
| 85:L5:1846:G:H2'  | 85:L5:1847:C:C6   | 2.45                     | 0.52              |
| 85:L5:1875:C:H2'  | 85:L5:1876:U:C6   | 2.45                     | 0.52              |
| 85:L5:2038:U:O2'  | 58:Lm:114:LYS:O   | 2.26                     | 0.52              |
| 85:L5:2284:G:OP1  | 46:La:7:LYS:NZ    | 2.43                     | 0.52              |
| 85:L5:2520:C:H2'  | 85:L5:2521:G:H8   | 1.73                     | 0.52              |
| 85:L5:2709:C:H5'  | 38:LR:43:LYS:HD2  | 1.91                     | 0.52              |
| 85:L5:2725:A:N6   | 38:LR:88:ARG:O    | 2.43                     | 0.52              |
| 85:L5:2751:G:H2'  | 85:L5:2752:G:H8   | 1.74                     | 0.52              |
| 85:L5:2773:G:OP1  | 56:Lk:39:SER:OG   | 2.27                     | 0.52              |
| 85:L5:4102:C:C4'  | 85:L5:4106:G:H2'  | 2.39                     | 0.52              |
| 85:L5:5023:C:H3'  | 85:L5:5024:C:H4'  | 1.92                     | 0.52              |
| 31:LJ:10:ASN:N    | 31:LJ:11:PRO:HD2  | 2.25                     | 0.52              |
| 45:LZ:25:ILE:HD13 | 45:LZ:41:ALA:HB1  | 1.91                     | 0.52              |
| 50:Le:72:SER:O    | 50:Le:72:SER:OG   | 2.23                     | 0.52              |
| 53:Lh:107:GLN:O   | 53:Lh:111:GLU:HG2 | 2.10                     | 0.52              |
| 60:Lo:54:PRO:O    | 82:PE:75:C:O2'    | 2.19                     | 0.52              |
| 62:Lr:52:GLU:N    | 62:Lr:52:GLU:OE2  | 2.43                     | 0.52              |
| 65:SD:69:LEU:HB3  | 65:SD:86:LEU:CD1  | 2.40                     | 0.52              |
| 70:SS:74:PRO:HA   | 70:SS:77:TYR:HB2  | 1.91                     | 0.52              |
| 79:S2:59:U:H1'    | 79:S2:501:C:H5'   | 1.92                     | 0.52              |
| 79:S2:1098:C:H2'  | 79:S2:1099:G:C8   | 2.45                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 79:S2:1337:C:H2'   | 79:S2:1338:G:H8    | 1.74                     | 0.52              |
| 79:S2:1418:C:O3'   | 79:S2:1419:C:H2'   | 2.09                     | 0.52              |
| 79:S2:1499:U:H2'   | 79:S2:1500:G:H8    | 1.75                     | 0.52              |
| 83:Ls:24:TYR:CD2   | 83:Ls:90:PHE:HB3   | 2.45                     | 0.52              |
| 87:IW:77:LYS:HB3   | 87:IW:79:GLN:HE22  | 1.74                     | 0.52              |
| 1:CH:125:GLU:OE1   | 1:CH:131:LYS:HG3   | 2.10                     | 0.51              |
| 1:cH:95:LEU:O      | 1:cH:99:ILE:HG12   | 2.10                     | 0.51              |
| 3:sI:61:ASP:O      | 3:sI:78:ILE:N      | 2.38                     | 0.51              |
| 4:sL:128:VAL:HG13  | 4:sL:140:PHE:CD1   | 2.45                     | 0.51              |
| 7:sJ:95:ASP:OD1    | 7:sJ:95:ASP:N      | 2.40                     | 0.51              |
| 8:sY:87:PRO:HG2    | 8:sY:90:ARG:CZ     | 2.39                     | 0.51              |
| 8:sY:93:ARG:NE     | 79:s2:575:A:OP1    | 2.40                     | 0.51              |
| 10:sA:174:MET:HE1  | 10:sA:175:TRP:CG   | 2.45                     | 0.51              |
| 12:sH:83:LEU:HD23  | 12:sH:87:PHE:HD1   | 1.73                     | 0.51              |
| 17:sO:103:ASN:HD22 | 17:sO:142:ARG:CG   | 2.20                     | 0.51              |
| 18:sW:112:ASP:CG   | 18:sW:113:HIS:N    | 2.68                     | 0.51              |
| 21:l8:111:U:O3'    | 21:l8:112:G:H8     | 1.93                     | 0.51              |
| 23:lB:90:VAL:HG13  | 23:lB:161:ARG:HB2  | 1.91                     | 0.51              |
| 28:lG:71:TYR:CE1   | 34:lN:25:VAL:HG21  | 2.43                     | 0.51              |
| 34:lN:47:LYS:HZ2   | 85:l5:279:A:H5''   | 1.75                     | 0.51              |
| 35:lO:118:MET:HE3  | 35:lO:119:VAL:N    | 2.25                     | 0.51              |
| 42:lV:74:LYS:HZ3   | 85:l5:3798:U:P     | 2.33                     | 0.51              |
| 48:lc:37:MET:HE2   | 48:lc:37:MET:HA    | 1.90                     | 0.51              |
| 51:lf:88:PHE:CD2   | 51:lf:92:LEU:HD21  | 2.44                     | 0.51              |
| 53:lh:4:ILE:HD11   | 53:lh:53:SER:HB3   | 1.92                     | 0.51              |
| 59:ln:20:MET:HA    | 59:ln:23:ARG:HB3   | 1.92                     | 0.51              |
| 62:lr:9:VAL:HG13   | 62:lr:10:VAL:HG13  | 1.91                     | 0.51              |
| 62:lr:38:PHE:O     | 62:lr:45:HIS:NE2   | 2.34                     | 0.51              |
| 62:lr:63:VAL:HG12  | 62:lr:79:ARG:HB3   | 1.92                     | 0.51              |
| 70:sS:114:LEU:HD23 | 70:sS:122:GLY:N    | 2.25                     | 0.51              |
| 72:sU:24:LEU:HB3   | 72:sU:112:VAL:HG12 | 1.92                     | 0.51              |
| 72:sU:62:ARG:NH2   | 79:s2:1547:C:O3'   | 2.43                     | 0.51              |
| 75:sg:14:HIS:CD2   | 75:sg:41:ILE:HD13  | 2.45                     | 0.51              |
| 76:sM:25:ALA:HB2   | 76:sM:111:VAL:HG23 | 1.91                     | 0.51              |
| 79:s2:509:G:H2'    | 79:s2:510:G:C8     | 2.45                     | 0.51              |
| 79:s2:1230:C:H2'   | 79:s2:1231:C:H6    | 1.75                     | 0.51              |
| 79:s2:1430:C:H2'   | 79:s2:1431:G:C8    | 2.44                     | 0.51              |
| 80:cB:766:LYS:HG3  | 80:cB:792:GLU:HB3  | 1.93                     | 0.51              |
| 83:ls:12:ASN:O     | 83:ls:15:LEU:HG    | 2.10                     | 0.51              |
| 83:ls:82:ILE:HG21  | 83:ls:88:PHE:HZ    | 1.74                     | 0.51              |
| 85:l5:189:G:N3     | 85:l5:253:G:N2     | 2.58                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 85:l5:1086:C:H2'   | 85:l5:1087:A:C8    | 2.44                     | 0.51              |
| 85:l5:1816:C:C4    | 85:l5:1817:U:C4    | 2.99                     | 0.51              |
| 85:l5:3917:A:H2'   | 85:l5:3918:G:C8    | 2.41                     | 0.51              |
| 80:CB:846:GLU:OE1  | 80:CB:846:GLU:N    | 2.40                     | 0.51              |
| 2:SE:161:GLN:O     | 2:SE:170:THR:OG1   | 2.28                     | 0.51              |
| 2:SE:201:HIS:NE2   | 79:S2:857:U:H4'    | 2.25                     | 0.51              |
| 4:SL:85:THR:HA     | 4:SL:112:HIS:HA    | 1.92                     | 0.51              |
| 6:SG:21:GLU:HG2    | 6:SG:22:ARG:HD3    | 1.91                     | 0.51              |
| 7:SJ:50:LEU:HD12   | 7:SJ:53:ILE:HD11   | 1.92                     | 0.51              |
| 10:SA:7:VAL:HG11   | 13:SV:42:VAL:O     | 2.09                     | 0.51              |
| 16:SN:33:VAL:O     | 16:SN:37:ILE:HG12  | 2.10                     | 0.51              |
| 85:L5:162:A:H2'    | 85:L5:163:A:C8     | 2.45                     | 0.51              |
| 85:L5:288:G:H2'    | 85:L5:289:C:H6     | 1.75                     | 0.51              |
| 85:L5:923:C:H2'    | 85:L5:925:C:H5     | 1.75                     | 0.51              |
| 85:L5:1402:C:N4    | 85:L5:1415:G:O6    | 2.43                     | 0.51              |
| 85:L5:1646:A:H2'   | 85:L5:1647:U:H6    | 1.75                     | 0.51              |
| 85:L5:2521:G:O3'   | 52:Lg:25:THR:OG1   | 2.27                     | 0.51              |
| 85:L5:4770:U:H2'   | 85:L5:4771:C:C6    | 2.46                     | 0.51              |
| 23:LB:55:HIS:NE2   | 87:LW:16:GLY:HA3   | 2.25                     | 0.51              |
| 23:LB:214:ASP:HB3  | 23:LB:363:ILE:HG22 | 1.92                     | 0.51              |
| 23:LB:261:ARG:HE   | 35:LO:64:THR:HG21  | 1.75                     | 0.51              |
| 30:LI:48:LEU:O     | 30:LI:139:ARG:HA   | 2.10                     | 0.51              |
| 37:LQ:50:ARG:NH2   | 37:LQ:139:LEU:O    | 2.43                     | 0.51              |
| 39:LS:132:ILE:HG23 | 39:LS:136:LYS:HB2  | 1.91                     | 0.51              |
| 41:LU:19:LEU:O     | 41:LU:20:LYS:HG3   | 2.10                     | 0.51              |
| 44:LY:42:TYR:CD2   | 44:LY:119:LEU:HD12 | 2.45                     | 0.51              |
| 46:La:75:LEU:H     | 46:La:75:LEU:HD12  | 1.76                     | 0.51              |
| 51:Lf:40:GLU:HA    | 51:Lf:43:LEU:HD23  | 1.92                     | 0.51              |
| 60:Lo:97:LYS:HB3   | 60:Lo:99:ARG:NH2   | 2.24                     | 0.51              |
| 66:SF:166:ILE:HA   | 79:S2:1599:U:C4    | 2.45                     | 0.51              |
| 71:ST:10:ASN:OD1   | 71:ST:13:GLU:HG2   | 2.10                     | 0.51              |
| 71:ST:101:ARG:HH12 | 79:S2:1565:C:H3'   | 1.75                     | 0.51              |
| 77:SZ:94:LYS:HD3   | 77:SZ:96:LEU:HD22  | 1.91                     | 0.51              |
| 87:IW:13:ILE:CD1   | 87:IW:32:LEU:HD13  | 2.40                     | 0.51              |
| 8:sY:64:PHE:HE1    | 79:s2:580:U:H5''   | 1.75                     | 0.51              |
| 8:sY:91:LEU:HB2    | 8:sY:97:TYR:HB3    | 1.92                     | 0.51              |
| 8:sY:108:LYS:NZ    | 79:s2:506:G:OP1    | 2.36                     | 0.51              |
| 11:sB:97:LEU:HB2   | 11:sB:232:HIS:CE1  | 2.45                     | 0.51              |
| 13:sV:81:LYS:O     | 13:sV:81:LYS:HD2   | 2.10                     | 0.51              |
| 27:IF:91:PHE:CE1   | 27:IF:244:ILE:HD11 | 2.45                     | 0.51              |
| 32:IL:92:ARG:NE    | 85:l5:109:G:H5'    | 2.25                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 34:IN:193:ARG:NH2  | 85:l5:28:C:OP2     | 2.42                     | 0.51              |
| 39:IS:80:ILE:HD12  | 39:lS:129:VAL:HG22 | 1.91                     | 0.51              |
| 41:IU:82:TYR:CZ    | 85:l5:2631:U:C2    | 2.98                     | 0.51              |
| 42:IV:97:TYR:HE2   | 87:IW:21:TYR:CE2   | 2.29                     | 0.51              |
| 44:IY:26:ARG:NH1   | 44:IY:75:ARG:O     | 2.41                     | 0.51              |
| 47:lb:103:LYS:HE3  | 85:l5:1708:G:N7    | 2.25                     | 0.51              |
| 50:le:90:MET:CA    | 50:le:90:MET:CE    | 2.83                     | 0.51              |
| 65:sD:76:ARG:HG3   | 67:sK:22:VAL:HG11  | 1.91                     | 0.51              |
| 71:sT:59:SER:HG    | 71:sT:79:TYR:HH    | 1.59                     | 0.51              |
| 79:s2:373:G:O6     | 79:s2:392:A:N6     | 2.42                     | 0.51              |
| 79:s2:867:G:H2'    | 79:s2:868:G:N3     | 2.25                     | 0.51              |
| 79:s2:1395:C:H1'   | 79:s2:1474:A:C5    | 2.45                     | 0.51              |
| 80:cB:225:LEU:HD11 | 80:cB:260:LEU:HB3  | 1.91                     | 0.51              |
| 80:cB:641:TRP:CH2  | 80:cB:645:GLU:HG2  | 2.45                     | 0.51              |
| 80:cB:698:ARG:CZ   | 80:cB:817:TRP:HB2  | 2.40                     | 0.51              |
| 85:l5:288:G:H2'    | 85:l5:289:C:C6     | 2.45                     | 0.51              |
| 85:l5:351:C:H2'    | 85:l5:352:G:C8     | 2.46                     | 0.51              |
| 85:l5:677:G:H2'    | 85:l5:678:C:C6     | 2.44                     | 0.51              |
| 85:l5:678:C:H2'    | 85:l5:679:C:C6     | 2.46                     | 0.51              |
| 85:l5:1269:G:N1    | 85:l5:2106:G:H1'   | 2.24                     | 0.51              |
| 85:l5:1340:C:H2'   | 85:l5:1341:U:C6    | 2.45                     | 0.51              |
| 85:l5:3658:C:H2'   | 85:l5:3659:G:H8    | 1.74                     | 0.51              |
| 85:l5:3754:G:H2'   | 85:l5:3755:G:H8    | 1.75                     | 0.51              |
| 85:l5:4608:G:H3'   | 85:l5:4609:G:H8    | 1.75                     | 0.51              |
| 80:CB:108:HIS:CE1  | 85:L5:4606:G:H4'   | 2.46                     | 0.51              |
| 80:CB:587:SER:HA   | 80:CB:736:ALA:HB2  | 1.91                     | 0.51              |
| 80:CB:739:ARG:NH2  | 80:CB:823:ASP:OD1  | 2.41                     | 0.51              |
| 80:CB:827:ASN:OD1  | 80:CB:828:SER:N    | 2.43                     | 0.51              |
| 2:SE:87:MET:O      | 2:SE:87:MET:SD     | 2.68                     | 0.51              |
| 6:SG:217:MET:N     | 6:SG:219:GLU:OE2   | 2.43                     | 0.51              |
| 10:SA:20:ALA:HB3   | 64:SR:91:LEU:HD23  | 1.93                     | 0.51              |
| 11:SB:67:PHE:N     | 11:SB:85:LYS:O     | 2.38                     | 0.51              |
| 12:SH:57:ARG:HH22  | 12:SH:91:HIS:N     | 2.09                     | 0.51              |
| 12:SH:121:THR:OG1  | 79:S2:688:U:OP2    | 2.29                     | 0.51              |
| 12:SH:167:GLU:N    | 12:SH:167:GLU:OE1  | 2.44                     | 0.51              |
| 14:Sa:23:CYS:SG    | 14:Sa:74:CYS:HB3   | 2.50                     | 0.51              |
| 14:Sa:101:PHE:CD1  | 14:Sa:101:PHE:O    | 2.63                     | 0.51              |
| 16:SN:106:ARG:HA   | 16:SN:106:ARG:NH1  | 2.25                     | 0.51              |
| 18:SW:113:HIS:HA   | 18:SW:116:ALA:HB3  | 1.93                     | 0.51              |
| 85:L5:352:G:C6     | 24:LC:196:MET:HE1  | 2.45                     | 0.51              |
| 85:L5:1309:C:OP1   | 35:LO:92:THR:OG1   | 2.26                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 85:L5:1336:G:H2'   | 85:L5:2346:C:H42   | 1.75                     | 0.51              |
| 85:L5:1752:G:H2'   | 85:L5:1753:G:C8    | 2.45                     | 0.51              |
| 85:L5:2630:U:H5''  | 41:LU:48:LYS:NZ    | 2.25                     | 0.51              |
| 85:L5:2655:C:C2    | 85:L5:2656:U:C5    | 2.98                     | 0.51              |
| 85:L5:2817:C:H2'   | 85:L5:2818:C:H6    | 1.75                     | 0.51              |
| 85:L5:4108:G:H2'   | 85:L5:4109:G:H2'   | 1.91                     | 0.51              |
| 85:L5:4344:U:H2'   | 85:L5:4345:C:C6    | 2.45                     | 0.51              |
| 85:L5:4870:G:H2'   | 33:LM:91:TRP:CZ2   | 2.45                     | 0.51              |
| 20:L7:38:U:N3      | 20:L7:41:G:OP2     | 2.41                     | 0.51              |
| 21:L8:125:C:H1'    | 21:L8:126:C:H2'    | 1.91                     | 0.51              |
| 23:LB:103:LYS:HB2  | 23:LB:153:MET:CE   | 2.40                     | 0.51              |
| 24:LC:144:ILE:O    | 24:LC:144:ILE:HG13 | 2.09                     | 0.51              |
| 25:LD:208:MET:HB3  | 25:LD:223:PHE:CE2  | 2.44                     | 0.51              |
| 39:LS:69:GLU:OE1   | 39:LS:102:THR:N    | 2.36                     | 0.51              |
| 45:LZ:77:TYR:HB3   | 48:Lc:39:ARG:CZ    | 2.40                     | 0.51              |
| 55:Lj:56:ARG:NE    | 55:Lj:56:ARG:HA    | 2.25                     | 0.51              |
| 58:Lm:94:MET:HG2   | 58:Lm:105:PRO:HA   | 1.91                     | 0.51              |
| 59:Ln:15:ARG:HA    | 59:Ln:18:ARG:HD3   | 1.93                     | 0.51              |
| 61:Lp:11:VAL:HG13  | 61:Lp:14:TYR:HD2   | 1.75                     | 0.51              |
| 64:SR:120:THR:OG1  | 64:SR:121:GLN:N    | 2.43                     | 0.51              |
| 75:Sg:149:GLU:CD   | 75:Sg:170:TRP:HB3  | 2.34                     | 0.51              |
| 75:Sg:176:VAL:O    | 75:Sg:185:LYS:N    | 2.32                     | 0.51              |
| 75:Sg:188:HIS:CE1  | 75:Sg:219:TRP:CD1  | 2.99                     | 0.51              |
| 75:Sg:201:SER:HA   | 75:Sg:241:PHE:CD2  | 2.46                     | 0.51              |
| 75:Sg:259:TRP:HA   | 75:Sg:267:VAL:H    | 1.75                     | 0.51              |
| 79:S2:1474:A:H2'   | 79:S2:1475:G:C8    | 2.46                     | 0.51              |
| 79:S2:1758:G:N2    | 79:S2:1773:C:O4'   | 2.43                     | 0.51              |
| 84:Lt:33:GLY:H     | 84:Lt:34:PRO:HD2   | 1.75                     | 0.51              |
| 84:Lt:114:ARG:HG2  | 84:Lt:119:ARG:CZ   | 2.41                     | 0.51              |
| 1:cH:85:ARG:HG2    | 1:cH:95:LEU:HD12   | 1.93                     | 0.51              |
| 3:sI:76:THR:HG23   | 3:sI:108:PRO:HG2   | 1.93                     | 0.51              |
| 9:se:8:ARG:HH21    | 79:s2:616:A:P      | 2.34                     | 0.51              |
| 10:sA:185:MET:HE3  | 10:sA:185:MET:O    | 2.10                     | 0.51              |
| 13:sV:38:GLU:CD    | 13:sV:38:GLU:H     | 2.18                     | 0.51              |
| 19:sb:54:VAL:HG12  | 19:sb:63:LEU:HD13  | 1.92                     | 0.51              |
| 21:l8:28:C:H2'     | 21:l8:29:G:C8      | 2.45                     | 0.51              |
| 28:lG:31:LEU:HD21  | 45:lZ:53:VAL:HB    | 1.91                     | 0.51              |
| 28:lG:248:ALA:O    | 28:lG:252:LYS:HG2  | 2.09                     | 0.51              |
| 32:lL:126:LEU:HD11 | 53:lh:117:ARG:CZ   | 2.40                     | 0.51              |
| 35:lO:34:VAL:HG11  | 35:lO:112:TYR:CD2  | 2.46                     | 0.51              |
| 39:lS:51:LEU:HD21  | 40:lT:153:PRO:HA   | 1.92                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 49:ld:85:ARG:CZ    | 49:ld:117:LEU:HB3  | 2.40                     | 0.51              |
| 52:lg:110:GLN:O    | 52:lg:113:SER:OG   | 2.23                     | 0.51              |
| 64:sR:26:ASN:ND2   | 64:sR:59:LYS:HA    | 2.25                     | 0.51              |
| 64:sR:28:PHE:HB3   | 79:s2:1455:A:C8    | 2.41                     | 0.51              |
| 65:sD:205:PRO:HG2  | 79:s2:1388:A:N3    | 2.24                     | 0.51              |
| 68:sP:17:TYR:CE2   | 68:sP:18:ARG:HG3   | 2.46                     | 0.51              |
| 70:sS:65:GLU:N     | 70:sS:65:GLU:OE1   | 2.43                     | 0.51              |
| 79:s2:349:A:H2'    | 79:s2:350:C:C6     | 2.44                     | 0.51              |
| 79:s2:1562:C:H2'   | 79:s2:1563:G:H8    | 1.75                     | 0.51              |
| 79:s2:1764:G:H5'   | 79:s2:1765:C:H5''  | 1.93                     | 0.51              |
| 81:aP:1:G:H2'      | 81:aP:2:U:H6       | 1.74                     | 0.51              |
| 83:ls:59:THR:HG23  | 85:l5:1960:A:H5''  | 1.93                     | 0.51              |
| 84:lt:117:ARG:O    | 84:lt:119:ARG:HG3  | 2.10                     | 0.51              |
| 85:l5:395:A:H2'    | 85:l5:396:A:C8     | 2.45                     | 0.51              |
| 85:l5:1552:G:H1'   | 85:l5:1575:A:N6    | 2.26                     | 0.51              |
| 85:l5:1950:U:H2'   | 85:l5:1951:G:C8    | 2.46                     | 0.51              |
| 85:l5:2557:G:H2'   | 85:l5:2558:C:C6    | 2.45                     | 0.51              |
| 85:l5:2693:G:OP2   | 85:l5:2694:G:O2'   | 2.22                     | 0.51              |
| 85:l5:3606:U:H2'   | 85:l5:3607:U:H6    | 1.74                     | 0.51              |
| 85:l5:3770:U:H2'   | 85:l5:3771:C:C6    | 2.45                     | 0.51              |
| 85:l5:3921:U:H1'   | 85:l5:4543:G:H21   | 1.75                     | 0.51              |
| 80:CB:327:ASP:OD1  | 80:CB:328:LYS:N    | 2.43                     | 0.51              |
| 80:CB:626:GLN:HG2  | 80:CB:631:ARG:HB2  | 1.92                     | 0.51              |
| 2:SE:183:VAL:HG12  | 2:SE:191:ARG:H     | 1.75                     | 0.51              |
| 3:SI:5:ARG:HD3     | 79:S2:380:G:H1'    | 1.92                     | 0.51              |
| 6:SG:74:ARG:HD2    | 6:SG:96:SER:HB3    | 1.91                     | 0.51              |
| 6:SG:118:GLU:OE2   | 6:SG:119:LYS:NZ    | 2.35                     | 0.51              |
| 6:SG:175:LYS:HB3   | 79:S2:65:C:OP2     | 2.10                     | 0.51              |
| 11:SB:164:ILE:HG22 | 11:SB:204:ILE:HD11 | 1.92                     | 0.51              |
| 85:L5:132:G:N2     | 85:L5:136:C:O2'    | 2.37                     | 0.51              |
| 85:L5:364:G:H5''   | 55:Lj:56:ARG:CZ    | 2.41                     | 0.51              |
| 85:L5:497:G:N2     | 85:L5:498:C:H41    | 2.09                     | 0.51              |
| 85:L5:908:G:H2'    | 85:L5:909:A:C8     | 2.45                     | 0.51              |
| 85:L5:1569:U:H2'   | 85:L5:1570:G:H8    | 1.76                     | 0.51              |
| 85:L5:4577:U:H2'   | 85:L5:4578:G:H8    | 1.75                     | 0.51              |
| 85:L5:4586:G:H2'   | 85:L5:4587:G:H8    | 1.74                     | 0.51              |
| 23:LB:173:LEU:HD21 | 23:LB:342:LYS:HD3  | 1.91                     | 0.51              |
| 24:LC:2:ALA:HA     | 24:LC:3:CYS:SG     | 2.50                     | 0.51              |
| 25:LD:287:PHE:CD2  | 30:LI:210:ARG:HD2  | 2.46                     | 0.51              |
| 26:LE:283:PRO:HB2  | 51:Lf:41:PHE:HE2   | 1.74                     | 0.51              |
| 31:LJ:94:LEU:HD11  | 31:LJ:98:ASN:HB2   | 1.91                     | 0.51              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 31:LJ:111:GLU:OE1  | 31:LJ:113:ILE:N   | 2.43                     | 0.51              |
| 33:LM:89:THR:HG23  | 33:LM:92:ALA:H    | 1.74                     | 0.51              |
| 34:LN:10:LEU:HA    | 54:Li:44:ILE:HD11 | 1.92                     | 0.51              |
| 35:LO:118:MET:HE1  | 39:LS:169:THR:HA  | 1.93                     | 0.51              |
| 64:SR:27:ASP:OD1   | 64:SR:30:THR:HG23 | 2.10                     | 0.51              |
| 65:SD:224:SER:HG   | 75:Sg:188:HIS:CD2 | 2.27                     | 0.51              |
| 68:SP:57:LEU:O     | 68:SP:61:ARG:HG2  | 2.10                     | 0.51              |
| 75:Sg:131:LEU:HD21 | 75:Sg:140:TYR:HB3 | 1.92                     | 0.51              |
| 79:S2:360:A:H2     | 79:S2:363:A:H5'   | 1.75                     | 0.51              |
| 79:S2:1051:G:H2'   | 79:S2:1052:A:H8   | 1.76                     | 0.51              |
| 81:AP:6:C:H2'      | 81:AP:7:G:C8      | 2.45                     | 0.51              |
| 83:Ls:47:LEU:HA    | 83:Ls:50:LYS:HE2  | 1.92                     | 0.51              |
| 1:CH:72:ARG:NH1    | 1:CH:113:ARG:HB3  | 2.26                     | 0.51              |
| 1:cH:44:TRP:CD1    | 9:se:53:LYS:HG2   | 2.46                     | 0.51              |
| 4:sL:154:GLN:NE2   | 16:sN:133:ARG:O   | 2.44                     | 0.51              |
| 10:sA:82:THR:O     | 10:sA:82:THR:OG1  | 2.29                     | 0.51              |
| 13:sV:65:SER:O     | 13:sV:69:ILE:HG13 | 2.10                     | 0.51              |
| 16:sN:140:LYS:HG2  | 16:sN:141:TYR:N   | 2.24                     | 0.51              |
| 18:sW:87:GLU:HA    | 18:sW:90:GLN:HG3  | 1.91                     | 0.51              |
| 19:sb:13:GLU:OE1   | 19:sb:14:GLU:N    | 2.43                     | 0.51              |
| 20:l7:97:G:O5'     | 27:lF:134:ARG:NH1 | 2.43                     | 0.51              |
| 21:l8:36:G:H2'     | 53:lh:89:ARG:HH11 | 1.74                     | 0.51              |
| 21:l8:96:C:H5''    | 53:lh:66:LYS:HG2  | 1.92                     | 0.51              |
| 22:lA:70:LYS:O     | 22:lA:71:LYS:HD3  | 2.09                     | 0.51              |
| 24:lC:283:LYS:NZ   | 37:lQ:24:TYR:HB2  | 2.26                     | 0.51              |
| 26:lE:74:SER:HB2   | 47:lb:118:LEU:HB3 | 1.92                     | 0.51              |
| 27:lF:132:MET:HA   | 27:lF:135:ILE:CD1 | 2.37                     | 0.51              |
| 28:lG:251:ALA:HA   | 28:lG:254:GLU:OE2 | 2.11                     | 0.51              |
| 29:lH:95:VAL:HG23  | 29:lH:177:ASP:HA  | 1.93                     | 0.51              |
| 30:lI:148:VAL:HG22 | 30:lI:152:LEU:CD2 | 2.40                     | 0.51              |
| 33:lM:14:TYR:O     | 33:lM:56:GLN:N    | 2.39                     | 0.51              |
| 33:lM:91:TRP:CE2   | 85:l5:4870:G:H5'' | 2.45                     | 0.51              |
| 33:lM:104:MET:HE3  | 33:lM:105:THR:N   | 2.25                     | 0.51              |
| 34:lN:14:LYS:NZ    | 85:l5:279:A:O2'   | 2.44                     | 0.51              |
| 35:lO:191:LYS:HD2  | 35:lO:192:TYR:CZ  | 2.46                     | 0.51              |
| 37:lQ:172:ARG:NH1  | 46:la:56:VAL:O    | 2.44                     | 0.51              |
| 38:IR:95:TRP:CE2   | 85:l5:1572:U:H4'  | 2.46                     | 0.51              |
| 54:li:55:ARG:HA    | 54:li:58:MET:SD   | 2.50                     | 0.51              |
| 56:lk:35:LYS:HB3   | 56:lk:42:LEU:HD11 | 1.91                     | 0.51              |
| 64:sR:32:LYS:HG2   | 79:s2:1453:C:C2   | 2.45                     | 0.51              |
| 64:sR:46:LEU:HD13  | 79:s2:1370:A:C5   | 2.46                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 65:sD:123:LEU:HA   | 65:sD:126:ILE:HG12 | 1.93                     | 0.51              |
| 69:sQ:9:SER:O      | 69:sQ:99:TYR:OH    | 2.29                     | 0.51              |
| 75:sg:129:ILE:HG23 | 75:sg:142:VAL:HB   | 1.92                     | 0.51              |
| 79:s2:293:C:O2'    | 79:s2:294:U:H3'    | 2.10                     | 0.51              |
| 79:s2:1318:G:H2'   | 79:s2:1319:U:C6    | 2.45                     | 0.51              |
| 80:cB:308:LYS:HB3  | 80:cB:311:GLU:CD   | 2.35                     | 0.51              |
| 80:cB:676:LYS:HA   | 80:cB:679:VAL:CG1  | 2.41                     | 0.51              |
| 81:aP:15:G:N2      | 81:aP:21:A:H1'     | 2.25                     | 0.51              |
| 81:aP:28:U:H2'     | 81:aP:29:C:O4'     | 2.09                     | 0.51              |
| 85:l5:1307:A:H2'   | 85:l5:1308:C:C6    | 2.45                     | 0.51              |
| 85:l5:1382:G:H2'   | 85:l5:1383:G:H8    | 1.74                     | 0.51              |
| 85:l5:4063:U:H2'   | 85:l5:4064:C:N1    | 2.26                     | 0.51              |
| 85:l5:4322:G:N2    | 85:l5:4325:A:OP2   | 2.37                     | 0.51              |
| 85:l5:4345:C:H2'   | 85:l5:4346:U:H6    | 1.74                     | 0.51              |
| 85:l5:4716:C:H2'   | 85:l5:4717:A:C8    | 2.45                     | 0.51              |
| 80:CB:494:MET:HE2  | 80:CB:494:MET:HA   | 1.92                     | 0.51              |
| 80:CB:605:LYS:HD2  | 80:CB:705:HIS:NE2  | 2.26                     | 0.51              |
| 80:CB:632:ALA:HB3  | 80:CB:633:ARG:HH11 | 1.76                     | 0.51              |
| 2:SE:147:ILE:HD12  | 2:SE:167:GLY:O     | 2.11                     | 0.51              |
| 6:SG:155:GLN:NE2   | 79:S2:76:U:OP2     | 2.44                     | 0.51              |
| 10:SA:85:ARG:HH21  | 64:SR:81:ARG:HH12  | 1.59                     | 0.51              |
| 17:SO:32:HIS:CD2   | 79:S2:975:G:H4'    | 2.33                     | 0.51              |
| 85:L5:1578:U:OP1   | 85:L5:3637:U:O2'   | 2.28                     | 0.51              |
| 85:L5:1699:A:H61   | 85:L5:1706:A:H4'   | 1.76                     | 0.51              |
| 85:L5:2483:G:O6    | 85:L5:2495:U:O4    | 2.29                     | 0.51              |
| 85:L5:2491:C:O2'   | 85:L5:2492:C:O4'   | 2.27                     | 0.51              |
| 85:L5:2599:G:P     | 52:Lg:40:LYS:HD2   | 2.51                     | 0.51              |
| 85:L5:2671:C:OP1   | 61:Lp:46:LYS:NZ    | 2.35                     | 0.51              |
| 85:L5:3623:C:O2    | 38:LR:82:LYS:NZ    | 2.42                     | 0.51              |
| 85:L5:3784:A:O2'   | 85:L5:3785:A:H3'   | 2.11                     | 0.51              |
| 85:L5:4238:G:H2'   | 85:L5:4239:A:C8    | 2.44                     | 0.51              |
| 85:L5:4704:C:H2'   | 85:L5:4705:A:C8    | 2.46                     | 0.51              |
| 85:L5:4704:C:H2'   | 85:L5:4705:A:H8    | 1.75                     | 0.51              |
| 85:L5:4896:G:H5''  | 33:LM:128:LYS:NZ   | 2.26                     | 0.51              |
| 24:LC:11:TYR:HE2   | 24:LC:149:GLU:HB3  | 1.75                     | 0.51              |
| 29:LH:12:ILE:HG23  | 29:LH:16:VAL:HG23  | 1.92                     | 0.51              |
| 30:LI:191:ILE:HG22 | 30:LI:198:LYS:HB2  | 1.92                     | 0.51              |
| 31:LJ:63:ARG:NH1   | 60:Lo:103:VAL:HG13 | 2.21                     | 0.51              |
| 35:LO:168:TYR:CE2  | 35:LO:172:LYS:HD2  | 2.46                     | 0.51              |
| 45:LZ:70:SER:H     | 45:LZ:111:ARG:NH1  | 2.08                     | 0.51              |
| 48:Lc:62:TYR:CE2   | 48:Lc:66:LEU:HD23  | 2.46                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 60:Lo:88:CYS:SG    | 60:Lo:89:LYS:N     | 2.83                     | 0.51              |
| 66:SF:52:SER:OG    | 66:SF:70:GLU:OE2   | 2.26                     | 0.51              |
| 70:SS:5:ILE:HD11   | 70:SS:9:PHE:HD1    | 1.76                     | 0.51              |
| 71:ST:112:MET:SD   | 71:ST:112:MET:N    | 2.83                     | 0.51              |
| 75:Sg:44:LYS:HG2   | 75:Sg:54:ILE:HB    | 1.91                     | 0.51              |
| 79:S2:207:G:H3'    | 79:S2:208:G:C8     | 2.43                     | 0.51              |
| 79:S2:1592:C:H2'   | 79:S2:1593:C:H6    | 1.75                     | 0.51              |
| 87:LW:46:PRO:HB2   | 87:LW:52:THR:HG21  | 1.91                     | 0.51              |
| 87:LW:102:LYS:HA   | 87:LW:105:ARG:HB2  | 1.92                     | 0.51              |
| 11:sB:127:VAL:HG11 | 11:sB:176:VAL:HG11 | 1.93                     | 0.51              |
| 15:sC:117:ARG:O    | 79:s2:1699:A:N6    | 2.42                     | 0.51              |
| 25:ID:59:ASP:OD1   | 25:ID:81:HIS:N     | 2.44                     | 0.51              |
| 27:IF:31:LYS:O     | 27:IF:35:LYS:HG3   | 2.10                     | 0.51              |
| 31:IJ:119:TYR:CD2  | 70:sS:105:ASN:HB3  | 2.45                     | 0.51              |
| 38:IR:31:GLU:N     | 38:IR:31:GLU:OE1   | 2.43                     | 0.51              |
| 38:IR:176:ARG:NH1  | 38:IR:180:LYS:HB2  | 2.25                     | 0.51              |
| 45:IZ:62:ILE:HD12  | 45:IZ:62:ILE:H     | 1.76                     | 0.51              |
| 64:sR:27:ASP:HB3   | 79:s2:1455:A:C5'   | 2.39                     | 0.51              |
| 64:sR:39:ALA:O     | 79:s2:1388:A:H1'   | 2.11                     | 0.51              |
| 79:s2:795:A:H2'    | 79:s2:796:G:C8     | 2.46                     | 0.51              |
| 79:s2:1007:C:H2'   | 79:s2:1008:A:C8    | 2.45                     | 0.51              |
| 79:s2:1119:A:H3'   | 79:s2:1120:U:C6    | 2.46                     | 0.51              |
| 85:l5:644:G:H2'    | 85:l5:645:G:O4'    | 2.11                     | 0.51              |
| 85:l5:1732:C:H2'   | 85:l5:1733:G:C8    | 2.46                     | 0.51              |
| 85:l5:1748:U:C4    | 85:l5:1783:C:C4    | 2.99                     | 0.51              |
| 85:l5:3758:U:H2'   | 85:l5:3765:G:N2    | 2.25                     | 0.51              |
| 85:l5:4070:U:H2'   | 85:l5:4071:U:C6    | 2.46                     | 0.51              |
| 85:l5:4740:G:C6    | 85:l5:4959:U:O2    | 2.64                     | 0.51              |
| 80:CB:403:PRO:HA   | 80:CB:410:PHE:HD2  | 1.76                     | 0.51              |
| 2:SE:122:LYS:HG2   | 2:SE:123:LEU:N     | 2.24                     | 0.51              |
| 3:SI:124:LYS:HB3   | 3:SI:125:LYS:HZ2   | 1.75                     | 0.51              |
| 3:SI:132:GLU:HA    | 3:SI:135:GLU:HG2   | 1.91                     | 0.51              |
| 4:SL:23:VAL:HG22   | 4:SL:24:LEU:H      | 1.76                     | 0.51              |
| 4:SL:84:ARG:HG2    | 4:SL:112:HIS:HE1   | 1.75                     | 0.51              |
| 6:SG:149:LYS:HG2   | 6:SG:150:GLU:HG3   | 1.92                     | 0.51              |
| 7:SJ:32:ILE:HA     | 7:SJ:37:LEU:HD13   | 1.92                     | 0.51              |
| 14:Sa:84:VAL:HG22  | 14:Sa:85:ARG:H     | 1.75                     | 0.51              |
| 85:L5:18:C:H2'     | 85:L5:19:G:C8      | 2.45                     | 0.51              |
| 85:L5:272:U:H2'    | 85:L5:273:U:C6     | 2.46                     | 0.51              |
| 85:L5:351:C:C4     | 85:L5:352:G:C6     | 2.98                     | 0.51              |
| 85:L5:1352:C:H2'   | 85:L5:1353:G:O4'   | 2.10                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 85:L5:1395:U:H2'  | 85:L5:1396:G:O4'  | 2.10                     | 0.51              |
| 85:L5:1427:A:OP2  | 85:L5:1457:G:N1   | 2.44                     | 0.51              |
| 85:L5:1562:G:H5'  | 85:L5:1563:A:OP2  | 2.11                     | 0.51              |
| 85:L5:1812:C:C1'  | 47:Lb:57:MET:HE1  | 2.40                     | 0.51              |
| 85:L5:3811:G:O2'  | 85:L5:3814:U:OP2  | 2.27                     | 0.51              |
| 85:L5:4177:C:H2'  | 85:L5:4178:A:H8   | 1.75                     | 0.51              |
| 85:L5:4565:C:H2'  | 85:L5:4566:U:H6   | 1.76                     | 0.51              |
| 24:LC:33:ARG:NH1  | 24:LC:35:ASP:OD2  | 2.43                     | 0.51              |
| 24:LC:34:PRO:HG3  | 62:Lr:9:VAL:HG13  | 1.93                     | 0.51              |
| 27:LF:124:LYS:HB3 | 27:LF:201:PHE:CE2 | 2.45                     | 0.51              |
| 28:LG:232:GLU:HA  | 28:LG:235:ARG:HB3 | 1.93                     | 0.51              |
| 31:LJ:32:ARG:O    | 31:LJ:35:ARG:HG2  | 2.11                     | 0.51              |
| 53:Lh:107:GLN:HA  | 53:Lh:110:LYS:HD2 | 1.93                     | 0.51              |
| 64:SR:93:GLN:HE21 | 64:SR:96:ILE:HB   | 1.75                     | 0.51              |
| 70:SS:88:LYS:HB3  | 70:SS:95:TYR:CE1  | 2.45                     | 0.51              |
| 72:SU:72:GLU:OE1  | 72:SU:73:GLY:N    | 2.44                     | 0.51              |
| 72:SU:80:PHE:HB3  | 74:Sd:52:PHE:HD2  | 1.76                     | 0.51              |
| 79:S2:452:G:H2'   | 79:S2:453:C:H6    | 1.75                     | 0.51              |
| 79:S2:940:U:H2'   | 79:S2:941:C:C6    | 2.45                     | 0.51              |
| 81:AP:1:G:H2'     | 81:AP:2:U:C6      | 2.45                     | 0.51              |
| 87:IW:14:TYR:HB3  | 87:IW:15:PRO:HD2  | 1.92                     | 0.51              |
| 3:sI:110:ARG:HH21 | 3:sI:122:GLY:HA3  | 1.76                     | 0.51              |
| 11:sB:30:TRP:CD1  | 17:sO:19:PRO:HG3  | 2.46                     | 0.51              |
| 11:sB:151:ARG:NH2 | 79:s2:1101:U:O5'  | 2.44                     | 0.51              |
| 12:sH:62:ILE:HB   | 12:sH:94:PHE:HD2  | 1.75                     | 0.51              |
| 15:sC:110:MET:HG2 | 15:sC:125:LYS:HB2 | 1.92                     | 0.51              |
| 21:l8:155:C:OP2   | 28:lG:89:ARG:NH1  | 2.43                     | 0.51              |
| 24:lC:317:ASN:HB2 | 85:l5:716:C:OP1   | 2.10                     | 0.51              |
| 26:lE:270:TYR:CE1 | 33:lM:107:PHE:HD1 | 2.29                     | 0.51              |
| 30:lI:87:MET:HE3  | 30:lI:88:ARG:H    | 1.75                     | 0.51              |
| 37:lQ:72:LEU:HD12 | 37:lQ:75:ARG:HH12 | 1.76                     | 0.51              |
| 38:lR:42:ARG:NH1  | 85:l5:2525:U:OP1  | 2.38                     | 0.51              |
| 39:lS:152:PHE:CD2 | 39:lS:152:PHE:C   | 2.89                     | 0.51              |
| 40:lT:147:GLU:OE1 | 40:lT:147:GLU:N   | 2.41                     | 0.51              |
| 49:ld:45:ALA:O    | 49:ld:49:ILE:HG23 | 2.10                     | 0.51              |
| 65:sD:7:LYS:HD2   | 72:sU:86:LYS:HE2  | 1.93                     | 0.51              |
| 68:sP:29:SER:OG   | 68:sP:30:TYR:N    | 2.42                     | 0.51              |
| 71:sT:73:GLY:O    | 71:sT:76:THR:HG22 | 2.10                     | 0.51              |
| 74:sd:44:ARG:NH2  | 79:s2:1337:C:H5'  | 2.25                     | 0.51              |
| 76:sM:33:ARG:NH2  | 79:s2:1284:A:N7   | 2.59                     | 0.51              |
| 76:sM:54:SER:OG   | 76:sM:80:ASP:O    | 2.28                     | 0.51              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 77:sZ:59:CYS:HB2  | 77:sZ:60:LYS:NZ    | 2.26                     | 0.51              |
| 79:s2:88:G:H2'    | 79:s2:89:C:H6      | 1.73                     | 0.51              |
| 79:s2:327:G:H4'   | 79:s2:328:U:O5'    | 2.11                     | 0.51              |
| 79:s2:1703:C:H2'  | 79:s2:1704:C:O4'   | 2.09                     | 0.51              |
| 80:cB:769:HIS:HB3 | 85:l5:1981:G:H21   | 1.75                     | 0.51              |
| 85:l5:500:G:O4'   | 85:l5:504:G:N2     | 2.35                     | 0.51              |
| 85:l5:1366:G:O2'  | 85:l5:1367:C:O2    | 2.29                     | 0.51              |
| 85:l5:1461:C:H2'  | 85:l5:1462:A:C8    | 2.45                     | 0.51              |
| 85:l5:1562:G:H5'  | 85:l5:1563:A:OP2   | 2.11                     | 0.51              |
| 85:l5:2704:C:H2'  | 85:l5:2705:G:C8    | 2.46                     | 0.51              |
| 85:l5:2743:A:H2'  | 85:l5:2744:A:C8    | 2.46                     | 0.51              |
| 85:l5:3807:A:H2'  | 85:l5:3808:C:H6    | 1.74                     | 0.51              |
| 85:l5:4159:C:H2'  | 85:l5:4160:C:C6    | 2.46                     | 0.51              |
| 85:l5:4563:U:H2'  | 85:l5:4564:A:C8    | 2.43                     | 0.51              |
| 12:SH:49:LYS:O    | 12:SH:61:ILE:N     | 2.35                     | 0.51              |
| 12:SH:77:VAL:HA   | 12:SH:80:VAL:HG22  | 1.91                     | 0.51              |
| 19:Sb:23:ARG:NH1  | 19:Sb:27:SER:OG    | 2.43                     | 0.51              |
| 85:L5:288:G:H2'   | 85:L5:289:C:C6     | 2.45                     | 0.51              |
| 85:L5:371:A:H2'   | 85:L5:372:A:C8     | 2.45                     | 0.51              |
| 85:L5:700:G:H2'   | 85:L5:701:G:C8     | 2.45                     | 0.51              |
| 85:L5:1938:C:H4'  | 85:L5:1939:A:O4'   | 2.10                     | 0.51              |
| 85:L5:2418:A:N1   | 85:L5:2429:A:O2'   | 2.36                     | 0.51              |
| 85:L5:2775:C:H2'  | 85:L5:2776:G:C8    | 2.45                     | 0.51              |
| 85:L5:3695:U:H2'  | 85:L5:3696:C:C6    | 2.45                     | 0.51              |
| 85:L5:3972:A:H1'  | 85:L5:4050:A:N6    | 2.25                     | 0.51              |
| 85:L5:4234:A:H2   | 85:L5:4271:A:C5    | 2.29                     | 0.51              |
| 85:L5:4563:U:H2'  | 85:L5:4564:A:H8    | 1.73                     | 0.51              |
| 41:LU:43:LEU:O    | 41:LU:46:ARG:N     | 2.44                     | 0.51              |
| 42:LV:129:TRP:HB2 | 42:LV:132:ILE:HG12 | 1.93                     | 0.51              |
| 46:La:132:ARG:HA  | 46:La:135:GLU:OE2  | 2.11                     | 0.51              |
| 47:Lb:13:SER:HA   | 47:Lb:16:TRP:NE1   | 2.26                     | 0.51              |
| 48:Lc:58:SER:HA   | 48:Lc:61:GLU:OE1   | 2.10                     | 0.51              |
| 50:Le:55:MET:SD   | 50:Le:56:PRO:HD2   | 2.51                     | 0.51              |
| 66:SF:91:ARG:HH21 | 66:SF:92:ILE:HG22  | 1.76                     | 0.51              |
| 71:ST:65:TYR:CD2  | 71:ST:66:LEU:HD22  | 2.44                     | 0.51              |
| 71:ST:103:VAL:O   | 71:ST:107:LEU:HG   | 2.10                     | 0.51              |
| 73:Sc:29:GLN:HE22 | 73:Sc:45:ASN:HB3   | 1.75                     | 0.51              |
| 75:Sg:15:ASN:HA   | 75:Sg:305:ASN:HD22 | 1.76                     | 0.51              |
| 79:S2:155:G:H2'   | 79:S2:156:G:H8     | 1.76                     | 0.51              |
| 79:S2:185:G:O6    | 79:S2:214:U:O4     | 2.28                     | 0.51              |
| 79:S2:874:G:H2'   | 79:S2:875:A:H8     | 1.76                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 79:S2:1067:C:H3'   | 79:S2:1068:G:H8    | 1.75                     | 0.51              |
| 79:S2:1107:G:C6    | 79:S2:1126:G:C6    | 2.98                     | 0.51              |
| 79:S2:1783:C:O2    | 87:LW:71:ARG:NH1   | 2.43                     | 0.51              |
| 1:CH:104:GLN:C     | 65:SD:178:ARG:HH12 | 2.18                     | 0.51              |
| 1:cH:44:TRP:HD1    | 9:se:53:LYS:HG2    | 1.76                     | 0.51              |
| 2:sE:67:GLN:HB3    | 2:sE:69:PHE:HE1    | 1.76                     | 0.51              |
| 2:sE:153:LEU:O     | 2:sE:174:LYS:NZ    | 2.39                     | 0.51              |
| 6:sG:10:THR:HB     | 6:sG:128:THR:OG1   | 2.11                     | 0.51              |
| 7:sJ:176:LYS:NZ    | 79:s2:587:A:OP1    | 2.44                     | 0.51              |
| 10:sA:11:LYS:HZ2   | 10:sA:184:ARG:HH22 | 1.59                     | 0.51              |
| 15:sC:82:TYR:CE2   | 15:sC:164:PRO:HD3  | 2.45                     | 0.51              |
| 15:sC:188:CYS:HB3  | 15:sC:239:ALA:HB2  | 1.92                     | 0.51              |
| 19:sb:81:ARG:HH11  | 19:sb:82:LYS:N     | 2.09                     | 0.51              |
| 20:l7:6:C:H4'      | 25:lD:52:ILE:HD13  | 1.93                     | 0.51              |
| 24:lC:217:ILE:HD11 | 24:lC:221:PHE:CE2  | 2.46                     | 0.51              |
| 24:lC:252:TRP:CZ3  | 24:lC:260:LEU:HD21 | 2.46                     | 0.51              |
| 26:lE:95:PRO:HA    | 26:lE:104:THR:HG22 | 1.92                     | 0.51              |
| 28:lG:43:GLN:HE22  | 85:l5:4116:C:H3'   | 1.76                     | 0.51              |
| 29:lH:63:ASN:ND2   | 29:lH:66:GLU:OE2   | 2.44                     | 0.51              |
| 34:lN:140:LYS:HE2  | 34:lN:144:ARG:HH21 | 1.75                     | 0.51              |
| 35:lO:44:SER:OG    | 35:lO:45:GLY:N     | 2.40                     | 0.51              |
| 37:lQ:63:LEU:HD12  | 37:lQ:66:MET:HE3   | 1.93                     | 0.51              |
| 37:lQ:152:PHE:CZ   | 85:l5:1847:C:H4'   | 2.46                     | 0.51              |
| 38:lR:134:ASN:HD21 | 85:l5:2897:G:P     | 2.34                     | 0.51              |
| 39:lS:131:GLU:C    | 39:lS:132:ILE:HD13 | 2.35                     | 0.51              |
| 44:lY:47:MET:HE3   | 44:lY:48:PRO:CD    | 2.40                     | 0.51              |
| 50:le:67:LYS:NZ    | 85:l5:2319:C:OP1   | 2.43                     | 0.51              |
| 58:lm:79:GLU:OE2   | 58:lm:81:SER:N     | 2.33                     | 0.51              |
| 60:lo:99:ARG:HH12  | 60:lo:102:GLN:CB   | 2.13                     | 0.51              |
| 61:lp:48:LYS:NZ    | 61:lp:49:ARG:O     | 2.44                     | 0.51              |
| 62:lr:2:SER:OG     | 62:lr:3:ALA:N      | 2.40                     | 0.51              |
| 75:sg:178:ASN:OD1  | 75:sg:183:LYS:N    | 2.33                     | 0.51              |
| 76:sM:94:ILE:O     | 76:sM:94:ILE:HG13  | 2.09                     | 0.51              |
| 78:sf:89:LYS:NZ    | 79:s2:1269:G:O3'   | 2.44                     | 0.51              |
| 79:s2:15:U:H2'     | 79:s2:16:G:O4'     | 2.11                     | 0.51              |
| 79:s2:59:U:O2'     | 79:s2:61:A:N7      | 2.34                     | 0.51              |
| 79:s2:160:U:O2'    | 79:s2:161:U:H3'    | 2.10                     | 0.51              |
| 79:s2:215:G:H2'    | 79:s2:216:C:C6     | 2.46                     | 0.51              |
| 79:s2:910:G:H2'    | 79:s2:911:C:C6     | 2.46                     | 0.51              |
| 79:s2:942:G:H2'    | 79:s2:943:U:C6     | 2.45                     | 0.51              |
| 80:cB:233:VAL:HG21 | 80:cB:253:VAL:HG12 | 1.93                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 80:cB:396:MET:CB   | 80:cB:485:ILE:HB   | 2.40                     | 0.51              |
| 82:pE:6:G:H2'      | 82:pE:7:A:H8       | 1.76                     | 0.51              |
| 85:l5:474:C:H2'    | 85:l5:475:G:C8     | 2.45                     | 0.51              |
| 85:l5:2104:G:H3'   | 85:l5:2105:A:C8    | 2.46                     | 0.51              |
| 85:l5:2810:U:H2'   | 85:l5:2811:G:O4'   | 2.11                     | 0.51              |
| 85:l5:3920:U:H2'   | 85:l5:3921:U:C6    | 2.46                     | 0.51              |
| 85:l5:4062:A:H2'   | 85:l5:4063:U:C5    | 2.46                     | 0.51              |
| 85:l5:4595:G:H2'   | 85:l5:4596:C:H6    | 1.76                     | 0.51              |
| 85:l5:4992:G:H2'   | 85:l5:4993:G:H8    | 1.73                     | 0.51              |
| 80:CB:368:ARG:HH11 | 80:CB:371:LEU:HD11 | 1.76                     | 0.51              |
| 80:CB:396:MET:SD   | 80:CB:416:VAL:HG22 | 2.50                     | 0.51              |
| 80:CB:451:ILE:HD12 | 80:CB:458:VAL:HG11 | 1.93                     | 0.51              |
| 80:CB:485:ILE:HD12 | 80:CB:486:THR:N    | 2.26                     | 0.51              |
| 80:CB:503:PRO:HB2  | 80:CB:547:ALA:HB1  | 1.92                     | 0.51              |
| 80:CB:756:VAL:O    | 80:CB:759:ILE:HG22 | 2.11                     | 0.51              |
| 80:CB:770:VAL:HG22 | 80:CB:786:ALA:HB2  | 1.92                     | 0.51              |
| 2:SE:59:ASP:O      | 2:SE:62:LYS:HG3    | 2.11                     | 0.51              |
| 5:SX:101:LEU:HB3   | 5:SX:124:LYS:HB2   | 1.93                     | 0.51              |
| 6:SG:41:LEU:HB3    | 6:SG:45:TRP:CG     | 2.46                     | 0.51              |
| 7:SJ:5:ARG:HB3     | 79:S2:38:A:H5''    | 1.93                     | 0.51              |
| 10:SA:63:ARG:HA    | 10:SA:66:VAL:HG22  | 1.93                     | 0.51              |
| 10:SA:65:ILE:O     | 10:SA:68:ILE:HG13  | 2.11                     | 0.51              |
| 10:SA:208:GLU:O    | 10:SA:212:LYS:NZ   | 2.36                     | 0.51              |
| 11:SB:103:MET:HG2  | 11:SB:188:LEU:HD21 | 1.92                     | 0.51              |
| 12:SH:31:GLU:OE2   | 12:SH:37:LYS:NZ    | 2.41                     | 0.51              |
| 12:SH:169:LYS:HB2  | 12:SH:173:PHE:CZ   | 2.46                     | 0.51              |
| 13:SV:59:ILE:HA    | 13:SV:62:MET:SD    | 2.51                     | 0.51              |
| 13:SV:80:SER:HB2   | 13:SV:83:PHE:CE2   | 2.46                     | 0.51              |
| 18:SW:44:HIS:HB3   | 18:SW:46:TYR:CE1   | 2.45                     | 0.51              |
| 18:SW:53:ILE:CG2   | 18:SW:60:LYS:HB2   | 2.41                     | 0.51              |
| 85:L5:10:A:H2'     | 85:L5:11:G:H8      | 1.76                     | 0.51              |
| 85:L5:248:C:H2'    | 85:L5:249:C:H6     | 1.76                     | 0.51              |
| 85:L5:968:C:H5''   | 26:LE:110:ARG:NH1  | 2.25                     | 0.51              |
| 85:L5:1080:C:N3    | 85:L5:1220:G:N1    | 2.58                     | 0.51              |
| 85:L5:2081:C:H2'   | 85:L5:2082:G:H8    | 1.76                     | 0.51              |
| 85:L5:2386:U:H4'   | 38:LR:24:LEU:HD12  | 1.91                     | 0.51              |
| 85:L5:4176:C:H2'   | 85:L5:4177:C:H6    | 1.76                     | 0.51              |
| 85:L5:5002:U:H2'   | 85:L5:5003:U:C6    | 2.46                     | 0.51              |
| 85:L5:5040:U:OP2   | 23:LB:396:ARG:NH1  | 2.43                     | 0.51              |
| 21:L8:153:C:H2'    | 21:L8:154:G:H8     | 1.73                     | 0.51              |
| 27:LF:131:ASN:O    | 27:LF:135:ILE:HG13 | 2.10                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 29:LH:64:ARG:HA    | 29:LH:67:LEU:HB2   | 1.91                     | 0.51              |
| 29:LH:177:ASP:O    | 29:LH:180:TYR:OH   | 2.23                     | 0.51              |
| 32:LL:175:ASN:OD1  | 32:LL:175:ASN:N    | 2.37                     | 0.51              |
| 42:LV:87:SER:HB3   | 42:LV:95:PHE:HB3   | 1.93                     | 0.51              |
| 65:SD:156:LEU:HD11 | 79:S2:1384:C:H5'   | 1.92                     | 0.51              |
| 73:Sc:21:THR:N     | 73:Sc:27:CYS:O     | 2.28                     | 0.51              |
| 75:Sg:199:THR:O    | 75:Sg:208:ALA:N    | 2.38                     | 0.51              |
| 77:SZ:79:ILE:HG21  | 77:SZ:84:ALA:HB2   | 1.92                     | 0.51              |
| 78:Sf:123:SER:O    | 78:Sf:127:GLY:N    | 2.43                     | 0.51              |
| 79:S2:909:G:H2'    | 79:S2:910:G:C8     | 2.46                     | 0.51              |
| 79:S2:1103:C:H2'   | 79:S2:1104:G:H8    | 1.76                     | 0.51              |
| 79:S2:1289:U:H2'   | 79:S2:1290:G:H8    | 1.74                     | 0.51              |
| 1:CH:88:LYS:HG3    | 1:CH:90:LEU:HG     | 1.91                     | 0.51              |
| 1:cH:54:ILE:HG13   | 9:se:59:SER:O      | 2.10                     | 0.51              |
| 4:sL:82:MET:HE3    | 4:sL:83:GLN:O      | 2.11                     | 0.51              |
| 5:sX:81:ILE:HD12   | 5:sX:82:THR:H      | 1.76                     | 0.51              |
| 6:sG:7:PHE:CE1     | 6:sG:113:ILE:HD13  | 2.45                     | 0.51              |
| 8:sY:19:GLN:NE2    | 8:sY:81:TYR:CD1    | 2.79                     | 0.51              |
| 10:sA:17:LYS:CE    | 64:sR:91:LEU:HG    | 2.41                     | 0.51              |
| 10:sA:211:GLU:N    | 10:sA:211:GLU:OE1  | 2.43                     | 0.51              |
| 16:sN:39:LYS:HA    | 16:sN:42:LYS:NZ    | 2.26                     | 0.51              |
| 16:sN:92:ILE:HG13  | 16:sN:149:LEU:HD11 | 1.92                     | 0.51              |
| 23:IB:140:GLU:HA   | 23:IB:143:LYS:HE2  | 1.91                     | 0.51              |
| 23:IB:302:ASN:ND2  | 23:IB:314:ILE:N    | 2.54                     | 0.51              |
| 26:IE:168:LEU:HG   | 26:IE:174:LEU:HB2  | 1.92                     | 0.51              |
| 31:IJ:7:GLU:HA     | 31:IJ:10:ASN:OD1   | 2.10                     | 0.51              |
| 33:IM:6:PHE:O      | 33:IM:11:ARG:NE    | 2.43                     | 0.51              |
| 33:IM:122:ILE:HD11 | 35:IO:189:ILE:HD11 | 1.92                     | 0.51              |
| 40:IT:130:ARG:NH2  | 85:I5:1802:A:N3    | 2.40                     | 0.51              |
| 45:IZ:116:VAL:HA   | 45:IZ:119:GLU:OE2  | 2.11                     | 0.51              |
| 47:Ib:56:LYS:HE3   | 85:I5:1812:C:H4'   | 1.92                     | 0.51              |
| 69:sQ:13:PHE:CD2   | 79:s2:1442:U:O2'   | 2.64                     | 0.51              |
| 75:sg:139:LYS:O    | 75:sg:140:TYR:HD1  | 1.94                     | 0.51              |
| 79:s2:88:G:H2'     | 79:s2:89:C:C6      | 2.46                     | 0.51              |
| 79:s2:1023:A:H2'   | 79:s2:1024:A:C8    | 2.46                     | 0.51              |
| 80:cB:10:ARG:NH1   | 80:cB:463:ASP:OD1  | 2.43                     | 0.51              |
| 84:lt:125:LEU:HG   | 84:lt:127:GLY:H    | 1.75                     | 0.51              |
| 85:I5:153:G:H2'    | 85:I5:154:G:H8     | 1.76                     | 0.51              |
| 85:I5:186:G:N2     | 85:I5:1365:C:O2'   | 2.44                     | 0.51              |
| 85:I5:1095:A:H2'   | 85:I5:1096:C:H6    | 1.75                     | 0.51              |
| 85:I5:1373:A:H2'   | 85:I5:1374:G:H8    | 1.74                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 85:L5:1402:C:C2    | 85:L5:1415:G:N2    | 2.74                     | 0.51              |
| 85:L5:1855:G:H2'   | 85:L5:1856:C:C6    | 2.46                     | 0.51              |
| 85:L5:1978:C:H2'   | 85:L5:1979:A:C8    | 2.46                     | 0.51              |
| 85:L5:3662:A:C8    | 85:L5:3664:G:C4    | 2.99                     | 0.51              |
| 85:L5:4262:C:H2'   | 85:L5:4263:C:H6    | 1.75                     | 0.51              |
| 85:L5:4941:G:H2'   | 85:L5:4942:C:C6    | 2.45                     | 0.51              |
| 80:CB:176:GLN:HE21 | 80:CB:180:ARG:HH11 | 1.59                     | 0.51              |
| 2:SE:164:LEU:C     | 2:SE:166:THR:H     | 2.17                     | 0.51              |
| 4:SL:27:GLU:C      | 4:SL:29:GLY:HA2    | 2.36                     | 0.51              |
| 5:SX:119:ARG:NH1   | 79:S2:1192:U:OP2   | 2.44                     | 0.51              |
| 12:SH:25:GLN:O     | 12:SH:29:GLU:HG3   | 2.10                     | 0.51              |
| 13:SV:68:SER:O     | 13:SV:72:LEU:HG    | 2.10                     | 0.51              |
| 85:L5:197:A:N1     | 85:L5:225:G:O2'    | 2.40                     | 0.51              |
| 85:L5:1415:G:H2'   | 85:L5:1416:G:C8    | 2.46                     | 0.51              |
| 85:L5:1519:C:H2'   | 85:L5:1520:C:H6    | 1.75                     | 0.51              |
| 85:L5:1655:C:OP2   | 46:La:26:ARG:NH1   | 2.43                     | 0.51              |
| 85:L5:1985:G:N2    | 85:L5:2003:G:HO2'  | 2.09                     | 0.51              |
| 85:L5:2498:C:H2'   | 85:L5:2499:C:H6    | 1.76                     | 0.51              |
| 85:L5:2505:C:N4    | 85:L5:4084:G:H4'   | 2.26                     | 0.51              |
| 85:L5:3923:A:H2'   | 85:L5:3924:C:C6    | 2.46                     | 0.51              |
| 85:L5:4070:U:H2'   | 85:L5:4071:U:C6    | 2.46                     | 0.51              |
| 85:L5:4344:U:H2'   | 85:L5:4345:C:H6    | 1.76                     | 0.51              |
| 85:L5:4612:C:C2    | 29:LH:120:GLU:HB2  | 2.46                     | 0.51              |
| 20:L7:63:C:H5'     | 20:L7:64:G:H5''    | 1.92                     | 0.51              |
| 27:LF:105:VAL:HA   | 27:LF:108:VAL:HG12 | 1.92                     | 0.51              |
| 27:LF:115:ARG:NH1  | 37:LQ:5:ILE:HD13   | 2.26                     | 0.51              |
| 31:LJ:88:LYS:HG2   | 31:LJ:92:TYR:HE2   | 1.76                     | 0.51              |
| 33:LM:30:VAL:O     | 39:LS:98:ARG:NH2   | 2.44                     | 0.51              |
| 35:LO:37:ARG:HB2   | 35:LO:108:ILE:HD11 | 1.92                     | 0.51              |
| 46:La:74:ASN:OD1   | 46:La:114:LYS:N    | 2.41                     | 0.51              |
| 46:La:131:ARG:HG2  | 46:La:135:GLU:OE1  | 2.11                     | 0.51              |
| 62:Lr:66:ARG:HD3   | 62:Lr:69:GLY:H     | 1.75                     | 0.51              |
| 66:SF:33:ILE:HG13  | 73:Sc:11:LEU:HD12  | 1.93                     | 0.51              |
| 68:SP:38:SER:HA    | 70:SS:88:LYS:NZ    | 2.25                     | 0.51              |
| 70:SS:132:ARG:HH21 | 79:S2:1609:C:H3'   | 1.74                     | 0.51              |
| 71:ST:102:ARG:HH22 | 79:S2:1565:C:P     | 2.33                     | 0.51              |
| 74:Sd:14:PHE:HD2   | 79:S2:1661:A:N7    | 2.09                     | 0.51              |
| 76:SM:120:ALA:O    | 76:SM:124:ILE:HG12 | 2.10                     | 0.51              |
| 77:SZ:47:LEU:HA    | 77:SZ:78:LYS:HE3   | 1.92                     | 0.51              |
| 79:S2:198:U:H2'    | 79:S2:199:C:H2'    | 1.91                     | 0.51              |
| 79:S2:459:C:H3'    | 79:S2:460:A:H8     | 1.76                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 79:S2:549:C:H2'    | 79:S2:550:C:C6     | 2.45                     | 0.51              |
| 79:S2:804:U:H3     | 79:S2:859:G:H1     | 1.59                     | 0.51              |
| 79:S2:1545:A:H2'   | 79:S2:1546:G:C8    | 2.46                     | 0.51              |
| 79:S2:1577:G:H1'   | 79:S2:1582:C:O2    | 2.10                     | 0.51              |
| 79:S2:1774:C:C4    | 79:S2:1775:U:H1'   | 2.46                     | 0.51              |
| 1:cH:133:ARG:HD2   | 1:cH:134:GLY:H     | 1.75                     | 0.51              |
| 15:sC:166:ARG:HH22 | 15:sC:255:LEU:HD11 | 1.76                     | 0.51              |
| 18:sW:85:ASP:OD1   | 18:sW:85:ASP:N     | 2.44                     | 0.51              |
| 20:l7:8:G:H2'      | 20:l7:9:C:O4'      | 2.11                     | 0.51              |
| 24:lC:284:MET:HG3  | 24:lC:287:THR:HB   | 1.93                     | 0.51              |
| 25:lD:152:ARG:NH2  | 85:l5:4239:A:O2'   | 2.44                     | 0.51              |
| 32:lL:60:ARG:HD2   | 32:lL:67:HIS:O     | 2.11                     | 0.51              |
| 36:lP:22:LEU:HD13  | 36:lP:146:ILE:HG22 | 1.93                     | 0.51              |
| 36:lP:107:LEU:HD11 | 36:lP:152:GLU:OE1  | 2.10                     | 0.51              |
| 38:lR:108:ARG:O    | 38:lR:111:GLU:HG3  | 2.09                     | 0.51              |
| 38:lR:175:GLU:O    | 38:lR:178:GLN:HG3  | 2.11                     | 0.51              |
| 40:lT:2:THR:OG1    | 85:l5:4220:A:OP2   | 2.18                     | 0.51              |
| 51:lf:83:MET:HE1   | 85:l5:1917:A:P     | 2.51                     | 0.51              |
| 55:lj:50:SER:OG    | 55:lj:53:ALA:HB3   | 2.11                     | 0.51              |
| 61:lp:10:ILE:HG22  | 61:lp:27:LYS:HG3   | 1.93                     | 0.51              |
| 63:lz:155:ILE:HD13 | 63:lz:168:ALA:O    | 2.11                     | 0.51              |
| 63:lz:209:THR:OG1  | 85:l5:4052:C:O2    | 2.21                     | 0.51              |
| 64:sR:12:ALA:HA    | 79:s2:1372:U:H2'   | 1.92                     | 0.51              |
| 67:sK:43:LEU:HD11  | 79:s2:1274:G:C5    | 2.46                     | 0.51              |
| 75:sg:255:SER:HA   | 75:sg:272:GLN:HE22 | 1.76                     | 0.51              |
| 76:sM:52:LEU:HD21  | 76:sM:62:VAL:HG13  | 1.92                     | 0.51              |
| 77:sZ:69:THR:H     | 77:sZ:72:VAL:HG12  | 1.76                     | 0.51              |
| 79:s2:301:A:N6     | 79:s2:302:A:H62    | 2.08                     | 0.51              |
| 79:s2:793:G:H2'    | 79:s2:794:A:H8     | 1.76                     | 0.51              |
| 79:s2:822:U:C2     | 79:s2:826:A:N6     | 2.79                     | 0.51              |
| 79:s2:1681:U:H2'   | 79:s2:1682:C:C6    | 2.45                     | 0.51              |
| 79:s2:1690:U:H2'   | 79:s2:1691:U:H6    | 1.76                     | 0.51              |
| 80:cB:256:MET:HA   | 80:cB:259:LYS:HB3  | 1.92                     | 0.51              |
| 80:cB:430:MET:HA   | 80:cB:441:ASP:O    | 2.11                     | 0.51              |
| 80:cB:602:LEU:HD13 | 80:cB:707:VAL:HG12 | 1.92                     | 0.51              |
| 81:aP:3:C:H42      | 81:aP:70:A:N6      | 2.07                     | 0.51              |
| 83:ls:120:GLU:OE2  | 83:ls:122:THR:OG1  | 2.29                     | 0.51              |
| 84:lt:137:GLN:CD   | 84:lt:137:GLN:H    | 2.19                     | 0.51              |
| 85:l5:1646:A:H2'   | 85:l5:1647:U:C6    | 2.46                     | 0.51              |
| 85:l5:2727:C:H2'   | 85:l5:2728:U:C6    | 2.46                     | 0.51              |
| 85:l5:4395:U:O2'   | 85:l5:4447:C:N4    | 2.44                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 85:L5:4723:A:H2'   | 85:L5:4724:A:C8    | 2.46                     | 0.51              |
| 80:CB:10:ARG:HA    | 80:CB:13:MET:SD    | 2.51                     | 0.51              |
| 80:CB:481:LYS:HZ1  | 80:CB:533:MET:C    | 2.19                     | 0.51              |
| 80:CB:760:TYR:O    | 80:CB:764:ASN:ND2  | 2.43                     | 0.51              |
| 5:SX:84:PHE:HD1    | 5:SX:105:PHE:CZ    | 2.26                     | 0.51              |
| 6:SG:31:ARG:O      | 6:SG:34:THR:OG1    | 2.23                     | 0.51              |
| 6:SG:63:MET:HE3    | 6:SG:99:GLY:O      | 2.11                     | 0.51              |
| 10:SA:167:GLY:O    | 10:SA:170:SER:OG   | 2.20                     | 0.51              |
| 10:SA:186:ARG:HG3  | 13:SV:46:PHE:CZ    | 2.46                     | 0.51              |
| 12:SH:167:GLU:CD   | 12:SH:168:HIS:HD1  | 2.19                     | 0.51              |
| 13:SV:21:ASN:ND2   | 18:SW:66:THR:O     | 2.39                     | 0.51              |
| 15:SC:209:VAL:HA   | 15:SC:212:LYS:HE2  | 1.93                     | 0.51              |
| 18:SW:23:ARG:HE    | 18:SW:24:GLN:N     | 2.09                     | 0.51              |
| 85:L5:315:G:C8     | 46:La:62:HIS:HB2   | 2.46                     | 0.51              |
| 85:L5:654:C:H5'    | 24:LC:268:ARG:HH22 | 1.76                     | 0.51              |
| 85:L5:1077:C:OP1   | 85:L5:1215:C:O2'   | 2.27                     | 0.51              |
| 85:L5:2375:A:OP1   | 49:Ld:63:ARG:NE    | 2.37                     | 0.51              |
| 85:L5:2496:G:H2'   | 85:L5:2497:C:H6    | 1.76                     | 0.51              |
| 85:L5:2540:C:H2'   | 85:L5:2541:G:C8    | 2.46                     | 0.51              |
| 85:L5:2558:C:H2'   | 85:L5:2559:G:C8    | 2.46                     | 0.51              |
| 85:L5:3919:C:OP1   | 22:LA:2:GLY:N      | 2.43                     | 0.51              |
| 85:L5:4566:U:O2'   | 23:LB:269:ALA:O    | 2.22                     | 0.51              |
| 85:L5:4654:C:H2'   | 85:L5:4655:A:C8    | 2.46                     | 0.51              |
| 23:LB:393:LYS:HG3  | 23:LB:396:ARG:NH2  | 2.25                     | 0.51              |
| 24:LC:67:TRP:NE1   | 24:LC:71:ARG:HD2   | 2.26                     | 0.51              |
| 24:LC:179:ASP:OD1  | 24:LC:207:PRO:HD3  | 2.11                     | 0.51              |
| 25:LD:48:LYS:HD2   | 25:LD:145:TYR:HE2  | 1.74                     | 0.51              |
| 26:LE:174:LEU:HD11 | 26:LE:186:LEU:HD12 | 1.92                     | 0.51              |
| 26:LE:212:LEU:HA   | 26:LE:216:TYR:HD2  | 1.75                     | 0.51              |
| 29:LH:168:LYS:O    | 29:LH:169:ASN:ND2  | 2.44                     | 0.51              |
| 32:LL:108:GLU:H    | 32:LL:108:GLU:CD   | 2.11                     | 0.51              |
| 32:LL:154:VAL:HG22 | 32:LL:155:MET:CE   | 2.41                     | 0.51              |
| 37:LQ:186:TYR:HE2  | 37:LQ:188:ASN:ND2  | 2.08                     | 0.51              |
| 39:LS:54:MET:HE1   | 39:LS:58:SER:O     | 2.11                     | 0.51              |
| 60:Lo:56:PHE:HB3   | 60:Lo:59:LYS:HZ3   | 1.75                     | 0.51              |
| 65:SD:15:GLY:HA2   | 65:SD:18:LYS:HE3   | 1.92                     | 0.51              |
| 66:SF:40:ALA:HA    | 66:SF:45:TYR:OH    | 2.11                     | 0.51              |
| 66:SF:40:ALA:HB3   | 66:SF:68:ILE:N     | 2.26                     | 0.51              |
| 66:SF:103:LEU:HD13 | 77:SZ:67:LEU:HD21  | 1.93                     | 0.51              |
| 69:SQ:105:LYS:HG2  | 69:SQ:109:LYS:HE3  | 1.92                     | 0.51              |
| 70:SS:98:VAL:HG22  | 70:SS:103:LEU:HD22 | 1.93                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 79:S2:1318:G:H2'   | 79:S2:1319:U:C6    | 2.46                     | 0.51              |
| 3:sI:51:GLY:HA3    | 79:s2:445:A:H5'    | 1.92                     | 0.51              |
| 3:sI:157:LYS:HD3   | 3:sI:158:ILE:H     | 1.75                     | 0.51              |
| 4:sL:74:SER:HA     | 4:sL:127:THR:HA    | 1.93                     | 0.51              |
| 8:sY:18:LEU:CD1    | 8:sY:85:ASN:HD22   | 2.24                     | 0.51              |
| 10:sA:206:ASP:HB2  | 10:sA:207:PRO:HD3  | 1.93                     | 0.51              |
| 14:sa:13:LYS:HZ3   | 79:s2:1132:C:H2'   | 1.76                     | 0.51              |
| 21:l8:75:G:O2'     | 57:ll:29:MET:HE1   | 2.11                     | 0.51              |
| 25:lD:122:GLN:O    | 25:lD:248:ARG:NH2  | 2.43                     | 0.51              |
| 25:lD:181:PRO:HD2  | 25:lD:195:HIS:ND1  | 2.26                     | 0.51              |
| 28:lG:210:GLU:OE1  | 28:lG:210:GLU:N    | 2.38                     | 0.51              |
| 29:lH:180:TYR:HB3  | 58:lm:89:TYR:HD1   | 1.75                     | 0.51              |
| 30:ll:98:ARG:HH21  | 85:l5:1865:G:P     | 2.33                     | 0.51              |
| 31:lJ:48:PRO:HB2   | 31:lJ:70:VAL:HG22  | 1.93                     | 0.51              |
| 31:lJ:151:ILE:HD11 | 31:lJ:156:ARG:HG3  | 1.93                     | 0.51              |
| 33:lM:39:ASP:OD2   | 33:lM:47:ARG:HA    | 2.11                     | 0.51              |
| 36:lP:18:ARG:C     | 36:lP:94:MET:HE1   | 2.36                     | 0.51              |
| 39:lS:60:GLU:CD    | 40:lT:136:ARG:HH22 | 2.18                     | 0.51              |
| 41:lU:40:GLU:OE2   | 41:lU:65:ARG:NH1   | 2.44                     | 0.51              |
| 48:lc:45:LEU:HD23  | 48:lc:46:VAL:N     | 2.26                     | 0.51              |
| 53:lh:105:LYS:HA   | 53:lh:108:GLN:CD   | 2.36                     | 0.51              |
| 56:lk:52:LYS:O     | 56:lk:56:LEU:HG    | 2.11                     | 0.51              |
| 63:lz:118:LYS:O    | 63:lz:121:PRO:HD2  | 2.11                     | 0.51              |
| 67:sK:4:PRO:HA     | 79:s2:1314:U:H6    | 1.75                     | 0.51              |
| 69:sQ:75:GLY:O     | 79:s2:1544:C:O2'   | 2.26                     | 0.51              |
| 70:sS:137:LYS:NZ   | 79:s2:1521:C:N3    | 2.54                     | 0.51              |
| 79:s2:96:C:H2'     | 79:s2:97:U:C6      | 2.45                     | 0.51              |
| 79:s2:1590:C:H3'   | 79:s2:1591:C:H6    | 1.75                     | 0.51              |
| 80:cB:135:VAL:HG21 | 80:cB:184:ASN:OD1  | 2.11                     | 0.51              |
| 80:cB:287:ARG:HG2  | 80:cB:290:CYS:SG   | 2.51                     | 0.51              |
| 80:cB:716:ARG:HB2  | 80:cB:716:ARG:NH1  | 2.26                     | 0.51              |
| 83:ls:91:THR:OG1   | 83:ls:93:GLU:OE1   | 2.28                     | 0.51              |
| 85:l5:323:C:H2'    | 85:l5:324:A:H8     | 1.76                     | 0.51              |
| 85:l5:474:C:H2'    | 85:l5:475:G:H8     | 1.76                     | 0.51              |
| 85:l5:1197:C:H2'   | 85:l5:1198:G:C8    | 2.46                     | 0.51              |
| 85:l5:1617:G:H1'   | 85:l5:2513:A:N6    | 2.25                     | 0.51              |
| 85:l5:2073:C:C2    | 85:l5:2074:C:C5    | 2.99                     | 0.51              |
| 85:l5:2109:G:H2'   | 85:l5:2110:C:C6    | 2.46                     | 0.51              |
| 85:l5:2306:G:N2    | 85:l5:2331:G:O2'   | 2.43                     | 0.51              |
| 85:l5:2448:G:H2'   | 85:l5:2449:A:C8    | 2.46                     | 0.51              |
| 85:l5:2756:G:H2'   | 85:l5:2757:A:C8    | 2.46                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 85:L5:2904:U:H3'   | 85:L5:2904:U:OP2   | 2.10                     | 0.51              |
| 80:CB:675:ILE:HG12 | 80:CB:679:VAL:HG23 | 1.92                     | 0.51              |
| 2:SE:141:THR:HG22  | 2:SE:145:ARG:O     | 2.11                     | 0.51              |
| 10:SA:52:LYS:NZ    | 10:SA:53:ARG:HE    | 2.09                     | 0.51              |
| 10:SA:57:LYS:HZ3   | 13:SV:70:LEU:HD21  | 1.76                     | 0.51              |
| 15:SC:69:LEU:HD22  | 15:SC:269:PHE:CD1  | 2.46                     | 0.51              |
| 15:SC:94:ILE:HD11  | 15:SC:159:LYS:CB   | 2.40                     | 0.51              |
| 85:L5:280:G:H1     | 34:LN:15:GLN:NE2   | 2.09                     | 0.51              |
| 85:L5:1175:A:H2    | 85:L5:1185:G:H1    | 1.58                     | 0.51              |
| 85:L5:1567:U:H2'   | 85:L5:1568:C:C6    | 2.46                     | 0.51              |
| 85:L5:1834:U:N3    | 40:LT:126:VAL:O    | 2.44                     | 0.51              |
| 85:L5:2267:U:C2    | 62:Lr:24:THR:HG21  | 2.45                     | 0.51              |
| 85:L5:2375:A:H2'   | 85:L5:2376:A:H8    | 1.75                     | 0.51              |
| 85:L5:2443:G:P     | 85:L5:2516:G:H22   | 2.34                     | 0.51              |
| 85:L5:2474:G:N2    | 85:L5:2502:G:O2'   | 2.43                     | 0.51              |
| 85:L5:2744:A:H2'   | 85:L5:2745:A:C8    | 2.46                     | 0.51              |
| 85:L5:2858:A:H2'   | 85:L5:2859:G:H8    | 1.76                     | 0.51              |
| 85:L5:3606:U:H4'   | 38:LR:89:MET:SD    | 2.50                     | 0.51              |
| 85:L5:3857:G:OP1   | 36:LP:85:LYS:N     | 2.44                     | 0.51              |
| 85:L5:4089:G:H2'   | 85:L5:4090:G:H8    | 1.75                     | 0.51              |
| 85:L5:4277:G:H4'   | 40:LT:47:THR:HA    | 1.92                     | 0.51              |
| 85:L5:4518:A:OP2   | 23:LB:258:HIS:HB2  | 2.11                     | 0.51              |
| 85:L5:4637:G:H2'   | 85:L5:4638:U:C6    | 2.46                     | 0.51              |
| 85:L5:4683:U:OP2   | 85:L5:4706:G:N1    | 2.39                     | 0.51              |
| 21:L8:8:U:H2'      | 21:L8:9:A:H8       | 1.75                     | 0.51              |
| 40:LT:48:VAL:HG11  | 40:LT:94:GLU:HG3   | 1.92                     | 0.51              |
| 47:Lb:40:LEU:CA    | 47:Lb:43:MET:HG2   | 2.41                     | 0.51              |
| 50:Le:79:VAL:HG21  | 50:Le:85:LEU:CD1   | 2.41                     | 0.51              |
| 52:Lg:15:THR:HG22  | 52:Lg:18:ASN:HB2   | 1.93                     | 0.51              |
| 66:SF:79:HIS:N     | 66:SF:82:ASN:OD1   | 2.44                     | 0.51              |
| 67:SK:60:GLU:OE2   | 79:S2:1497:G:N2    | 2.43                     | 0.51              |
| 70:SS:26:ILE:HD12  | 70:SS:59:LEU:HD21  | 1.92                     | 0.51              |
| 72:SU:56:MET:CE    | 79:S2:1580:A:H5'   | 2.39                     | 0.51              |
| 75:Sg:172:LYS:HA   | 75:Sg:194:TYR:HA   | 1.93                     | 0.51              |
| 77:SZ:80:ARG:O     | 79:S2:1598:G:O2'   | 2.23                     | 0.51              |
| 77:SZ:94:LYS:NZ    | 77:SZ:96:LEU:HB3   | 2.26                     | 0.51              |
| 79:S2:517:C:H2'    | 79:S2:518:G:O4'    | 2.11                     | 0.51              |
| 79:S2:963:A:H2'    | 79:S2:964:A:C8     | 2.46                     | 0.51              |
| 79:S2:980:A:H2'    | 79:S2:981:A:H8     | 1.76                     | 0.51              |
| 79:S2:1686:G:H2'   | 79:S2:1687:C:H6    | 1.75                     | 0.51              |
| 79:S2:1700:C:O2    | 79:S2:1834:A:N6    | 2.43                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 83:Ls:28:PHE:CE2   | 83:Ls:95:LEU:HB2   | 2.46                     | 0.51              |
| 83:Ls:143:ILE:HD13 | 83:Ls:158:VAL:HG21 | 1.93                     | 0.51              |
| 87:IW:33:ASN:O     | 87:IW:37:GLU:HG2   | 2.10                     | 0.51              |
| 1:CH:38:VAL:HG13   | 86:Se:44:ASN:HB2   | 1.93                     | 0.50              |
| 1:CH:117:ASN:ND2   | 1:CH:119:GLN:HG2   | 2.26                     | 0.50              |
| 2:sE:60:GLU:O      | 2:sE:64:ILE:HG12   | 2.11                     | 0.50              |
| 4:sL:97:ARG:CZ     | 79:s2:421:G:H5''   | 2.41                     | 0.50              |
| 11:sB:125:VAL:HG11 | 11:sB:172:MET:HE1  | 1.93                     | 0.50              |
| 12:sH:17:ASP:OD1   | 12:sH:17:ASP:N     | 2.41                     | 0.50              |
| 14:sa:5:ARG:NH2    | 79:s2:1864:U:H3'   | 2.26                     | 0.50              |
| 22:lA:179:ILE:HB   | 85:l5:3653:A:H4'   | 1.92                     | 0.50              |
| 23:lB:53:MET:CB    | 23:lB:77:THR:HA    | 2.41                     | 0.50              |
| 25:lD:40:ASP:OD1   | 25:lD:41:LYS:N     | 2.44                     | 0.50              |
| 25:lD:180:PHE:HB3  | 25:lD:195:HIS:CE1  | 2.46                     | 0.50              |
| 31:lJ:13:ARG:O     | 31:lJ:136:ARG:NH1  | 2.45                     | 0.50              |
| 33:lM:118:MET:HA   | 33:lM:121:ARG:HB2  | 1.92                     | 0.50              |
| 43:lX:62:ARG:NH2   | 85:l5:16:G:OP1     | 2.44                     | 0.50              |
| 52:lg:25:THR:HG23  | 52:lg:27:GLY:N     | 2.26                     | 0.50              |
| 53:lh:28:LEU:O     | 53:lh:28:LEU:HD23  | 2.11                     | 0.50              |
| 63:lz:157:PHE:HD2  | 63:lz:167:VAL:HG21 | 1.76                     | 0.50              |
| 64:sR:8:THR:HA     | 64:sR:11:LYS:HE3   | 1.92                     | 0.50              |
| 67:sK:31:LYS:HD3   | 67:sK:39:ASN:HA    | 1.93                     | 0.50              |
| 70:sS:60:THR:HG22  | 70:sS:63:GLU:OE2   | 2.11                     | 0.50              |
| 70:sS:67:VAL:O     | 70:sS:70:ILE:N     | 2.44                     | 0.50              |
| 71:sT:18:LEU:O     | 71:sT:22:LEU:HG    | 2.11                     | 0.50              |
| 71:sT:131:LEU:O    | 71:sT:134:ILE:HG22 | 2.10                     | 0.50              |
| 77:sZ:94:LYS:HG3   | 77:sZ:96:LEU:HD22  | 1.93                     | 0.50              |
| 79:s2:185:G:H2'    | 79:s2:186:C:H6     | 1.76                     | 0.50              |
| 79:s2:555:A:N3     | 79:s2:556:U:H5     | 2.09                     | 0.50              |
| 79:s2:949:G:H2'    | 79:s2:950:C:H6     | 1.76                     | 0.50              |
| 79:s2:1287:A:C5    | 79:s2:1288:U:H1'   | 2.46                     | 0.50              |
| 79:s2:1386:A:H8    | 79:s2:1386:A:O5'   | 1.94                     | 0.50              |
| 80:cB:572:LYS:HE2  | 80:cB:572:LYS:HA   | 1.93                     | 0.50              |
| 85:l5:424:U:H2'    | 85:l5:425:U:C6     | 2.46                     | 0.50              |
| 85:l5:1568:C:H2'   | 85:l5:1569:U:H6    | 1.76                     | 0.50              |
| 85:l5:1687:U:H2'   | 85:l5:1688:G:C8    | 2.46                     | 0.50              |
| 85:l5:1777:C:H2'   | 85:l5:1778:C:C6    | 2.45                     | 0.50              |
| 85:l5:2299:G:C2    | 85:l5:2336:G:C5    | 2.99                     | 0.50              |
| 85:l5:2732:G:H2'   | 85:l5:2733:C:H6    | 1.76                     | 0.50              |
| 85:l5:3967:G:H5''  | 85:l5:3969:G:C2    | 2.47                     | 0.50              |
| 85:l5:4461:C:H1'   | 85:l5:4516:G:N2    | 2.26                     | 0.50              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 85:L5:4770:U:H2'   | 85:L5:4771:C:C6   | 2.46                     | 0.50              |
| 85:L5:4929:C:H2'   | 85:L5:4930:C:C6   | 2.46                     | 0.50              |
| 85:L5:4986:G:H2'   | 85:L5:4987:C:C6   | 2.46                     | 0.50              |
| 80:CB:594:LYS:HG3  | 80:CB:598:LYS:HG3 | 1.93                     | 0.50              |
| 2:SE:15:PRO:HD2    | 2:SE:18:TRP:CD2   | 2.46                     | 0.50              |
| 3:SI:74:ARG:NH2    | 79:S2:301:A:O2'   | 2.43                     | 0.50              |
| 8:SY:54:VAL:HG22   | 8:SY:76:TYR:HB2   | 1.93                     | 0.50              |
| 86:Se:8:ARG:HD3    | 79:S2:616:A:H5'   | 1.92                     | 0.50              |
| 10:SA:114:ALA:O    | 10:SA:117:ARG:NH2 | 2.44                     | 0.50              |
| 19:Sb:54:VAL:HG22  | 19:Sb:64:CYS:SG   | 2.51                     | 0.50              |
| 85:L5:20:U:P       | 21:L8:36:G:H22    | 2.34                     | 0.50              |
| 85:L5:150:U:OP2    | 28:LG:200:THR:OG1 | 2.28                     | 0.50              |
| 85:L5:1478:C:H2'   | 85:L5:1479:G:C8   | 2.42                     | 0.50              |
| 85:L5:1681:G:H2'   | 85:L5:1682:A:H8   | 1.76                     | 0.50              |
| 85:L5:1730:U:H1'   | 40:LT:101:SER:HB3 | 1.92                     | 0.50              |
| 85:L5:2017:A:O2'   | 85:L5:2018:C:H6   | 1.94                     | 0.50              |
| 85:L5:2419:C:H2'   | 85:L5:2420:A:C8   | 2.46                     | 0.50              |
| 85:L5:2496:G:H2'   | 85:L5:2497:C:C6   | 2.46                     | 0.50              |
| 85:L5:2617:G:H2'   | 85:L5:2618:G:O4'  | 2.11                     | 0.50              |
| 85:L5:4082:G:H2'   | 85:L5:4083:U:C6   | 2.46                     | 0.50              |
| 85:L5:4215:C:O2    | 40:LT:60:LYS:NZ   | 2.44                     | 0.50              |
| 85:L5:4246:G:H2'   | 85:L5:4247:G:C8   | 2.46                     | 0.50              |
| 85:L5:4301:U:H4'   | 40:LT:54:HIS:CD2  | 2.45                     | 0.50              |
| 85:L5:4342:C:O3'   | 60:Lo:37:GLY:HA3  | 2.11                     | 0.50              |
| 85:L5:4573:G:H2'   | 85:L5:4574:U:C6   | 2.46                     | 0.50              |
| 85:L5:4981:G:OP2   | 85:L5:4981:G:N2   | 2.42                     | 0.50              |
| 20:L7:118:C:H2'    | 20:L7:119:U:C6    | 2.46                     | 0.50              |
| 21:L8:66:A:H2'     | 21:L8:67:U:C6     | 2.45                     | 0.50              |
| 22:LA:114:CYS:HB2  | 22:LA:169:VAL:CG1 | 2.40                     | 0.50              |
| 24:LC:209:ILE:HG13 | 24:LC:221:PHE:CE1 | 2.46                     | 0.50              |
| 24:LC:209:ILE:HG21 | 24:LC:221:PHE:HE1 | 1.75                     | 0.50              |
| 27:LF:114:LEU:HD22 | 27:LF:119:ASN:O   | 2.11                     | 0.50              |
| 29:LH:110:SER:HA   | 29:LH:128:MET:HE3 | 1.93                     | 0.50              |
| 32:LL:209:LYS:HG3  | 32:LL:210:LYS:HG2 | 1.92                     | 0.50              |
| 34:LN:123:GLU:CB   | 34:LN:128:LYS:HA  | 2.40                     | 0.50              |
| 35:LO:3:GLU:N      | 35:LO:31:ARG:HE   | 2.08                     | 0.50              |
| 37:LQ:186:TYR:HE2  | 37:LQ:188:ASN:HB3 | 1.76                     | 0.50              |
| 43:LX:101:ASP:OD2  | 43:LX:102:VAL:N   | 2.44                     | 0.50              |
| 50:Le:79:VAL:HG22  | 50:Le:98:GLU:O    | 2.11                     | 0.50              |
| 64:SR:72:LYS:NZ    | 64:SR:76:GLU:HG2  | 2.26                     | 0.50              |
| 66:SF:77:MET:SD    | 66:SF:85:LYS:N    | 2.84                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 69:SQ:98:LYS:HB3   | 69:SQ:99:TYR:CD2   | 2.46                     | 0.50              |
| 70:SS:68:ILE:O     | 70:SS:72:GLN:NE2   | 2.33                     | 0.50              |
| 75:Sg:152:SER:OG   | 75:Sg:153:CYS:N    | 2.42                     | 0.50              |
| 75:Sg:220:ASP:HB3  | 75:Sg:227:LEU:HD11 | 1.93                     | 0.50              |
| 79:S2:57:U:OP1     | 79:S2:504:G:O2'    | 2.29                     | 0.50              |
| 79:S2:644:G:H2'    | 79:S2:645:C:C6     | 2.47                     | 0.50              |
| 79:S2:1589:A:H2'   | 79:S2:1590:C:O4'   | 2.11                     | 0.50              |
| 3:sI:178:ARG:HG2   | 3:sI:181:GLN:HG3   | 1.94                     | 0.50              |
| 6:sG:56:ASN:OD1    | 6:sG:60:GLY:HA2    | 2.11                     | 0.50              |
| 10:sA:54:THR:HG22  | 10:sA:162:PRO:HD2  | 1.93                     | 0.50              |
| 11:sB:154:SER:OG   | 64:sR:134:PRO:HB2  | 2.12                     | 0.50              |
| 15:sC:270:THR:O    | 15:sC:274:VAL:HG13 | 2.11                     | 0.50              |
| 18:sW:2:VAL:HG12   | 18:sW:3:ARG:H      | 1.76                     | 0.50              |
| 20:l7:28:C:O3'     | 31:lJ:138:GLY:HA2  | 2.11                     | 0.50              |
| 23:lB:116:ARG:HD3  | 23:lB:122:TRP:CG   | 2.46                     | 0.50              |
| 23:lB:302:ASN:HD21 | 23:lB:314:ILE:HG22 | 1.77                     | 0.50              |
| 24:lC:140:LYS:HZ3  | 24:lC:242:PRO:HD2  | 1.74                     | 0.50              |
| 25:lD:196:ARG:NH2  | 25:lD:200:MET:SD   | 2.84                     | 0.50              |
| 36:lP:72:GLN:NE2   | 85:l5:4970:C:O3'   | 2.44                     | 0.50              |
| 41:lU:105:ASN:OD1  | 41:lU:106:SER:N    | 2.44                     | 0.50              |
| 42:lV:68:GLY:O     | 42:lV:73:ARG:NH2   | 2.22                     | 0.50              |
| 45:lZ:74:VAL:HG13  | 45:lZ:101:PHE:CE2  | 2.46                     | 0.50              |
| 50:le:102:ASN:ND2  | 85:l5:2307:A:H5''  | 2.23                     | 0.50              |
| 61:lp:47:MET:HE2   | 61:lp:47:MET:HA    | 1.93                     | 0.50              |
| 70:sS:134:GLN:OE1  | 70:sS:134:GLN:N    | 2.41                     | 0.50              |
| 71:sT:49:ASP:OD1   | 71:sT:51:ASN:N     | 2.42                     | 0.50              |
| 74:sd:21:CYS:SG    | 74:sd:22:ARG:N     | 2.83                     | 0.50              |
| 75:sg:24:THR:HG23  | 75:sg:27:PHE:H     | 1.76                     | 0.50              |
| 76:sM:126:GLU:HA   | 76:sM:129:LYS:HE3  | 1.91                     | 0.50              |
| 79:s2:535:G:O2'    | 79:s2:536:A:N7     | 2.41                     | 0.50              |
| 80:cB:207:PRO:HG2  | 80:cB:261:TRP:CZ2  | 2.46                     | 0.50              |
| 80:cB:302:ASP:OD1  | 80:cB:303:ALA:N    | 2.44                     | 0.50              |
| 80:cB:336:LEU:O    | 80:cB:340:MET:HG3  | 2.12                     | 0.50              |
| 80:cB:635:LEU:C    | 80:cB:641:TRP:HB3  | 2.36                     | 0.50              |
| 80:cB:743:PRO:HG3  | 80:cB:817:TRP:CH2  | 2.47                     | 0.50              |
| 83:ls:30:VAL:O     | 83:ls:87:GLY:N     | 2.35                     | 0.50              |
| 83:ls:97:GLU:OE2   | 83:ls:98:ILE:HG12  | 2.10                     | 0.50              |
| 85:l5:1095:A:H2'   | 85:l5:1096:C:C6    | 2.45                     | 0.50              |
| 85:l5:1279:A:O2'   | 85:l5:1281:G:N7    | 2.41                     | 0.50              |
| 85:l5:1589:C:H2'   | 85:l5:1590:C:C6    | 2.46                     | 0.50              |
| 85:l5:3684:G:H2'   | 85:l5:3685:C:C6    | 2.46                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 85:l5:3722:G:H2'  | 85:l5:3723:A:C8   | 2.46                     | 0.50              |
| 85:l5:4127:A:N6   | 85:l5:4156:G:H2'  | 2.25                     | 0.50              |
| 85:l5:4577:U:H2'  | 85:l5:4578:G:C8   | 2.45                     | 0.50              |
| 85:l5:4596:C:C4   | 85:l5:4597:U:C4   | 2.99                     | 0.50              |
| 2:SE:139:LEU:HD12 | 2:SE:140:VAL:N    | 2.25                     | 0.50              |
| 3:SI:159:SER:O    | 3:SI:163:GLU:HG3  | 2.12                     | 0.50              |
| 7:SJ:113:GLN:OE1  | 7:SJ:113:GLN:N    | 2.33                     | 0.50              |
| 11:SB:206:PRO:HD3 | 79:S2:1121:G:H21  | 1.75                     | 0.50              |
| 12:SH:27:LEU:O    | 12:SH:30:LEU:HB3  | 2.11                     | 0.50              |
| 16:SN:39:LYS:HZ1  | 16:SN:43:LYS:HB2  | 1.75                     | 0.50              |
| 85:L5:16:G:P      | 43:LX:62:ARG:HH22 | 2.34                     | 0.50              |
| 85:L5:106:A:H1'   | 85:L5:336:A:N3    | 2.26                     | 0.50              |
| 85:L5:424:U:H2'   | 85:L5:425:U:C6    | 2.47                     | 0.50              |
| 85:L5:1084:C:H2'  | 85:L5:1085:C:H6   | 1.76                     | 0.50              |
| 85:L5:2544:G:H22  | 21:L8:124:U:H5'   | 1.76                     | 0.50              |
| 85:L5:4194:U:O2'  | 30:LI:116:ARG:NH2 | 2.45                     | 0.50              |
| 85:L5:4291:G:H4'  | 85:L5:4292:A:H5'' | 1.92                     | 0.50              |
| 85:L5:4354:U:O4   | 46:La:61:TYR:N    | 2.41                     | 0.50              |
| 85:L5:4507:A:O3'  | 42:LV:62:MET:HE1  | 2.10                     | 0.50              |
| 85:L5:4591:U:H2'  | 85:L5:4592:C:C6   | 2.46                     | 0.50              |
| 20:L7:110:G:H2'   | 20:L7:111:C:C6    | 2.46                     | 0.50              |
| 21:L8:19:C:H2'    | 21:L8:20:A:C8     | 2.40                     | 0.50              |
| 21:L8:90:C:H1'    | 44:LY:24:HIS:HB3  | 1.93                     | 0.50              |
| 22:LA:28:ARG:HB2  | 22:LA:123:ARG:HB3 | 1.92                     | 0.50              |
| 23:LB:156:TYR:O   | 23:LB:158:GLN:NE2 | 2.45                     | 0.50              |
| 23:LB:386:LYS:O   | 23:LB:386:LYS:NZ  | 2.39                     | 0.50              |
| 27:LF:62:ARG:NH1  | 27:LF:66:ARG:HH21 | 2.09                     | 0.50              |
| 32:LL:28:GLN:OE1  | 34:LN:202:ARG:NE  | 2.38                     | 0.50              |
| 60:Lo:19:GLN:O    | 60:Lo:21:HIS:ND1  | 2.43                     | 0.50              |
| 79:S2:386:C:H2'   | 79:S2:387:C:H6    | 1.76                     | 0.50              |
| 79:S2:1255:G:OP1  | 79:S2:1256:G:O2'  | 2.19                     | 0.50              |
| 79:S2:1359:U:H2'  | 79:S2:1360:U:C6   | 2.46                     | 0.50              |
| 79:S2:1435:C:O2'  | 79:S2:1437:C:N4   | 2.45                     | 0.50              |
| 79:S2:1615:U:H2'  | 79:S2:1616:U:C6   | 2.47                     | 0.50              |
| 3:sI:104:ILE:HG22 | 3:sI:171:LEU:HB2  | 1.94                     | 0.50              |
| 4:sL:86:ILE:N     | 4:sL:111:VAL:O    | 2.44                     | 0.50              |
| 6:sG:177:GLN:OE1  | 6:sG:178:ARG:N    | 2.43                     | 0.50              |
| 6:sG:223:LYS:NZ   | 6:sG:223:LYS:O    | 2.39                     | 0.50              |
| 11:sB:89:GLU:HG2  | 11:sB:90:ASP:N    | 2.27                     | 0.50              |
| 19:sb:35:VAL:HG22 | 19:sb:79:PHE:HB3  | 1.93                     | 0.50              |
| 20:l7:34:C:H1'    | 25:lD:203:ASN:OD1 | 2.11                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 21:l8:150:C:H42    | 28:lG:53:ARG:HA    | 1.76                     | 0.50              |
| 22:lA:47:ASP:C     | 22:lA:47:ASP:OD2   | 2.54                     | 0.50              |
| 26:lE:203:ILE:HD12 | 26:lE:206:VAL:HG11 | 1.92                     | 0.50              |
| 27:lF:93:ILE:HG22  | 27:lF:141:ALA:O    | 2.12                     | 0.50              |
| 27:lF:94:ARG:HB2   | 27:lF:114:LEU:HD12 | 1.93                     | 0.50              |
| 28:lG:120:LYS:HZ2  | 28:lG:125:LYS:CB   | 2.25                     | 0.50              |
| 31:lJ:66:GLU:HA    | 60:lo:103:VAL:CG1  | 2.42                     | 0.50              |
| 33:lM:122:ILE:HD11 | 35:lO:189:ILE:CD1  | 2.41                     | 0.50              |
| 36:lP:18:ARG:NH2   | 36:lP:147:GLU:OE2  | 2.45                     | 0.50              |
| 38:lR:172:ARG:HH22 | 79:s2:909:G:P      | 2.33                     | 0.50              |
| 39:lS:15:ARG:HD2   | 39:lS:25:PRO:HG2   | 1.93                     | 0.50              |
| 43:lX:94:ASN:OD1   | 43:lX:146:ALA:N    | 2.43                     | 0.50              |
| 45:lZ:113:GLU:OE1  | 45:lZ:113:GLU:HA   | 2.11                     | 0.50              |
| 56:lk:5:ILE:HD11   | 56:lk:43:TYR:CD1   | 2.47                     | 0.50              |
| 64:sR:11:LYS:HB2   | 79:s2:1373:C:C6    | 2.47                     | 0.50              |
| 66:sF:88:MET:HE1   | 79:s2:1536:G:P     | 2.52                     | 0.50              |
| 67:sK:55:ARG:HH12  | 79:s2:1278:A:H5'   | 1.75                     | 0.50              |
| 68:sP:16:THR:OG1   | 68:sP:17:TYR:N     | 2.44                     | 0.50              |
| 71:sT:10:ASN:OD1   | 71:sT:12:GLN:HB2   | 2.11                     | 0.50              |
| 75:sg:14:HIS:HD2   | 75:sg:41:ILE:HD13  | 1.76                     | 0.50              |
| 75:sg:147:HIS:CD2  | 75:sg:169:GLY:HA3  | 2.47                     | 0.50              |
| 75:sg:191:HIS:NE2  | 75:sg:213:ASP:OD1  | 2.45                     | 0.50              |
| 79:s2:499:G:N1     | 79:s2:504:G:C6     | 2.79                     | 0.50              |
| 79:s2:618:C:H2'    | 79:s2:619:A:O4'    | 2.11                     | 0.50              |
| 79:s2:929:G:N2     | 79:s2:1104:G:O2'   | 2.44                     | 0.50              |
| 79:s2:1563:G:H2'   | 79:s2:1564:C:H6    | 1.76                     | 0.50              |
| 79:s2:1616:U:H2'   | 79:s2:1617:G:O4'   | 2.10                     | 0.50              |
| 79:s2:1779:G:N2    | 79:s2:1780:G:C6    | 2.80                     | 0.50              |
| 79:s2:1826:G:H5'   | 85:l5:3760:A:C6    | 2.47                     | 0.50              |
| 80:cB:693:CYS:SG   | 80:cB:835:VAL:HG12 | 2.51                     | 0.50              |
| 83:ls:78:LEU:HD12  | 83:ls:78:LEU:H     | 1.76                     | 0.50              |
| 85:l5:27:C:O3'     | 85:l5:60:G:N2      | 2.44                     | 0.50              |
| 85:l5:724:C:H2'    | 85:l5:725:G:C8     | 2.46                     | 0.50              |
| 85:l5:2033:A:O2'   | 85:l5:2034:G:O5'   | 2.28                     | 0.50              |
| 85:l5:2563:C:H2'   | 85:l5:2564:G:O4'   | 2.12                     | 0.50              |
| 85:l5:2864:A:H2'   | 85:l5:2865:U:H6    | 1.77                     | 0.50              |
| 85:l5:3761:C:H2'   | 85:l5:3762:U:O4'   | 2.11                     | 0.50              |
| 85:l5:3916:G:H2'   | 85:l5:3917:A:C8    | 2.45                     | 0.50              |
| 85:l5:4070:U:H2'   | 85:l5:4071:U:H6    | 1.75                     | 0.50              |
| 85:l5:4661:G:H2'   | 85:l5:4662:C:C6    | 2.46                     | 0.50              |
| 85:l5:4771:C:H2'   | 85:l5:4772:C:C6    | 2.46                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 85:L5:5056:A:H2'   | 85:L5:5057:C:C6    | 2.46                     | 0.50              |
| 80:CB:18:ASN:ND2   | 80:CB:94:ASP:H     | 1.97                     | 0.50              |
| 3:SI:110:ARG:O     | 3:SI:114:GLU:HG2   | 2.11                     | 0.50              |
| 6:SG:160:LYS:NZ    | 6:SG:161:PRO:O     | 2.44                     | 0.50              |
| 6:SG:209:TYR:HA    | 6:SG:212:LEU:HD12  | 1.92                     | 0.50              |
| 15:SC:196:ILE:N    | 15:SC:223:TYR:O    | 2.40                     | 0.50              |
| 17:SO:147:ARG:HH22 | 79:S2:1854:U:P     | 2.34                     | 0.50              |
| 85:L5:18:C:H4'     | 34:LN:138:PHE:CD2  | 2.46                     | 0.50              |
| 85:L5:82:U:H2'     | 85:L5:83:C:O4'     | 2.12                     | 0.50              |
| 85:L5:731:G:C6     | 85:L5:932:A:C4     | 2.99                     | 0.50              |
| 85:L5:991:C:H3'    | 85:L5:992:C:H4'    | 1.93                     | 0.50              |
| 85:L5:1924:C:H5''  | 33:LM:34:ASN:HD22  | 1.77                     | 0.50              |
| 85:L5:1984:A:H5'   | 85:L5:1986:U:P     | 2.52                     | 0.50              |
| 85:L5:2538:U:H2'   | 85:L5:2539:C:H6    | 1.76                     | 0.50              |
| 85:L5:4406:U:C2    | 85:L5:4407:G:C8    | 3.00                     | 0.50              |
| 85:L5:4460:U:H2'   | 85:L5:4461:C:C6    | 2.45                     | 0.50              |
| 85:L5:4499:G:C2    | 85:L5:4529:G:H1'   | 2.45                     | 0.50              |
| 85:L5:4605:A:C6    | 85:L5:4606:G:C2    | 2.99                     | 0.50              |
| 24:LC:152:LEU:HD21 | 24:LC:174:LEU:HD12 | 1.92                     | 0.50              |
| 24:LC:358:ALA:O    | 24:LC:361:LEU:HG   | 2.11                     | 0.50              |
| 26:LE:265:PRO:O    | 26:LE:266:GLN:NE2  | 2.45                     | 0.50              |
| 27:LF:127:LYS:HG2  | 40:LT:133:ALA:HB3  | 1.92                     | 0.50              |
| 30:LI:98:ARG:C     | 30:LI:123:GLN:OE1  | 2.55                     | 0.50              |
| 35:LO:58:LEU:HD12  | 35:LO:72:HIS:CD2   | 2.46                     | 0.50              |
| 50:Le:22:ARG:HD2   | 50:Le:36:ARG:HB2   | 1.94                     | 0.50              |
| 64:SR:98:VAL:HG11  | 64:SR:117:LEU:HD11 | 1.93                     | 0.50              |
| 66:SF:94:LYS:HA    | 66:SF:97:PHE:CD2   | 2.46                     | 0.50              |
| 71:ST:133:ARG:HG2  | 71:ST:137:GLN:NE2  | 2.26                     | 0.50              |
| 75:Sg:149:GLU:OE1  | 75:Sg:170:TRP:CD1  | 2.65                     | 0.50              |
| 78:Sf:88:PRO:HG2   | 78:Sf:89:LYS:HD2   | 1.92                     | 0.50              |
| 79:S2:1114:U:O2'   | 79:S2:1115:U:H2'   | 2.10                     | 0.50              |
| 87:LW:87:LEU:HD13  | 87:LW:90:ILE:HD11  | 1.93                     | 0.50              |
| 87:LW:106:GLU:O    | 87:LW:110:ARG:HG2  | 2.11                     | 0.50              |
| 2:sE:147:ILE:HD13  | 2:sE:169:ILE:HD11  | 1.94                     | 0.50              |
| 3:sI:141:ARG:CZ    | 3:sI:141:ARG:HA    | 2.41                     | 0.50              |
| 7:sJ:136:ARG:HH11  | 28:LG:266:GLY:H    | 1.60                     | 0.50              |
| 14:sa:88:SER:O     | 14:sa:92:ARG:HB2   | 2.11                     | 0.50              |
| 19:sb:13:GLU:OE1   | 19:sb:13:GLU:N     | 2.44                     | 0.50              |
| 21:l8:5:U:H2'      | 21:l8:6:C:H6       | 1.76                     | 0.50              |
| 21:l8:125:C:O2     | 21:l8:126:C:O2'    | 2.30                     | 0.50              |
| 28:lG:120:LYS:NZ   | 28:lG:125:LYS:HG3  | 2.25                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 29:IH:61:TRP:CD1  | 33:IM:33:GLN:HE22 | 2.29                     | 0.50              |
| 32:IL:55:ILE:HD11 | 32:IL:116:ARG:HE  | 1.76                     | 0.50              |
| 32:IL:63:THR:HG21 | 46:la:66:ASN:CG   | 2.37                     | 0.50              |
| 42:IV:26:ILE:HG23 | 42:IV:39:ILE:HD11 | 1.94                     | 0.50              |
| 42:IV:40:ILE:HD11 | 85:l5:3799:A:C6   | 2.45                     | 0.50              |
| 44:IY:54:GLU:HB3  | 44:IY:67:ILE:HD11 | 1.93                     | 0.50              |
| 45:lZ:3:LYS:NZ    | 48:lc:40:GLN:HA   | 2.26                     | 0.50              |
| 45:lZ:46:ILE:HD11 | 45:lZ:68:ILE:HB   | 1.92                     | 0.50              |
| 48:lc:15:ASN:O    | 48:lc:19:GLN:HG2  | 2.11                     | 0.50              |
| 63:lz:202:ARG:NH2 | 63:lz:205:TYR:OH  | 2.43                     | 0.50              |
| 72:sU:30:LYS:HE2  | 72:sU:30:LYS:H    | 1.77                     | 0.50              |
| 75:sg:243:PRO:HG2 | 75:sg:295:GLY:H   | 1.76                     | 0.50              |
| 79:s2:569:A:H2'   | 79:s2:570:C:O4'   | 2.11                     | 0.50              |
| 79:s2:943:U:C2    | 79:s2:944:A:C8    | 3.00                     | 0.50              |
| 79:s2:1112:U:H2'  | 79:s2:1113:A:C8   | 2.46                     | 0.50              |
| 79:s2:1215:C:H5   | 79:s2:1645:C:H2'  | 1.76                     | 0.50              |
| 79:s2:1758:G:N2   | 79:s2:1773:C:O4'  | 2.44                     | 0.50              |
| 80:cB:750:GLN:HB3 | 80:cB:781:MET:CE  | 2.41                     | 0.50              |
| 85:l5:167:C:H2'   | 85:l5:168:C:C6    | 2.47                     | 0.50              |
| 85:l5:920:C:H2'   | 85:l5:921:C:C6    | 2.47                     | 0.50              |
| 85:l5:1202:C:H3'  | 85:l5:1203:G:C5'  | 2.41                     | 0.50              |
| 85:l5:1872:G:O2'  | 85:l5:4219:A:N3   | 2.36                     | 0.50              |
| 85:l5:3614:G:H2'  | 85:l5:3617:G:H21  | 1.76                     | 0.50              |
| 85:l5:4254:G:O2'  | 85:l5:4256:A:H2   | 1.95                     | 0.50              |
| 85:l5:4481:U:H2'  | 85:l5:4482:U:H6   | 1.76                     | 0.50              |
| 85:l5:4892:A:H2'  | 85:l5:4893:A:O4'  | 2.12                     | 0.50              |
| 80:CB:343:TRP:CD2 | 80:CB:344:LEU:HG  | 2.47                     | 0.50              |
| 80:CB:422:SER:O   | 80:CB:425:LEU:HG  | 2.12                     | 0.50              |
| 80:CB:531:ASP:OD2 | 80:CB:553:HIS:NE2 | 2.39                     | 0.50              |
| 2:SE:44:LEU:O     | 2:SE:48:LEU:HG    | 2.12                     | 0.50              |
| 3:SI:48:VAL:HG11  | 3:SI:54:LYS:HG3   | 1.93                     | 0.50              |
| 3:SI:87:ASN:OD1   | 3:SI:88:ASN:N     | 2.44                     | 0.50              |
| 4:SL:41:GLY:HA3   | 79:S2:291:G:N3    | 2.27                     | 0.50              |
| 4:SL:86:ILE:O     | 4:SL:111:VAL:N    | 2.27                     | 0.50              |
| 5:SX:93:PHE:HE2   | 5:SX:134:TYR:HA   | 1.76                     | 0.50              |
| 7:SJ:132:GLN:C    | 7:SJ:133:ARG:HE   | 2.18                     | 0.50              |
| 10:SA:80:ARG:C    | 10:SA:84:GLN:HE22 | 2.20                     | 0.50              |
| 12:SH:145:ARG:HD2 | 18:SW:51:GLU:OE1  | 2.12                     | 0.50              |
| 15:SC:73:MET:SD   | 15:SC:96:PHE:CZ   | 3.05                     | 0.50              |
| 18:SW:22:LYS:NZ   | 19:Sb:2:PRO:O     | 2.45                     | 0.50              |
| 85:L5:40:G:N2     | 85:L5:4380:A:H62  | 2.10                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 85:L5:116:G:H2'    | 85:L5:117:C:C6     | 2.47                     | 0.50              |
| 85:L5:352:G:N2     | 21:L8:24:G:C6      | 2.80                     | 0.50              |
| 85:L5:468:U:O2     | 85:L5:686:A:N6     | 2.44                     | 0.50              |
| 85:L5:667:A:H5''   | 85:L5:668:C:H5''   | 1.94                     | 0.50              |
| 85:L5:2634:C:H2'   | 85:L5:2635:U:C6    | 2.46                     | 0.50              |
| 85:L5:2895:A:H2'   | 85:L5:2896:G:H8    | 1.75                     | 0.50              |
| 85:L5:4096:C:O2    | 85:L5:4111:U:C4    | 2.65                     | 0.50              |
| 85:L5:4761:G:H2'   | 85:L5:4762:A:C8    | 2.46                     | 0.50              |
| 20:L7:37:G:C2      | 20:L7:41:G:C2      | 2.99                     | 0.50              |
| 20:L7:60:G:C2      | 20:L7:61:G:C8      | 2.99                     | 0.50              |
| 27:LF:241:ASN:O    | 27:LF:245:ARG:HG2  | 2.12                     | 0.50              |
| 34:LN:91:GLN:O     | 34:LN:93:LYS:NZ    | 2.36                     | 0.50              |
| 34:LN:174:LEU:HA   | 34:LN:183:THR:HG21 | 1.94                     | 0.50              |
| 38:LR:119:MET:SD   | 38:LR:120:TYR:N    | 2.85                     | 0.50              |
| 40:LT:149:GLU:CD   | 40:LT:149:GLU:H    | 2.18                     | 0.50              |
| 43:LX:120:ASP:HB3  | 43:LX:144:TYR:OH   | 2.12                     | 0.50              |
| 43:LX:148:ASP:O    | 43:LX:152:LYS:HG2  | 2.11                     | 0.50              |
| 46:La:75:LEU:HA    | 46:La:78:LEU:HG    | 1.93                     | 0.50              |
| 48:Lc:12:GLU:HA    | 48:Lc:15:ASN:HD21  | 1.75                     | 0.50              |
| 62:Lr:86:ALA:O     | 62:Lr:89:THR:OG1   | 2.25                     | 0.50              |
| 63:Lz:62:LYS:HE3   | 63:Lz:62:LYS:HA    | 1.94                     | 0.50              |
| 64:SR:48:ASN:HD22  | 79:S2:1452:A:H5''  | 1.76                     | 0.50              |
| 66:SF:99:ILE:HA    | 66:SF:102:LEU:CG   | 2.42                     | 0.50              |
| 74:Sd:19:ARG:HD3   | 74:Sd:32:ARG:HH11  | 1.76                     | 0.50              |
| 79:S2:61:A:H1'     | 79:S2:316:G:H1'    | 1.92                     | 0.50              |
| 79:S2:329:G:H2'    | 79:S2:330:G:H8     | 1.77                     | 0.50              |
| 79:S2:373:G:H2'    | 79:S2:374:G:C8     | 2.46                     | 0.50              |
| 79:S2:813:A:H2'    | 79:S2:814:U:O4'    | 2.12                     | 0.50              |
| 1:CH:133:ARG:NH1   | 79:S2:533:A:O3'    | 2.45                     | 0.50              |
| 6:sG:58:LYS:HA     | 6:sG:107:SER:HB3   | 1.93                     | 0.50              |
| 14:sa:27:ALA:CB    | 17:sO:142:ARG:HH12 | 2.24                     | 0.50              |
| 17:sO:103:ASN:HD22 | 17:sO:142:ARG:HA   | 1.76                     | 0.50              |
| 19:sb:31:TYR:HB2   | 19:sb:81:ARG:NE    | 2.18                     | 0.50              |
| 27:lF:179:LEU:HD21 | 27:lF:207:PHE:CG   | 2.46                     | 0.50              |
| 28:lG:32:PHE:HE1   | 45:lZ:53:VAL:HG12  | 1.75                     | 0.50              |
| 29:lH:123:ILE:HD13 | 29:lH:125:ARG:NH2  | 2.27                     | 0.50              |
| 33:lM:19:PRO:HG2   | 33:lM:20:HIS:CE1   | 2.47                     | 0.50              |
| 35:lO:107:GLY:HA3  | 85:l5:4910:G:H22   | 1.77                     | 0.50              |
| 37:lQ:23:ILE:HD11  | 62:lr:8:MET:HB3    | 1.92                     | 0.50              |
| 37:lQ:89:ASP:OD1   | 37:lQ:91:ARG:NE    | 2.43                     | 0.50              |
| 42:lV:51:ARG:NH1   | 85:l5:4620:U:OP1   | 2.44                     | 0.50              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 56:lk:5:ILE:HD11   | 56:lk:43:TYR:HB3  | 1.93                     | 0.50              |
| 60:lo:4:VAL:HG13   | 60:lo:5:PRO:HD2   | 1.92                     | 0.50              |
| 61:lp:85:ARG:O     | 61:lp:88:GLU:HG2  | 2.11                     | 0.50              |
| 62:lr:22:LYS:N     | 85:l5:2289:C:O2   | 2.44                     | 0.50              |
| 64:sR:9:VAL:HA     | 79:s2:1372:U:N3   | 2.19                     | 0.50              |
| 66:sF:152:TRP:C    | 66:sF:152:TRP:CD1 | 2.89                     | 0.50              |
| 69:sQ:47:LEU:HB3   | 69:sQ:50:LYS:HB3  | 1.92                     | 0.50              |
| 72:sU:61:LEU:HD12  | 74:sd:34:TYR:CZ   | 2.47                     | 0.50              |
| 73:sc:13:ARG:HD2   | 73:sc:55:VAL:HG23 | 1.94                     | 0.50              |
| 77:sZ:52:LYS:HZ1   | 77:sZ:56:ASP:HB3  | 1.76                     | 0.50              |
| 79:s2:1107:G:C6    | 79:s2:1126:G:C6   | 3.00                     | 0.50              |
| 79:s2:1350:U:H2'   | 79:s2:1351:G:O4'  | 2.12                     | 0.50              |
| 79:s2:1534:C:O2'   | 79:s2:1599:U:O4   | 2.12                     | 0.50              |
| 79:s2:1772:C:H2'   | 79:s2:1772:C:O2   | 2.11                     | 0.50              |
| 82:pE:27:U:H2'     | 82:pE:28:C:H6     | 1.76                     | 0.50              |
| 82:pE:41:U:H2'     | 82:pE:42:G:C8     | 2.47                     | 0.50              |
| 84:lt:142:ASN:HB2  | 84:lt:148:PRO:HB3 | 1.94                     | 0.50              |
| 85:l5:497:G:H22    | 85:l5:658:C:H42   | 1.59                     | 0.50              |
| 85:l5:724:C:H2'    | 85:l5:725:G:H8    | 1.77                     | 0.50              |
| 85:l5:1072:C:N4    | 85:l5:1240:G:O6   | 2.32                     | 0.50              |
| 85:l5:1820:C:O2'   | 85:l5:1821:G:N7   | 2.39                     | 0.50              |
| 85:l5:1984:A:H5'   | 85:l5:1986:U:P    | 2.52                     | 0.50              |
| 85:l5:2060:G:H2'   | 85:l5:2061:U:C6   | 2.47                     | 0.50              |
| 85:l5:4389:C:H2'   | 85:l5:4390:A:H8   | 1.76                     | 0.50              |
| 85:l5:4631:G:H2'   | 85:l5:4632:U:C6   | 2.46                     | 0.50              |
| 80:CB:579:TYR:HA   | 80:CB:817:TRP:HZ3 | 1.77                     | 0.50              |
| 2:SE:166:THR:O     | 2:SE:168:LYS:HD2  | 2.11                     | 0.50              |
| 3:SI:92:ARG:NH2    | 85:L5:3612:C:OP1  | 2.44                     | 0.50              |
| 10:SA:180:ARG:HH12 | 10:SA:184:ARG:HD2 | 1.77                     | 0.50              |
| 11:SB:128:LYS:HA   | 11:SB:134:LEU:HA  | 1.93                     | 0.50              |
| 15:SC:84:PHE:CZ    | 15:SC:264:SER:HA  | 2.47                     | 0.50              |
| 85:L5:325:U:H2'    | 85:L5:326:C:H6    | 1.75                     | 0.50              |
| 85:L5:967:C:O2'    | 26:LE:110:ARG:NH1 | 2.43                     | 0.50              |
| 85:L5:1199:G:H2'   | 85:L5:1200:G:H8   | 1.77                     | 0.50              |
| 85:L5:1351:G:H2'   | 85:L5:1352:C:H6   | 1.75                     | 0.50              |
| 85:L5:1813:U:H5''  | 47:Lb:52:LYS:HE2  | 1.93                     | 0.50              |
| 85:L5:1926:C:H2'   | 85:L5:1927:U:C6   | 2.46                     | 0.50              |
| 85:L5:2780:C:H2'   | 85:L5:2781:G:C8   | 2.42                     | 0.50              |
| 85:L5:3848:U:H2'   | 85:L5:3849:A:C8   | 2.38                     | 0.50              |
| 85:L5:3944:G:H1    | 85:L5:4069:U:H3   | 1.60                     | 0.50              |
| 85:L5:4499:G:N3    | 85:L5:4529:G:H1'  | 2.27                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 85:L5:4603:C:P     | 29:LH:98:HIS:HD1   | 2.34                     | 0.50              |
| 85:L5:4759:C:H2'   | 85:L5:4760:G:C8    | 2.46                     | 0.50              |
| 20:L7:55:A:C4      | 20:L7:56:G:C8      | 3.00                     | 0.50              |
| 22:LA:96:LEU:O     | 22:LA:96:LEU:HD12  | 2.11                     | 0.50              |
| 28:LG:106:THR:HG23 | 28:LG:108:GLN:H    | 1.76                     | 0.50              |
| 30:LI:10:ARG:NH1   | 30:LI:160:PRO:HB2  | 2.27                     | 0.50              |
| 30:LI:41:ALA:O     | 30:LI:139:ARG:NH2  | 2.44                     | 0.50              |
| 33:LM:119:ARG:O    | 33:LM:123:ILE:HG12 | 2.12                     | 0.50              |
| 34:LN:37:HIS:HB3   | 34:LN:63:ARG:HB3   | 1.92                     | 0.50              |
| 36:LP:31:GLU:OE1   | 36:LP:61:ARG:N     | 2.31                     | 0.50              |
| 54:Li:45:ARG:HD2   | 54:Li:50:PHE:CZ    | 2.46                     | 0.50              |
| 66:SF:128:ILE:HD11 | 73:Sc:24:GLN:HG3   | 1.92                     | 0.50              |
| 66:SF:146:ARG:NH1  | 73:Sc:57:THR:HG21  | 2.26                     | 0.50              |
| 68:SP:108:LYS:O    | 68:SP:111:MET:HG3  | 2.12                     | 0.50              |
| 70:SS:49:ASP:O     | 70:SS:50:ILE:HD13  | 2.10                     | 0.50              |
| 70:SS:105:ASN:HB2  | 70:SS:108:ARG:NH2  | 2.22                     | 0.50              |
| 72:SU:22:ILE:HD12  | 72:SU:113:GLU:O    | 2.12                     | 0.50              |
| 79:S2:509:G:H2'    | 79:S2:510:G:C8     | 2.47                     | 0.50              |
| 79:S2:696:G:H3'    | 79:S2:733:C:H42    | 1.76                     | 0.50              |
| 79:S2:1337:C:H2'   | 79:S2:1338:G:C8    | 2.46                     | 0.50              |
| 79:S2:1361:G:OP2   | 79:S2:1362:U:O2'   | 2.27                     | 0.50              |
| 79:S2:1538:C:H2'   | 79:S2:1539:U:C6    | 2.47                     | 0.50              |
| 79:S2:1728:U:H2'   | 79:S2:1729:U:O4'   | 2.11                     | 0.50              |
| 79:S2:1740:C:H2'   | 79:S2:1741:U:H6    | 1.75                     | 0.50              |
| 81:AP:5:C:H2'      | 81:AP:6:C:C6       | 2.47                     | 0.50              |
| 1:CH:121:LEU:HD22  | 1:CH:133:ARG:NE    | 2.08                     | 0.50              |
| 2:sE:103:TYR:HE2   | 2:sE:109:PHE:CE1   | 2.30                     | 0.50              |
| 2:sE:140:VAL:HG12  | 2:sE:146:THR:HB    | 1.93                     | 0.50              |
| 5:sX:5:ARG:NH2     | 79:s2:1157:G:C1'   | 2.74                     | 0.50              |
| 5:sX:53:GLU:OE1    | 5:sX:53:GLU:C      | 2.55                     | 0.50              |
| 7:sJ:81:LEU:HB3    | 7:sJ:87:LEU:HB2    | 1.93                     | 0.50              |
| 10:sA:10:MET:CA    | 10:sA:55:TRP:HH2   | 2.23                     | 0.50              |
| 12:sH:103:LYS:HA   | 12:sH:116:ARG:NH2  | 2.27                     | 0.50              |
| 14:sa:29:CYS:SG    | 17:sO:146:ARG:NH1  | 2.84                     | 0.50              |
| 20:l7:117:G:OP1    | 25:lD:255:LYS:HD2  | 2.12                     | 0.50              |
| 21:l8:72:A:P       | 44:lY:51:LYS:HB2   | 2.51                     | 0.50              |
| 23:lB:374:PHE:HE2  | 85:l5:5050:C:N1    | 2.09                     | 0.50              |
| 24:lC:169:LEU:O    | 24:lC:173:LYS:HG2  | 2.11                     | 0.50              |
| 28:lG:105:GLU:HB2  | 28:lG:109:GLU:OE1  | 2.11                     | 0.50              |
| 40:lT:120:LYS:HB3  | 40:lT:120:LYS:HZ2  | 1.77                     | 0.50              |
| 50:le:36:ARG:NE    | 85:l5:1661:C:OP1   | 2.38                     | 0.50              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 52:lg:97:ILE:HG22 | 85:l5:4120:U:C4    | 2.47                     | 0.50              |
| 62:lr:17:LEU:HD23 | 62:lr:18:ILE:N     | 2.25                     | 0.50              |
| 65:sD:93:THR:O    | 65:sD:93:THR:OG1   | 2.30                     | 0.50              |
| 66:sF:166:ILE:H   | 66:sF:166:ILE:HD12 | 1.77                     | 0.50              |
| 70:sS:64:VAL:O    | 70:sS:67:VAL:HG22  | 2.12                     | 0.50              |
| 70:sS:86:ARG:NH2  | 79:s2:1610:G:O2'   | 2.32                     | 0.50              |
| 71:sT:12:GLN:NE2  | 79:s2:1541:G:N3    | 2.58                     | 0.50              |
| 71:sT:40:ALA:HB1  | 71:sT:95:GLY:HA2   | 1.93                     | 0.50              |
| 71:sT:71:GLY:H    | 71:sT:74:SER:HG    | 1.56                     | 0.50              |
| 76:sM:31:LEU:HD23 | 76:sM:109:VAL:HG21 | 1.93                     | 0.50              |
| 76:sM:68:LEU:HA   | 76:sM:71:GLU:OE1   | 2.12                     | 0.50              |
| 79:s2:472:C:H4'   | 79:s2:474:G:OP1    | 2.11                     | 0.50              |
| 79:s2:835:C:C5'   | 79:s2:836:G:H5'    | 2.40                     | 0.50              |
| 79:s2:1113:A:H2'  | 79:s2:1114:U:C2    | 2.47                     | 0.50              |
| 79:s2:1359:U:H2'  | 79:s2:1360:U:H6    | 1.76                     | 0.50              |
| 79:s2:1693:G:H2'  | 79:s2:1694:U:C6    | 2.47                     | 0.50              |
| 79:s2:1705:C:H2'  | 79:s2:1706:G:C8    | 2.46                     | 0.50              |
| 81:aP:25:C:H2'    | 81:aP:26:G:H5'     | 1.94                     | 0.50              |
| 82:pE:6:G:H2'     | 82:pE:7:A:C8       | 2.46                     | 0.50              |
| 83:ls:57:LYS:N    | 85:l5:2020:U:H5''  | 2.27                     | 0.50              |
| 85:l5:995:C:O2'   | 85:l5:1049:C:N4    | 2.44                     | 0.50              |
| 85:l5:1468:C:H2'  | 85:l5:1469:C:H6    | 1.76                     | 0.50              |
| 85:l5:1786:A:H2'  | 85:l5:1789:C:C5    | 2.47                     | 0.50              |
| 85:l5:1992:U:O2   | 85:l5:2002:A:H5''  | 2.11                     | 0.50              |
| 85:l5:2108:G:H2'  | 85:l5:2109:G:H8    | 1.77                     | 0.50              |
| 85:l5:2553:A:OP2  | 85:l5:2574:G:O2'   | 2.24                     | 0.50              |
| 85:l5:2611:A:H5'  | 85:l5:2688:G:H4'   | 1.93                     | 0.50              |
| 85:l5:3967:G:OP2  | 85:l5:3969:G:N2    | 2.43                     | 0.50              |
| 85:l5:4251:A:H2'  | 85:l5:4252:C:O4'   | 2.11                     | 0.50              |
| 80:CB:265:TYR:CD1 | 80:CB:287:ARG:HA   | 2.47                     | 0.50              |
| 2:SE:56:LEU:N     | 2:SE:60:GLU:OE1    | 2.40                     | 0.50              |
| 4:SL:113:LEU:HD13 | 4:SL:142:VAL:HG21  | 1.93                     | 0.50              |
| 11:SB:38:MET:HE1  | 11:SB:231:LEU:HG   | 1.94                     | 0.50              |
| 11:SB:157:GLN:OE1 | 11:SB:160:GLN:N    | 2.39                     | 0.50              |
| 13:SV:65:SER:O    | 13:SV:69:ILE:HG12  | 2.12                     | 0.50              |
| 85:L5:1328:G:H2'  | 85:L5:1329:G:C8    | 2.46                     | 0.50              |
| 85:L5:1558:A:H2'  | 85:L5:1559:G:C8    | 2.46                     | 0.50              |
| 85:L5:1815:G:O6   | 47:Lb:49:HIS:NE2   | 2.37                     | 0.50              |
| 85:L5:2465:C:H2'  | 85:L5:2466:G:C8    | 2.46                     | 0.50              |
| 85:L5:2633:U:H2'  | 85:L5:2634:C:H6    | 1.75                     | 0.50              |
| 85:L5:3910:C:H2'  | 85:L5:3911:C:H6    | 1.76                     | 0.50              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 85:L5:4092:G:H2'  | 85:L5:4093:G:N3    | 2.27                     | 0.50              |
| 85:L5:4414:A:O2'  | 85:L5:4427:G:N2    | 2.30                     | 0.50              |
| 85:L5:4551:U:H2'  | 85:L5:4552:U:H6    | 1.77                     | 0.50              |
| 85:L5:4760:G:OP1  | 35:LO:117:ARG:NH2  | 2.42                     | 0.50              |
| 21:L8:134:G:OP1   | 43:LX:67:ARG:NH1   | 2.45                     | 0.50              |
| 23:LB:48:GLY:N    | 23:LB:345:LEU:O    | 2.44                     | 0.50              |
| 24:LC:146:GLU:HG2 | 24:LC:175:LYS:HB3  | 1.93                     | 0.50              |
| 30:LI:177:ASN:HB2 | 30:LI:180:GLU:OE1  | 2.11                     | 0.50              |
| 31:LJ:35:ARG:HE   | 31:LJ:124:GLY:N    | 2.09                     | 0.50              |
| 32:LL:96:ILE:HG21 | 32:LL:98:VAL:HG23  | 1.94                     | 0.50              |
| 37:LQ:90:VAL:HG23 | 46:La:77:LYS:NZ    | 2.26                     | 0.50              |
| 40:LT:102:ARG:O   | 40:LT:106:LEU:HD23 | 2.12                     | 0.50              |
| 41:LU:48:LYS:HB3  | 41:LU:51:GLY:HA2   | 1.94                     | 0.50              |
| 46:La:38:LEU:HD21 | 46:La:53:PHE:CE2   | 2.47                     | 0.50              |
| 61:Lp:25:MET:CE   | 79:S2:1040:G:H4'   | 2.42                     | 0.50              |
| 64:SR:76:GLU:OE1  | 64:SR:80:ARG:CZ    | 2.59                     | 0.50              |
| 65:SD:76:ARG:HG3  | 65:SD:77:PHE:CD1   | 2.46                     | 0.50              |
| 68:SP:59:ARG:NH1  | 79:S2:1299:A:OP1   | 2.45                     | 0.50              |
| 68:SP:93:MET:HE2  | 68:SP:93:MET:HA    | 1.94                     | 0.50              |
| 71:ST:6:VAL:HG21  | 71:ST:65:TYR:CE2   | 2.46                     | 0.50              |
| 71:ST:106:ALA:O   | 71:ST:110:LEU:HG   | 2.12                     | 0.50              |
| 73:Sc:44:ARG:HD3  | 73:Sc:45:ASN:H     | 1.76                     | 0.50              |
| 76:SM:14:VAL:HG23 | 76:SM:126:GLU:HG3  | 1.93                     | 0.50              |
| 77:SZ:80:ARG:HB3  | 79:S2:1598:G:H2'   | 1.92                     | 0.50              |
| 79:S2:51:U:H2'    | 79:S2:52:G:C8      | 2.46                     | 0.50              |
| 79:S2:218:U:N3    | 79:S2:304:C:O2     | 2.45                     | 0.50              |
| 79:S2:1279:C:H2'  | 79:S2:1280:G:H8    | 1.77                     | 0.50              |
| 79:S2:1284:A:H5'' | 79:S2:1286:G:O4'   | 2.11                     | 0.50              |
| 79:S2:1560:U:O2'  | 79:S2:1583:C:O2'   | 2.21                     | 0.50              |
| 79:S2:1651:A:H2'  | 79:S2:1652:G:C8    | 2.46                     | 0.50              |
| 79:S2:1729:U:O4   | 79:S2:1805:G:O6    | 2.30                     | 0.50              |
| 83:Ls:110:ALA:O   | 83:Ls:112:ARG:NH1  | 2.45                     | 0.50              |
| 84:Lt:127:GLY:HA2 | 84:Lt:130:LYS:CG   | 2.41                     | 0.50              |
| 1:CH:36:GLU:HG3   | 1:CH:37:ASP:N      | 2.26                     | 0.50              |
| 4:sL:59:LYS:HZ3   | 4:sL:134:LEU:HB3   | 1.77                     | 0.50              |
| 5:sX:22:TRP:HH2   | 79:s2:359:U:C5'    | 2.23                     | 0.50              |
| 7:sJ:85:GLY:HA3   | 7:sJ:108:ARG:HH21  | 1.76                     | 0.50              |
| 7:sJ:127:ARG:HE   | 9:se:31:ARG:CZ     | 2.25                     | 0.50              |
| 10:sA:3:GLY:HA3   | 13:sV:79:VAL:HG22  | 1.93                     | 0.50              |
| 11:sB:151:ARG:H   | 64:sR:133:GLY:H    | 1.59                     | 0.50              |
| 12:sH:62:ILE:HB   | 12:sH:94:PHE:CD2   | 2.47                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 15:sC:73:MET:HE3   | 15:sC:76:LYS:NZ    | 2.26                     | 0.50              |
| 17:sO:75:MET:O     | 17:sO:79:GLN:HG2   | 2.12                     | 0.50              |
| 22:lA:5:ILE:HG12   | 22:lA:8:GLN:HG3    | 1.94                     | 0.50              |
| 22:lA:176:ASP:OD1  | 22:lA:176:ASP:N    | 2.43                     | 0.50              |
| 24:lC:10:VAL:O     | 24:lC:18:SER:OG    | 2.28                     | 0.50              |
| 24:lC:297:GLU:CD   | 24:lC:298:ILE:HD12 | 2.37                     | 0.50              |
| 25:lD:42:ASN:HB3   | 40:lT:67:VAL:HG22  | 1.94                     | 0.50              |
| 26:lE:270:TYR:CD1  | 33:lM:107:PHE:HD1  | 2.29                     | 0.50              |
| 30:lI:174:THR:HG22 | 30:lI:176:PHE:H    | 1.77                     | 0.50              |
| 38:lR:103:ARG:HH22 | 85:l5:2668:G:P     | 2.35                     | 0.50              |
| 53:lh:78:TYR:HE2   | 85:l5:16:G:O3'     | 1.95                     | 0.50              |
| 59:ln:1:MET:HE3    | 59:ln:2:ARG:HB3    | 1.92                     | 0.50              |
| 59:ln:1:MET:HB3    | 59:ln:6:ARG:CZ     | 2.41                     | 0.50              |
| 60:lo:11:PHE:HB2   | 60:lo:18:HIS:CE1   | 2.47                     | 0.50              |
| 62:lr:93:ILE:HA    | 62:lr:96:MET:CG    | 2.42                     | 0.50              |
| 66:sF:103:LEU:HD22 | 77:sZ:66:LYS:NZ    | 2.26                     | 0.50              |
| 66:sF:169:ILE:HD12 | 79:s2:1535:U:H5''  | 1.94                     | 0.50              |
| 70:sS:77:TYR:O     | 70:sS:77:TYR:CD2   | 2.64                     | 0.50              |
| 78:sf:95:ARG:HG3   | 79:s2:1305:C:OP2   | 2.12                     | 0.50              |
| 79:s2:429:C:H2'    | 79:s2:430:C:C6     | 2.46                     | 0.50              |
| 79:s2:1204:A:O2'   | 79:s2:1700:C:OP2   | 2.28                     | 0.50              |
| 79:s2:1266:C:C2    | 79:s2:1517:G:N2    | 2.80                     | 0.50              |
| 79:s2:1756:C:N4    | 79:s2:1775:U:O4    | 2.43                     | 0.50              |
| 80:cB:152:LYS:HZ3  | 80:cB:359:PRO:HG3  | 1.77                     | 0.50              |
| 80:cB:225:LEU:CD2  | 80:cB:260:LEU:HD23 | 2.41                     | 0.50              |
| 80:cB:407:LYS:HG3  | 80:cB:408:GLY:N    | 2.27                     | 0.50              |
| 85:l5:270:U:H2'    | 85:l5:271:C:H6     | 1.77                     | 0.50              |
| 85:l5:287:U:H2'    | 85:l5:288:G:H8     | 1.77                     | 0.50              |
| 85:l5:741:C:H2'    | 85:l5:742:G:O4'    | 2.11                     | 0.50              |
| 85:l5:751:G:H2'    | 85:l5:752:G:O4'    | 2.12                     | 0.50              |
| 85:l5:2034:G:H2'   | 85:l5:2035:C:H6    | 1.77                     | 0.50              |
| 85:l5:2250:C:H2'   | 85:l5:2251:G:C8    | 2.46                     | 0.50              |
| 85:l5:2832:A:H2'   | 85:l5:2833:A:C8    | 2.46                     | 0.50              |
| 85:l5:3937:C:H3'   | 85:l5:3938:G:H2'   | 1.94                     | 0.50              |
| 85:l5:4406:U:C2    | 85:l5:4407:G:C8    | 3.00                     | 0.50              |
| 85:l5:4537:C:H2'   | 85:l5:4538:G:C8    | 2.44                     | 0.50              |
| 85:l5:4592:C:H2'   | 85:l5:4593:C:C6    | 2.46                     | 0.50              |
| 85:l5:5004:C:H2'   | 85:l5:5005:G:O4'   | 2.11                     | 0.50              |
| 80:CB:45:ILE:HD11  | 80:CB:77:LEU:C     | 2.37                     | 0.50              |
| 80:CB:72:SER:O     | 80:CB:400:LYS:NZ   | 2.37                     | 0.50              |
| 80:CB:802:SER:HA   | 85:L5:4605:A:N7    | 2.27                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:SE:229:GLY:HA2   | 2:SE:235:TRP:CD1   | 2.47                     | 0.50              |
| 6:SG:23:LYS:O      | 6:SG:26:THR:OG1    | 2.18                     | 0.50              |
| 15:SC:166:ARG:HG3  | 15:SC:181:PRO:HG3  | 1.92                     | 0.50              |
| 16:SN:83:ASP:OD1   | 16:SN:84:LEU:N     | 2.45                     | 0.50              |
| 17:SO:66:ARG:CZ    | 79:S2:962:A:H4'    | 2.41                     | 0.50              |
| 19:Sb:81:ARG:HH11  | 19:Sb:81:ARG:HA    | 1.77                     | 0.50              |
| 85:L5:23:C:OP2     | 55:Lj:46:LYS:NZ    | 2.38                     | 0.50              |
| 85:L5:268:G:H2'    | 85:L5:269:G:C8     | 2.43                     | 0.50              |
| 85:L5:324:A:H2'    | 85:L5:325:U:C6     | 2.47                     | 0.50              |
| 85:L5:413:G:OP2    | 57:Ll:36:ARG:NH1   | 2.45                     | 0.50              |
| 85:L5:710:G:H2'    | 85:L5:711:A:C8     | 2.46                     | 0.50              |
| 85:L5:1341:U:H2'   | 85:L5:1342:A:H8    | 1.77                     | 0.50              |
| 85:L5:1397:A:N7    | 46:La:114:LYS:HD2  | 2.26                     | 0.50              |
| 85:L5:1471:U:H2'   | 85:L5:1472:C:C6    | 2.46                     | 0.50              |
| 85:L5:1534:A:H2'   | 85:L5:1637:A:C6    | 2.47                     | 0.50              |
| 85:L5:1613:A:H5''  | 22:LA:183:GLY:CA   | 2.42                     | 0.50              |
| 85:L5:1701:A:P     | 85:L5:1703:C:H42   | 2.34                     | 0.50              |
| 85:L5:1762:C:N4    | 85:L5:1770:A:H2    | 2.01                     | 0.50              |
| 85:L5:1921:C:C6    | 39:LS:161:ARG:HD3  | 2.47                     | 0.50              |
| 85:L5:2562:G:O2'   | 85:L5:2565:A:N6    | 2.44                     | 0.50              |
| 85:L5:3685:C:H5'   | 22:LA:193:ARG:CZ   | 2.42                     | 0.50              |
| 85:L5:4192:A:H2'   | 85:L5:4193:C:H6    | 1.76                     | 0.50              |
| 85:L5:4458:C:H2'   | 85:L5:4459:U:C6    | 2.47                     | 0.50              |
| 85:L5:4685:U:H2'   | 85:L5:4686:G:C8    | 2.47                     | 0.50              |
| 85:L5:5039:U:OP2   | 87:LW:61:LYS:NZ    | 2.44                     | 0.50              |
| 21:L8:132:G:H2'    | 21:L8:133:G:H8     | 1.75                     | 0.50              |
| 25:LD:212:MET:HE1  | 25:LD:219:TYR:CE1  | 2.46                     | 0.50              |
| 26:LE:72:LYS:HE3   | 47:Lb:119:CYS:HA   | 1.93                     | 0.50              |
| 33:LM:41:PRO:CG    | 33:LM:74:ARG:HG2   | 2.42                     | 0.50              |
| 41:LU:100:LEU:HB3  | 41:LU:112:LEU:HD11 | 1.93                     | 0.50              |
| 46:La:75:LEU:O     | 46:La:78:LEU:HG    | 2.11                     | 0.50              |
| 52:Lg:101:LYS:O    | 52:Lg:104:VAL:HG12 | 2.11                     | 0.50              |
| 64:SR:46:LEU:O     | 64:SR:50:ILE:HG12  | 2.12                     | 0.50              |
| 67:SK:76:ILE:HG22  | 67:SK:80:ARG:HH12  | 1.77                     | 0.50              |
| 69:SQ:125:ARG:HD2  | 79:S2:1648:G:H5''  | 1.94                     | 0.50              |
| 72:SU:48:LEU:HD12  | 72:SU:93:SER:HB2   | 1.93                     | 0.50              |
| 72:SU:87:ARG:NH2   | 79:S2:1447:G:OP1   | 2.45                     | 0.50              |
| 75:Sg:159:ASN:ND2  | 75:Sg:161:SER:O    | 2.45                     | 0.50              |
| 75:Sg:163:PRO:C    | 75:Sg:164:ILE:HD13 | 2.36                     | 0.50              |
| 76:SM:124:ILE:HG22 | 76:SM:128:PHE:HE2  | 1.77                     | 0.50              |
| 79:S2:1018:U:H2'   | 79:S2:1019:C:H6    | 1.76                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 79:S2:1798:C:H2'   | 79:S2:1799:G:O4'   | 2.12                     | 0.50              |
| 1:CH:39:GLU:N      | 1:CH:39:GLU:OE2    | 2.44                     | 0.50              |
| 13:sV:27:LYS:HZ1   | 15:sC:161:SER:C    | 2.19                     | 0.50              |
| 13:sV:38:GLU:HB2   | 13:sV:47:ASN:ND2   | 2.27                     | 0.50              |
| 15:sC:230:THR:HG22 | 79:s2:5:U:P        | 2.52                     | 0.50              |
| 18:sW:57:ARG:NH2   | 79:s2:920:A:OP1    | 2.44                     | 0.50              |
| 20:l7:88:A:H2'     | 20:l7:89:G:C8      | 2.47                     | 0.50              |
| 21:l8:16:G:N2      | 85:l5:418:A:OP2    | 2.45                     | 0.50              |
| 21:l8:114:G:H2'    | 21:l8:115:G:H8     | 1.76                     | 0.50              |
| 22:lA:233:ARG:HB2  | 85:l5:4184:G:H5'   | 1.94                     | 0.50              |
| 25:lD:250:ASN:OD1  | 25:lD:250:ASN:N    | 2.45                     | 0.50              |
| 29:lH:23:ARG:O     | 29:lH:38:PHE:N     | 2.41                     | 0.50              |
| 30:lI:3:ARG:NH1    | 30:lI:63:GLU:OE2   | 2.45                     | 0.50              |
| 31:lJ:16:ARG:NH1   | 31:lJ:18:ARG:HG3   | 2.22                     | 0.50              |
| 32:lL:90:VAL:O     | 32:lL:93:THR:HG22  | 2.10                     | 0.50              |
| 32:lL:184:MET:HE1  | 85:l5:1487:G:C1'   | 2.41                     | 0.50              |
| 35:lO:163:LYS:O    | 35:lO:166:ILE:HG22 | 2.10                     | 0.50              |
| 37:lQ:146:ARG:NH2  | 85:l5:1347:G:OP1   | 2.35                     | 0.50              |
| 43:lX:114:LYS:HA   | 43:lX:119:ILE:O    | 2.12                     | 0.50              |
| 45:lZ:7:PRO:HA     | 45:lZ:25:ILE:HG23  | 1.93                     | 0.50              |
| 63:lz:198:TRP:CD1  | 63:lz:199:GLN:HG3  | 2.47                     | 0.50              |
| 65:sD:99:ILE:O     | 65:sD:103:GLU:HG2  | 2.11                     | 0.50              |
| 65:sD:193:ASP:OD1  | 65:sD:194:PRO:HD3  | 2.12                     | 0.50              |
| 66:sF:156:THR:O    | 66:sF:160:GLU:HG3  | 2.12                     | 0.50              |
| 69:sQ:45:ARG:HB3   | 69:sQ:48:GLN:HG2   | 1.94                     | 0.50              |
| 71:sT:126:GLN:O    | 71:sT:129:ARG:HB2  | 2.11                     | 0.50              |
| 72:sU:37:ALA:O     | 72:sU:40:ILE:HG12  | 2.11                     | 0.50              |
| 75:sg:159:ASN:ND2  | 75:sg:161:SER:O    | 2.44                     | 0.50              |
| 78:sf:87:THR:HA    | 79:s2:1507:G:H1    | 1.76                     | 0.50              |
| 79:s2:414:A:H2'    | 79:s2:415:A:H8     | 1.77                     | 0.50              |
| 79:s2:811:A:H2'    | 79:s2:812:A:C8     | 2.47                     | 0.50              |
| 79:s2:1094:C:H2'   | 79:s2:1095:C:H6    | 1.75                     | 0.50              |
| 79:s2:1852:C:H2'   | 79:s2:1853:C:C6    | 2.47                     | 0.50              |
| 80:cB:162:ARG:NH1  | 85:l5:4601:U:O3'   | 2.44                     | 0.50              |
| 80:cB:266:PHE:HA   | 80:cB:273:PHE:HA   | 1.93                     | 0.50              |
| 85:l5:665:C:H4'    | 85:l5:666:G:H5'    | 1.92                     | 0.50              |
| 85:l5:1243:C:C2    | 85:l5:1244:G:C8    | 2.99                     | 0.50              |
| 85:l5:2728:U:H2'   | 85:l5:2729:C:H6    | 1.75                     | 0.50              |
| 85:l5:3783:A:N7    | 85:l5:3792:G:C8    | 2.80                     | 0.50              |
| 85:l5:4093:G:C5    | 85:l5:4095:G:N2    | 2.80                     | 0.50              |
| 85:l5:4973:U:H3    | 85:l5:4985:U:H3    | 1.58                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 80:CB:686:ALA:HB2  | 80:CB:726:ARG:HG3  | 1.94                     | 0.50              |
| 2:SE:80:ILE:HG23   | 2:SE:81:THR:HG23   | 1.93                     | 0.50              |
| 3:SI:148:LYS:HZ2   | 3:SI:149:TYR:N     | 2.09                     | 0.50              |
| 4:SL:99:TYR:CD1    | 5:SX:13:LEU:HD13   | 2.46                     | 0.50              |
| 4:SL:126:VAL:HG23  | 4:SL:145:VAL:HG12  | 1.94                     | 0.50              |
| 5:SX:84:PHE:HD2    | 5:SX:85:VAL:N      | 2.09                     | 0.50              |
| 16:SN:39:LYS:O     | 16:SN:39:LYS:NZ    | 2.36                     | 0.50              |
| 85:L5:7:C:H2'      | 85:L5:8:U:C6       | 2.47                     | 0.50              |
| 85:L5:222:C:H2'    | 85:L5:223:G:O4'    | 2.12                     | 0.50              |
| 85:L5:418:A:C2     | 21:L8:17:A:H1'     | 2.46                     | 0.50              |
| 85:L5:680:G:H2'    | 85:L5:681:G:H8     | 1.77                     | 0.50              |
| 85:L5:703:G:H2'    | 85:L5:704:C:H4'    | 1.94                     | 0.50              |
| 85:L5:1534:A:H1'   | 55:Lj:11:ARG:NH2   | 2.27                     | 0.50              |
| 85:L5:1847:C:H2'   | 85:L5:1848:C:H6    | 1.76                     | 0.50              |
| 85:L5:1870:C:H2'   | 85:L5:1871:A:C8    | 2.46                     | 0.50              |
| 85:L5:4093:G:C8    | 85:L5:4094:G:C8    | 2.99                     | 0.50              |
| 85:L5:4661:G:H2'   | 85:L5:4662:C:C6    | 2.46                     | 0.50              |
| 85:L5:4710:C:H2'   | 85:L5:4711:C:C6    | 2.47                     | 0.50              |
| 23:LB:161:ARG:HA   | 23:LB:184:GLN:HA   | 1.94                     | 0.50              |
| 27:LF:30:ILE:O     | 27:LF:34:ARG:HG3   | 2.12                     | 0.50              |
| 38:LR:104:ARG:HA   | 38:LR:107:ARG:NH1  | 2.26                     | 0.50              |
| 43:LX:109:ILE:O    | 43:LX:113:VAL:HG12 | 2.12                     | 0.50              |
| 48:Lc:51:ASN:HD21  | 61:Lp:41:PHE:C     | 2.20                     | 0.50              |
| 56:Lk:33:LYS:HG2   | 56:Lk:46:VAL:HG22  | 1.93                     | 0.50              |
| 63:Lz:163:LEU:HD12 | 63:Lz:164:CYS:HB2  | 1.93                     | 0.50              |
| 66:SF:45:TYR:C     | 66:SF:45:TYR:CD1   | 2.89                     | 0.50              |
| 66:SF:140:ASP:OD2  | 73:Sc:46:VAL:HG22  | 2.11                     | 0.50              |
| 67:SK:83:LEU:HD13  | 67:SK:85:LEU:HG    | 1.93                     | 0.50              |
| 71:ST:133:ARG:HG2  | 71:ST:137:GLN:HE22 | 1.77                     | 0.50              |
| 73:Sc:12:ALA:HB1   | 73:Sc:32:VAL:HB    | 1.92                     | 0.50              |
| 75:Sg:31:ILE:HD11  | 75:Sg:43:TRP:HB2   | 1.93                     | 0.50              |
| 75:Sg:240:CYS:HG   | 75:Sg:291:TRP:CD1  | 2.30                     | 0.50              |
| 76:SM:64:LEU:O     | 76:SM:68:LEU:HG    | 2.12                     | 0.50              |
| 77:SZ:65:TYR:CA    | 77:SZ:111:ARG:HE   | 2.23                     | 0.50              |
| 79:S2:24:C:O2'     | 79:S2:25:A:O5'     | 2.30                     | 0.50              |
| 79:S2:434:G:H2'    | 79:S2:435:A:C8     | 2.46                     | 0.50              |
| 79:S2:1227:G:C2    | 79:S2:1228:A:C8    | 2.99                     | 0.50              |
| 79:S2:1271:C:N4    | 79:S2:1512:C:N3    | 2.60                     | 0.50              |
| 81:AP:52:G:H2'     | 81:AP:53:G:C8      | 2.47                     | 0.50              |
| 83:Ls:55:MET:HB3   | 83:Ls:87:GLY:HA2   | 1.94                     | 0.50              |
| 84:Lt:108:GLU:O    | 84:Lt:112:ILE:HG12 | 2.12                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:cH:42:LYS:HG3    | 9:se:42:PHE:CD1    | 2.47                     | 0.50              |
| 5:sX:105:PHE:HB2   | 5:sX:119:ARG:C     | 2.37                     | 0.50              |
| 6:sG:136:LYS:HD3   | 79:s2:65:C:H5      | 1.77                     | 0.50              |
| 6:sG:186:GLN:OE1   | 79:s2:319:C:N4     | 2.44                     | 0.50              |
| 10:sA:214:GLU:CD   | 10:sA:214:GLU:H    | 2.19                     | 0.50              |
| 14:sa:2:THR:OG1    | 14:sa:3:LYS:N      | 2.42                     | 0.50              |
| 14:sa:27:ALA:HB1   | 17:sO:144:GLY:HA3  | 1.94                     | 0.50              |
| 14:sa:75:VAL:HG21  | 79:s2:1862:G:N1    | 2.27                     | 0.50              |
| 18:sW:31:SER:O     | 18:sW:35:VAL:HG13  | 2.11                     | 0.50              |
| 21:l8:39:G:OP1     | 53:lh:86:LYS:NZ    | 2.42                     | 0.50              |
| 21:l8:145:C:H2'    | 21:l8:146:U:C6     | 2.47                     | 0.50              |
| 22:lA:29:LEU:HG    | 22:lA:124:GLY:H    | 1.77                     | 0.50              |
| 22:lA:82:ILE:HB    | 22:lA:86:GLN:HE21  | 1.77                     | 0.50              |
| 22:lA:189:TYR:CD1  | 22:lA:196:TRP:HB2  | 2.47                     | 0.50              |
| 24:lC:139:SER:O    | 62:lr:15:SER:N     | 2.39                     | 0.50              |
| 24:lC:292:ILE:HG22 | 24:lC:293:LEU:HD22 | 1.93                     | 0.50              |
| 25:lD:60:ILE:HB    | 25:lD:80:ALA:HB2   | 1.93                     | 0.50              |
| 34:lN:29:GLN:HG3   | 34:lN:30:TYR:HD1   | 1.77                     | 0.50              |
| 44:lY:30:MET:SD    | 44:lY:101:PRO:HG3  | 2.52                     | 0.50              |
| 49:ld:26:THR:HB    | 49:ld:85:ARG:HD2   | 1.93                     | 0.50              |
| 52:lg:90:ARG:NH2   | 85:l5:4122:G:O3'   | 2.45                     | 0.50              |
| 55:lj:34:CYS:HB3   | 55:lj:39:TYR:H     | 1.76                     | 0.50              |
| 56:lk:5:ILE:HD11   | 56:lk:43:TYR:HD1   | 1.76                     | 0.50              |
| 56:lk:19:ASP:OD2   | 85:l5:2773:G:H4'   | 2.12                     | 0.50              |
| 68:sP:58:LYS:HA    | 68:sP:61:ARG:HD2   | 1.94                     | 0.50              |
| 69:sQ:58:LEU:HB3   | 69:sQ:62:ARG:HD3   | 1.94                     | 0.50              |
| 77:sZ:82:SER:HA    | 77:sZ:85:ARG:HE    | 1.76                     | 0.50              |
| 79:s2:555:A:C2     | 79:s2:557:U:H1'    | 2.46                     | 0.50              |
| 79:s2:1734:G:O2'   | 79:s2:1800:A:N6    | 2.39                     | 0.50              |
| 79:s2:1750:C:H2'   | 79:s2:1751:C:O4'   | 2.12                     | 0.50              |
| 80:cB:319:LEU:HG   | 80:cB:321:ILE:HG23 | 1.93                     | 0.50              |
| 80:cB:749:ILE:HD11 | 80:cB:808:ALA:HB1  | 1.94                     | 0.50              |
| 83:ls:44:ARG:HH21  | 84:lt:124:GLU:HG2  | 1.77                     | 0.50              |
| 83:ls:165:ASP:OD1  | 83:ls:165:ASP:N    | 2.40                     | 0.50              |
| 85:l5:190:G:H2'    | 85:l5:191:G:H8     | 1.76                     | 0.50              |
| 85:l5:693:C:H2'    | 85:l5:694:C:H6     | 1.77                     | 0.50              |
| 85:l5:1244:G:H2'   | 85:l5:1245:C:H6    | 1.76                     | 0.50              |
| 85:l5:1806:G:H2'   | 85:l5:1807:C:H6    | 1.76                     | 0.50              |
| 85:l5:2654:C:H2'   | 85:l5:2655:C:C6    | 2.47                     | 0.50              |
| 85:l5:4768:G:O3'   | 85:l5:4873:G:N2    | 2.45                     | 0.50              |
| 85:l5:4957:C:H2'   | 85:l5:4958:C:C6    | 2.47                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:SE:140:VAL:O     | 2:SE:140:VAL:HG13  | 2.11                     | 0.50              |
| 10:SA:79:SER:HB3   | 10:SA:130:ASP:OD1  | 2.12                     | 0.50              |
| 10:SA:91:ALA:HA    | 10:SA:96:ALA:HB3   | 1.94                     | 0.50              |
| 11:SB:82:ARG:NH2   | 11:SB:191:ASP:HB2  | 2.27                     | 0.50              |
| 13:SV:50:PHE:CE2   | 13:SV:52:THR:HB    | 2.47                     | 0.50              |
| 14:Sa:74:CYS:SG    | 14:Sa:77:CYS:N     | 2.75                     | 0.50              |
| 85:L5:179:G:H2'    | 85:L5:180:C:C6     | 2.47                     | 0.50              |
| 85:L5:210:C:O2'    | 85:L5:233:U:O2'    | 2.27                     | 0.50              |
| 85:L5:350:C:H3'    | 24:LC:197:ARG:HH12 | 1.77                     | 0.50              |
| 85:L5:372:A:H4'    | 55:Lj:45:ARG:HH22  | 1.77                     | 0.50              |
| 85:L5:909:A:H2'    | 85:L5:910:G:H8     | 1.77                     | 0.50              |
| 85:L5:969:C:OP1    | 26:LE:110:ARG:NH2  | 2.45                     | 0.50              |
| 85:L5:2662:G:H2'   | 85:L5:2663:G:C8    | 2.47                     | 0.50              |
| 85:L5:2823:G:N7    | 38:LR:20:LYS:NZ    | 2.60                     | 0.50              |
| 85:L5:4095:G:H3'   | 85:L5:4110:C:C2    | 2.47                     | 0.50              |
| 85:L5:4101:C:C6    | 85:L5:4104:G:O3'   | 2.65                     | 0.50              |
| 85:L5:4593:C:H2'   | 85:L5:4594:U:H6    | 1.77                     | 0.50              |
| 85:L5:4680:G:H2'   | 85:L5:4681:A:H8    | 1.77                     | 0.50              |
| 85:L5:4711:C:H2'   | 85:L5:4712:C:C6    | 2.46                     | 0.50              |
| 21:L8:14:U:C4      | 21:L8:15:G:C6      | 3.00                     | 0.50              |
| 25:LD:51:MET:HB3   | 25:LD:146:LEU:HA   | 1.93                     | 0.50              |
| 28:LG:51:LEU:N     | 43:LX:41:ARG:O     | 2.44                     | 0.50              |
| 28:LG:159:HIS:CE1  | 28:LG:160:ASP:HB3  | 2.47                     | 0.50              |
| 31:LJ:95:ARG:HD3   | 31:LJ:95:ARG:H     | 1.76                     | 0.50              |
| 32:LL:47:ALA:O     | 32:LL:149:GLN:NE2  | 2.45                     | 0.50              |
| 35:LO:42:ASN:ND2   | 35:LO:135:PHE:CD2  | 2.79                     | 0.50              |
| 35:LO:62:MET:SD    | 35:LO:65:ASN:N     | 2.75                     | 0.50              |
| 40:LT:127:GLN:HE22 | 40:LT:129:LYS:C    | 2.19                     | 0.50              |
| 54:Li:6:PRO:O      | 54:Li:6:PRO:HD2    | 2.11                     | 0.50              |
| 54:Li:15:HIS:ND1   | 54:Li:15:HIS:O     | 2.45                     | 0.50              |
| 61:Lp:39:CYS:HB3   | 61:Lp:42:CYS:SG    | 2.51                     | 0.50              |
| 62:Lr:44:ILE:HG13  | 62:Lr:45:HIS:N     | 2.26                     | 0.50              |
| 66:SF:22:LYS:HG3   | 66:SF:23:TRP:CD2   | 2.47                     | 0.50              |
| 68:SP:28:MET:CE    | 68:SP:32:GLN:HG2   | 2.42                     | 0.50              |
| 69:SQ:58:LEU:HB3   | 69:SQ:62:ARG:HD2   | 1.93                     | 0.50              |
| 75:Sg:18:VAL:HG21  | 75:Sg:307:VAL:HG23 | 1.92                     | 0.50              |
| 76:SM:49:LEU:HD23  | 76:SM:114:TYR:OH   | 2.11                     | 0.50              |
| 77:SZ:50:PHE:HE1   | 77:SZ:55:TYR:CA    | 2.22                     | 0.50              |
| 77:SZ:55:TYR:O     | 77:SZ:58:LEU:HD12  | 2.11                     | 0.50              |
| 79:S2:221:A:H2'    | 79:S2:222:U:H6     | 1.76                     | 0.50              |
| 79:S2:612:U:H3'    | 79:S2:613:G:C8     | 2.47                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 79:S2:888:U:H4'    | 79:S2:889:U:H5'    | 1.94                     | 0.50              |
| 79:S2:945:U:H2'    | 79:S2:946:U:C6     | 2.47                     | 0.50              |
| 79:S2:1064:C:H2'   | 79:S2:1065:G:C8    | 2.44                     | 0.50              |
| 79:S2:1365:G:H2'   | 79:S2:1366:G:C8    | 2.47                     | 0.50              |
| 79:S2:1420:G:O2'   | 79:S2:1421:A:N3    | 2.44                     | 0.50              |
| 79:S2:1432:U:H5''  | 79:S2:1433:C:H5''  | 1.93                     | 0.50              |
| 79:S2:1722:G:H2'   | 79:S2:1723:G:C8    | 2.47                     | 0.50              |
| 83:Ls:121:VAL:O    | 83:Ls:160:LEU:HB3  | 2.12                     | 0.50              |
| 84:Lt:76:SER:OG    | 84:Lt:117:ARG:HG3  | 2.11                     | 0.50              |
| 87:IW:9:SER:O      | 87:IW:53:VAL:HG22  | 2.11                     | 0.50              |
| 2:sE:124:CYS:HB3   | 2:sE:141:THR:OG1   | 2.11                     | 0.49              |
| 7:sJ:115:PHE:CD2   | 7:sJ:123:ILE:HB    | 2.46                     | 0.49              |
| 8:sY:94:HIS:HD1    | 8:sY:96:LEU:HD23   | 1.77                     | 0.49              |
| 9:se:33:LYS:O      | 9:se:37:GLN:NE2    | 2.45                     | 0.49              |
| 10:sA:61:ALA:O     | 10:sA:65:ILE:HG12  | 2.12                     | 0.49              |
| 11:sB:225:LEU:O    | 11:sB:228:LEU:HG   | 2.11                     | 0.49              |
| 14:sa:12:LYS:NZ    | 79:s2:1859:A:OP1   | 2.45                     | 0.49              |
| 15:sC:60:TRP:CD1   | 15:sC:61:MET:C     | 2.90                     | 0.49              |
| 16:sN:115:LEU:O    | 16:sN:119:GLU:HG2  | 2.12                     | 0.49              |
| 18:sW:32:LYS:O     | 18:sW:36:ARG:HG3   | 2.12                     | 0.49              |
| 23:IB:57:VAL:HG22  | 23:IB:73:VAL:HG12  | 1.93                     | 0.49              |
| 25:ID:35:ARG:NH1   | 85:l5:4325:A:C5    | 2.80                     | 0.49              |
| 25:ID:206:ASP:N    | 25:ID:206:ASP:OD2  | 2.45                     | 0.49              |
| 27:IF:64:MET:HE3   | 27:IF:64:MET:N     | 2.27                     | 0.49              |
| 27:IF:154:ILE:HG21 | 27:IF:191:ILE:HD12 | 1.94                     | 0.49              |
| 28:IG:138:ALA:O    | 28:IG:142:THR:OG1  | 2.23                     | 0.49              |
| 32:IL:71:ARG:HG2   | 32:IL:72:ALA:N     | 2.26                     | 0.49              |
| 39:IS:71:SER:O     | 39:IS:76:LYS:NZ    | 2.39                     | 0.49              |
| 39:IS:82:LEU:HB3   | 39:IS:126:ILE:HD12 | 1.93                     | 0.49              |
| 44:IY:81:TYR:CD2   | 44:IY:96:HIS:HB2   | 2.47                     | 0.49              |
| 58:lm:94:MET:N     | 58:lm:103:LEU:O    | 2.34                     | 0.49              |
| 61:lp:14:TYR:HB3   | 61:lp:18:TYR:HE2   | 1.76                     | 0.49              |
| 65:sD:118:ALA:O    | 65:sD:122:VAL:HG13 | 2.12                     | 0.49              |
| 67:sK:8:ARG:NH2    | 79:s2:1314:U:H4'   | 2.27                     | 0.49              |
| 72:sU:67:LYS:HA    | 74:sd:44:ARG:HD2   | 1.94                     | 0.49              |
| 76:sM:22:LEU:HD21  | 76:sM:88:TRP:HE3   | 1.77                     | 0.49              |
| 76:sM:40:LYS:HE2   | 78:sf:130:VAL:HA   | 1.94                     | 0.49              |
| 77:sZ:104:ARG:NH2  | 79:s2:1594:A:H62   | 2.09                     | 0.49              |
| 79:s2:30:C:C4      | 79:s2:31:U:C4      | 3.00                     | 0.49              |
| 79:s2:207:G:C2     | 79:s2:208:G:H1'    | 2.47                     | 0.49              |
| 79:s2:461:U:H2'    | 79:s2:462:C:H6     | 1.75                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 79:s2:920:A:O2'    | 79:s2:922:A:O5'    | 2.30                     | 0.49              |
| 79:s2:1690:U:H2'   | 79:s2:1691:U:C6    | 2.47                     | 0.49              |
| 79:s2:1798:C:H2'   | 79:s2:1799:G:O4'   | 2.12                     | 0.49              |
| 80:cB:759:ILE:HG22 | 80:cB:800:LEU:HD11 | 1.94                     | 0.49              |
| 84:lt:16:ARG:HH22  | 84:lt:29:ALA:HB2   | 1.76                     | 0.49              |
| 85:l5:272:U:H2'    | 85:l5:273:U:H6     | 1.76                     | 0.49              |
| 85:l5:4143:G:C4    | 85:l5:4145:C:H1'   | 2.46                     | 0.49              |
| 85:l5:4261:C:H2'   | 85:l5:4262:C:H6    | 1.77                     | 0.49              |
| 80:CB:8:GLN:HB3    | 8:SY:130:LYS:CD    | 2.36                     | 0.49              |
| 80:CB:165:LEU:HD12 | 80:CB:166:GLU:N    | 2.26                     | 0.49              |
| 80:CB:551:GLU:O    | 80:CB:555:GLU:HG3  | 2.12                     | 0.49              |
| 2:SE:212:ASP:OD2   | 2:SE:216:ASN:HB2   | 2.12                     | 0.49              |
| 2:SE:227:VAL:C     | 2:SE:228:ILE:HD13  | 2.37                     | 0.49              |
| 10:SA:85:ARG:HG2   | 10:SA:89:LYS:NZ    | 2.27                     | 0.49              |
| 13:SV:58:ALA:O     | 13:SV:62:MET:HG3   | 2.12                     | 0.49              |
| 15:SC:267:GLN:N    | 15:SC:267:GLN:OE1  | 2.45                     | 0.49              |
| 16:SN:73:ARG:O     | 16:SN:76:LYS:HG3   | 2.12                     | 0.49              |
| 85:L5:154:G:H5''   | 53:Lh:105:LYS:NZ   | 2.27                     | 0.49              |
| 85:L5:310:G:H2'    | 85:L5:311:G:H8     | 1.77                     | 0.49              |
| 85:L5:507:G:C2     | 85:L5:652:G:C2     | 3.00                     | 0.49              |
| 85:L5:937:U:OP1    | 33:LM:46:ARG:NE    | 2.44                     | 0.49              |
| 85:L5:1424:G:H1'   | 47:Lb:29:TYR:CE2   | 2.42                     | 0.49              |
| 85:L5:1956:A:H2'   | 85:L5:1957:U:C6    | 2.47                     | 0.49              |
| 85:L5:2107:C:H2'   | 85:L5:2108:G:C8    | 2.47                     | 0.49              |
| 85:L5:2521:G:H2'   | 85:L5:2522:G:H8    | 1.77                     | 0.49              |
| 85:L5:2568:C:H2'   | 85:L5:2569:G:H8    | 1.76                     | 0.49              |
| 85:L5:3855:C:P     | 36:LP:82:ARG:HE    | 2.34                     | 0.49              |
| 85:L5:3968:U:O4    | 85:L5:4053:A:O2'   | 2.18                     | 0.49              |
| 85:L5:4112:C:H1'   | 85:L5:4113:U:OP1   | 2.12                     | 0.49              |
| 85:L5:4524:G:OP1   | 85:L5:4559:A:N6    | 2.42                     | 0.49              |
| 85:L5:4611:A:H2'   | 85:L5:4612:C:H6    | 1.77                     | 0.49              |
| 21:L8:146:U:H4'    | 43:LX:52:LEU:HD21  | 1.94                     | 0.49              |
| 23:LB:43:LEU:HD23  | 23:LB:185:VAL:HG23 | 1.94                     | 0.49              |
| 30:LI:53:VAL:HG13  | 30:LI:164:LYS:HB2  | 1.94                     | 0.49              |
| 55:Lj:51:ALA:HA    | 55:Lj:54:LYS:HD3   | 1.93                     | 0.49              |
| 68:SP:85:ILE:HD12  | 68:SP:85:ILE:H     | 1.76                     | 0.49              |
| 69:SQ:4:LYS:HE3    | 79:S2:1423:C:H5    | 1.77                     | 0.49              |
| 75:Sg:280:LYS:NZ   | 79:S2:1458:G:O3'   | 2.40                     | 0.49              |
| 79:S2:666:U:H2'    | 79:S2:667:U:C6     | 2.47                     | 0.49              |
| 79:S2:1013:U:H2'   | 79:S2:1014:G:C8    | 2.46                     | 0.49              |
| 79:S2:1112:U:O2    | 79:S2:1121:G:O6    | 2.29                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 79:S2:1862:G:H1'  | 79:S2:1863:A:H2'  | 1.94                     | 0.49              |
| 4:sL:84:ARG:O     | 4:sL:112:HIS:ND1  | 2.44                     | 0.49              |
| 8:sY:19:GLN:CD    | 8:sY:81:TYR:CD1   | 2.87                     | 0.49              |
| 11:sB:25:PHE:HA   | 11:sB:28:LYS:HG2  | 1.95                     | 0.49              |
| 11:sB:35:ALA:HB1  | 11:sB:39:PHE:HD2  | 1.77                     | 0.49              |
| 16:sN:39:LYS:HA   | 16:sN:42:LYS:HE3  | 1.94                     | 0.49              |
| 20:l7:119:U:H5    | 25:lD:258:LYS:HZ2 | 1.57                     | 0.49              |
| 21:l8:94:G:N3     | 55:lJ:82:THR:OG1  | 2.46                     | 0.49              |
| 23:lB:119:TYR:OH  | 23:lB:129:ALA:N   | 2.45                     | 0.49              |
| 24:lC:83:GLY:HA3  | 85:l5:368:C:O4'   | 2.12                     | 0.49              |
| 28:lG:60:TYR:O    | 28:lG:64:GLN:HG2  | 2.12                     | 0.49              |
| 30:lI:158:LYS:HE3 | 85:l5:4430:G:H1'  | 1.94                     | 0.49              |
| 31:lJ:12:MET:SD   | 31:lJ:137:PRO:HG2 | 2.51                     | 0.49              |
| 32:lL:25:TRP:CZ3  | 85:l5:1360:G:H5'' | 2.47                     | 0.49              |
| 32:lL:194:ILE:O   | 32:lL:198:ARG:HG3 | 2.11                     | 0.49              |
| 33:lM:104:MET:CE  | 33:lM:108:ASP:HB2 | 2.17                     | 0.49              |
| 35:lO:19:LEU:O    | 35:lO:23:VAL:HG12 | 2.11                     | 0.49              |
| 38:lR:143:HIS:CE1 | 85:l5:3597:G:H5'  | 2.46                     | 0.49              |
| 42:lV:46:LYS:NZ   | 85:l5:4510:A:OP1  | 2.44                     | 0.49              |
| 45:lZ:75:TYR:HD1  | 45:lZ:80:LEU:HD21 | 1.77                     | 0.49              |
| 51:lF:2:SER:N     | 85:l5:4946:U:O2'  | 2.33                     | 0.49              |
| 64:sR:60:ARG:HB2  | 79:s2:1464:C:H5'  | 1.93                     | 0.49              |
| 66:sF:48:TYR:HB2  | 69:sQ:53:GLU:OE2  | 2.12                     | 0.49              |
| 67:sK:57:TYR:HB3  | 67:sK:75:GLY:CA   | 2.42                     | 0.49              |
| 72:sU:19:ARG:NH2  | 79:s2:1433:C:O2   | 2.45                     | 0.49              |
| 75:sg:220:ASP:OD1 | 75:sg:222:ASN:N   | 2.45                     | 0.49              |
| 77:sZ:45:ASN:ND2  | 77:sZ:45:ASN:O    | 2.45                     | 0.49              |
| 79:s2:464:A:H5'   | 79:s2:465:A:N7    | 2.27                     | 0.49              |
| 79:s2:494:C:H42   | 79:s2:509:G:H21   | 1.58                     | 0.49              |
| 79:s2:509:G:H2'   | 79:s2:510:G:H8    | 1.76                     | 0.49              |
| 79:s2:557:U:H5'   | 79:s2:558:G:C8    | 2.40                     | 0.49              |
| 79:s2:946:U:H2'   | 79:s2:947:G:C8    | 2.47                     | 0.49              |
| 79:s2:1387:G:O5'  | 79:s2:1387:G:H8   | 1.95                     | 0.49              |
| 79:s2:1533:A:H2   | 79:s2:1536:G:N3   | 2.10                     | 0.49              |
| 79:s2:1756:C:P    | 79:s2:1757:G:H21  | 2.35                     | 0.49              |
| 79:s2:1784:G:C2'  | 79:s2:1785:C:H5'  | 2.42                     | 0.49              |
| 80:cB:364:ALA:O   | 80:cB:368:ARG:HB2 | 2.12                     | 0.49              |
| 80:cB:654:PRO:HA  | 80:cB:684:GLN:NE2 | 2.27                     | 0.49              |
| 83:ls:57:LYS:N    | 83:ls:60:MET:HE1  | 2.27                     | 0.49              |
| 83:ls:120:GLU:OE2 | 83:ls:159:GLN:NE2 | 2.45                     | 0.49              |
| 85:l5:254:G:H2'   | 85:l5:255:C:O4'   | 2.11                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 85:L5:342:G:H2'    | 85:L5:343:C:C6     | 2.46                     | 0.49              |
| 85:L5:966:A:H5'    | 85:L5:2092:G:H1    | 1.76                     | 0.49              |
| 85:L5:2638:G:H3'   | 85:L5:2638:G:N3    | 2.27                     | 0.49              |
| 85:L5:4038:C:C5    | 85:L5:4050:A:H5'   | 2.47                     | 0.49              |
| 85:L5:4878:C:H2'   | 85:L5:4879:C:H6    | 1.77                     | 0.49              |
| 80:CB:206:ASP:HB3  | 80:CB:209:LEU:HG   | 1.93                     | 0.49              |
| 2:SE:59:ASP:OD1    | 2:SE:60:GLU:N      | 2.45                     | 0.49              |
| 3:SI:46:VAL:HG22   | 3:SI:54:LYS:HB2    | 1.94                     | 0.49              |
| 3:SI:193:LYS:HZ3   | 3:SI:200:ARG:HH12  | 1.60                     | 0.49              |
| 4:SL:137:THR:OG1   | 79:S2:373:G:OP1    | 2.16                     | 0.49              |
| 6:SG:190:ARG:HH12  | 79:S2:333:G:H3'    | 1.77                     | 0.49              |
| 10:SA:34:MET:HE2   | 10:SA:149:ASN:O    | 2.13                     | 0.49              |
| 17:SO:97:LEU:HD23  | 17:SO:98:ARG:N     | 2.28                     | 0.49              |
| 85:L5:35:U:H4'     | 85:L5:1525:A:C2    | 2.46                     | 0.49              |
| 85:L5:47:A:H5''    | 32:LL:16:LYS:HD3   | 1.94                     | 0.49              |
| 85:L5:189:G:N3     | 85:L5:253:G:N2     | 2.60                     | 0.49              |
| 85:L5:295:A:C2     | 85:L5:317:A:H1'    | 2.48                     | 0.49              |
| 85:L5:1084:C:H2'   | 85:L5:1085:C:C6    | 2.47                     | 0.49              |
| 85:L5:1236:C:H2'   | 85:L5:1237:C:C6    | 2.47                     | 0.49              |
| 85:L5:1274:A:O2'   | 85:L5:1275:G:H8    | 1.95                     | 0.49              |
| 85:L5:1471:U:H2'   | 85:L5:1472:C:H6    | 1.78                     | 0.49              |
| 85:L5:1629:G:C2    | 85:L5:1631:A:C2    | 3.00                     | 0.49              |
| 85:L5:1720:C:H2'   | 85:L5:1721:G:O4'   | 2.11                     | 0.49              |
| 85:L5:1977:C:O2'   | 85:L5:1978:C:OP1   | 2.27                     | 0.49              |
| 85:L5:2285:A:H2'   | 85:L5:2286:G:H8    | 1.77                     | 0.49              |
| 85:L5:2475:G:N1    | 43:LX:50:LYS:HG2   | 2.26                     | 0.49              |
| 85:L5:2809:G:H4'   | 38:LR:63:CYS:SG    | 2.52                     | 0.49              |
| 85:L5:2857:A:H2'   | 85:L5:2858:A:O4'   | 2.12                     | 0.49              |
| 85:L5:3736:A:H2'   | 85:L5:3737:A:O4'   | 2.12                     | 0.49              |
| 85:L5:3771:C:O2'   | 85:L5:3772:U:H5'   | 2.11                     | 0.49              |
| 85:L5:3827:G:O2'   | 85:L5:3829:G:OP2   | 2.21                     | 0.49              |
| 23:LB:395:ASP:O    | 23:LB:399:LYS:HG3  | 2.11                     | 0.49              |
| 27:LF:86:GLU:CD    | 40:LT:136:ARG:H    | 2.20                     | 0.49              |
| 32:LL:142:GLU:HB2  | 32:LL:146:LEU:HD13 | 1.93                     | 0.49              |
| 34:LN:135:ILE:HD11 | 34:LN:142:ILE:HD12 | 1.95                     | 0.49              |
| 38:LR:44:LEU:HD13  | 38:LR:49:LEU:HD13  | 1.92                     | 0.49              |
| 54:Li:88:GLU:OE2   | 54:Li:92:ASN:ND2   | 2.42                     | 0.49              |
| 64:SR:7:LYS:HD3    | 79:S2:1373:C:OP1   | 2.12                     | 0.49              |
| 66:SF:40:ALA:C     | 66:SF:45:TYR:CE1   | 2.90                     | 0.49              |
| 68:SP:92:SER:O     | 68:SP:107:ILE:HG12 | 2.13                     | 0.49              |
| 69:SQ:110:ASP:OD1  | 69:SQ:111:ILE:N    | 2.44                     | 0.49              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 71:ST:78:ILE:HD12 | 79:S2:1587:G:C8    | 2.46                     | 0.49              |
| 79:S2:224:A:H2'   | 79:S2:225:G:C8     | 2.46                     | 0.49              |
| 79:S2:443:U:H2'   | 79:S2:444:G:O4'    | 2.12                     | 0.49              |
| 79:S2:1643:U:H2'  | 79:S2:1644:C:C6    | 2.47                     | 0.49              |
| 79:S2:1650:A:H2'  | 79:S2:1651:A:O4'   | 2.13                     | 0.49              |
| 79:S2:1811:C:H3'  | 79:S2:1812:U:H4'   | 1.93                     | 0.49              |
| 82:PE:9:A:H4'     | 82:PE:46:G:O3'     | 2.12                     | 0.49              |
| 1:CH:50:LYS:HE2   | 1:CH:52:HIS:O      | 2.13                     | 0.49              |
| 1:cH:57:ASN:OD1   | 79:s2:536:A:H1'    | 2.13                     | 0.49              |
| 2:sE:103:TYR:CE2  | 2:sE:109:PHE:CE1   | 3.00                     | 0.49              |
| 5:sX:125:VAL:HG22 | 5:sX:126:ALA:H     | 1.76                     | 0.49              |
| 6:sG:136:LYS:HD3  | 79:s2:65:C:C5      | 2.47                     | 0.49              |
| 7:sJ:128:VAL:HG22 | 7:sJ:132:GLN:NE2   | 2.27                     | 0.49              |
| 10:sA:63:ARG:NH1  | 13:sV:36:VAL:HA    | 2.27                     | 0.49              |
| 10:sA:66:VAL:HG21 | 10:sA:185:MET:HG3  | 1.94                     | 0.49              |
| 17:sO:74:ALA:HB3  | 17:sO:114:SER:HB3  | 1.93                     | 0.49              |
| 21:l8:1:C:H2'     | 21:l8:2:G:O4'      | 2.12                     | 0.49              |
| 21:l8:83:C:H42    | 44:lY:50:ARG:HH22  | 1.60                     | 0.49              |
| 22:lA:28:ARG:HB2  | 22:lA:123:ARG:HB2  | 1.93                     | 0.49              |
| 22:lA:131:GLY:H   | 22:lA:169:VAL:HG13 | 1.76                     | 0.49              |
| 25:lD:63:GLN:HB2  | 25:lD:74:ILE:HD11  | 1.94                     | 0.49              |
| 27:lF:188:GLU:N   | 27:lF:188:GLU:OE2  | 2.45                     | 0.49              |
| 31:lJ:32:ARG:NE   | 31:lJ:35:ARG:CZ    | 2.76                     | 0.49              |
| 32:lL:180:ALA:O   | 32:lL:184:MET:HG2  | 2.12                     | 0.49              |
| 33:lM:128:LYS:NZ  | 85:l5:4896:G:O3'   | 2.40                     | 0.49              |
| 34:lN:37:HIS:O    | 34:lN:63:ARG:N     | 2.45                     | 0.49              |
| 34:lN:51:LEU:HD12 | 34:lN:117:ASN:CG   | 2.37                     | 0.49              |
| 34:lN:158:HIS:HB3 | 34:lN:161:MET:SD   | 2.52                     | 0.49              |
| 35:lO:180:GLN:O   | 35:lO:183:LYS:HG2  | 2.12                     | 0.49              |
| 50:le:46:ARG:HA   | 50:le:55:MET:HE1   | 1.94                     | 0.49              |
| 51:lf:5:LEU:HD21  | 85:l5:4945:G:C2    | 2.48                     | 0.49              |
| 59:ln:2:ARG:HE    | 59:ln:4:LYS:HG2    | 1.76                     | 0.49              |
| 64:sR:32:LYS:HG3  | 79:s2:1454:A:O5'   | 2.11                     | 0.49              |
| 68:sP:108:LYS:HZ1 | 68:sP:110:GLU:HG2  | 1.76                     | 0.49              |
| 71:sT:128:GLN:NE2 | 79:s2:1415:C:O2'   | 2.43                     | 0.49              |
| 79:s2:224:A:N6    | 79:s2:298:G:O6     | 2.45                     | 0.49              |
| 79:s2:323:C:O2'   | 79:s2:325:C:N4     | 2.45                     | 0.49              |
| 79:s2:1198:G:H2'  | 79:s2:1199:A:H8    | 1.76                     | 0.49              |
| 79:s2:1275:G:H22  | 79:s2:1506:A:P     | 2.34                     | 0.49              |
| 79:s2:1593:C:H2'  | 79:s2:1594:A:C8    | 2.47                     | 0.49              |
| 79:s2:1714:U:H2'  | 79:s2:1715:A:C8    | 2.47                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 79:s2:1827:U:C2   | 79:s2:1828:C:C5   | 3.00                     | 0.49              |
| 80:cB:581:GLU:OE1 | 80:cB:692:LEU:HB2 | 2.12                     | 0.49              |
| 80:cB:604:MET:HE2 | 80:cB:604:MET:C   | 2.37                     | 0.49              |
| 81:aP:56:C:H2'    | 81:aP:57:G:C8     | 2.47                     | 0.49              |
| 85:l5:751:G:N2    | 85:l5:915:A:N3    | 2.60                     | 0.49              |
| 85:l5:1402:C:N4   | 85:l5:1415:G:O6   | 2.45                     | 0.49              |
| 85:l5:2864:A:H2'  | 85:l5:2865:U:C6   | 2.47                     | 0.49              |
| 85:l5:3707:U:H2'  | 85:l5:3708:C:C6   | 2.47                     | 0.49              |
| 85:l5:4111:U:H2'  | 85:l5:4112:C:C5   | 2.47                     | 0.49              |
| 85:l5:4130:C:H2'  | 85:l5:4131:G:H8   | 1.77                     | 0.49              |
| 85:l5:4140:C:N3   | 85:l5:4143:G:N1   | 2.60                     | 0.49              |
| 85:l5:4396:A:N6   | 85:l5:4447:C:O2   | 2.45                     | 0.49              |
| 85:l5:4577:U:H2'  | 85:l5:4578:G:H8   | 1.77                     | 0.49              |
| 85:l5:4629:U:HO2' | 87:IW:19:ARG:NH1  | 2.09                     | 0.49              |
| 80:CB:607:ARG:HG2 | 80:CB:701:ARG:HB3 | 1.93                     | 0.49              |
| 2:SE:11:ARG:NH1   | 2:SE:24:THR:OG1   | 2.45                     | 0.49              |
| 3:SI:98:LYS:HG3   | 3:SI:178:ARG:HD2  | 1.94                     | 0.49              |
| 3:SI:143:LYS:NZ   | 79:S2:203:G:H5''  | 2.28                     | 0.49              |
| 7:SJ:155:LYS:HE2  | 7:SJ:156:HIS:CE1  | 2.48                     | 0.49              |
| 10:SA:164:ASN:OD1 | 10:SA:166:LYS:N   | 2.34                     | 0.49              |
| 85:L5:18:C:H2'    | 85:L5:19:G:H8     | 1.77                     | 0.49              |
| 85:L5:496:G:O6    | 85:L5:497:G:N2    | 2.45                     | 0.49              |
| 85:L5:655:C:OP1   | 24:LC:268:ARG:NH1 | 2.44                     | 0.49              |
| 85:L5:939:G:H2'   | 85:L5:940:C:C6    | 2.47                     | 0.49              |
| 85:L5:1081:C:N3   | 85:L5:1219:G:N1   | 2.60                     | 0.49              |
| 85:L5:1577:G:H5'  | 85:L5:1578:U:H5'' | 1.94                     | 0.49              |
| 85:L5:1721:G:H2'  | 85:L5:1722:C:C6   | 2.47                     | 0.49              |
| 85:L5:2569:G:H2'  | 85:L5:2570:U:H6   | 1.77                     | 0.49              |
| 85:L5:2703:G:C6   | 85:L5:2714:G:C6   | 3.00                     | 0.49              |
| 85:L5:2705:G:H1   | 85:L5:2710:C:H41  | 1.61                     | 0.49              |
| 85:L5:2886:U:H2'  | 85:L5:2887:U:C6   | 2.47                     | 0.49              |
| 85:L5:4220:A:OP2  | 40:LT:2:THR:HB    | 2.12                     | 0.49              |
| 85:L5:4545:G:OP2  | 22:LA:214:GLY:N   | 2.40                     | 0.49              |
| 21:L8:26:C:H2'    | 21:L8:27:U:C6     | 2.47                     | 0.49              |
| 23:LB:50:LYS:O    | 23:LB:342:LYS:N   | 2.45                     | 0.49              |
| 24:LC:158:VAL:HA  | 24:LC:161:TYR:CD1 | 2.47                     | 0.49              |
| 25:LD:234:ASP:O   | 25:LD:236:MET:N   | 2.45                     | 0.49              |
| 35:LO:65:ASN:O    | 35:LO:67:SER:N    | 2.46                     | 0.49              |
| 39:LS:11:LYS:HG2  | 39:LS:63:TYR:CE2  | 2.46                     | 0.49              |
| 41:LU:105:ASN:HB3 | 41:LU:111:GLU:OE2 | 2.11                     | 0.49              |
| 49:Ld:26:THR:OG1  | 49:Ld:85:ARG:NH1  | 2.44                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 51:Lf:50:VAL:HG21 | 51:Lf:102:ARG:CZ  | 2.42                     | 0.49              |
| 51:Lf:51:TYR:CZ   | 51:Lf:68:ARG:HB2  | 2.47                     | 0.49              |
| 54:Li:60:LEU:HD23 | 54:Li:60:LEU:O    | 2.13                     | 0.49              |
| 63:Lz:47:LYS:HG3  | 63:Lz:159:MET:HE3 | 1.93                     | 0.49              |
| 63:Lz:47:LYS:HE3  | 63:Lz:194:LEU:HB2 | 1.94                     | 0.49              |
| 75:Sg:191:HIS:CE1 | 75:Sg:215:GLN:HB2 | 2.48                     | 0.49              |
| 77:SZ:60:LYS:NZ   | 77:SZ:64:ASN:HD22 | 2.10                     | 0.49              |
| 79:S2:414:A:H2'   | 79:S2:415:A:H8    | 1.77                     | 0.49              |
| 79:S2:534:G:H2'   | 79:S2:535:G:C8    | 2.47                     | 0.49              |
| 79:S2:1657:G:H1   | 79:S2:1667:U:H3   | 1.59                     | 0.49              |
| 79:S2:1819:A:H2'  | 79:S2:1820:G:C8   | 2.46                     | 0.49              |
| 79:S2:1846:G:H2'  | 79:S2:1847:G:C8   | 2.47                     | 0.49              |
| 1:CH:131:LYS:HB3  | 1:CH:139:LYS:CB   | 2.43                     | 0.49              |
| 4:sL:85:THR:HA    | 4:sL:113:LEU:H    | 1.78                     | 0.49              |
| 6:sG:198:ARG:HA   | 6:sG:201:LYS:HE3  | 1.94                     | 0.49              |
| 10:sA:71:PRO:HB3  | 10:sA:94:THR:O    | 2.12                     | 0.49              |
| 11:sB:71:LEU:HA   | 11:sB:74:LEU:HB3  | 1.95                     | 0.49              |
| 11:sB:109:LYS:NZ  | 11:sB:113:MET:SD  | 2.79                     | 0.49              |
| 12:sH:98:ARG:HG3  | 12:sH:125:VAL:HB  | 1.94                     | 0.49              |
| 16:sN:33:VAL:HG22 | 16:sN:37:ILE:HD11 | 1.95                     | 0.49              |
| 19:sb:37:CYS:HA   | 19:sb:77:CYS:HB3  | 1.94                     | 0.49              |
| 20:l7:13:A:OP2    | 20:l7:66:G:N2     | 2.35                     | 0.49              |
| 20:l7:48:G:H2'    | 20:l7:49:A:C8     | 2.48                     | 0.49              |
| 22:lA:200:ARG:NH2 | 85:l5:3651:A:OP2  | 2.37                     | 0.49              |
| 22:lA:245:ARG:HB3 | 22:lA:247:ARG:HG3 | 1.95                     | 0.49              |
| 25:lD:164:LYS:HD3 | 25:lD:180:PHE:CE1 | 2.48                     | 0.49              |
| 27:lF:46:ARG:O    | 27:lF:50:ILE:HG23 | 2.11                     | 0.49              |
| 28:lG:111:LYS:O   | 28:lG:115:LEU:HG  | 2.12                     | 0.49              |
| 32:lL:54:PRO:HB2  | 32:lL:97:SER:HB3  | 1.94                     | 0.49              |
| 39:lS:84:TYR:O    | 39:lS:90:THR:OG1  | 2.20                     | 0.49              |
| 39:lS:135:SER:OG  | 39:lS:136:LYS:HD2 | 2.13                     | 0.49              |
| 54:li:56:ARG:O    | 54:li:59:GLU:HG2  | 2.12                     | 0.49              |
| 55:lj:48:ASN:N    | 85:l5:52:G:OP1    | 2.35                     | 0.49              |
| 62:lr:17:LEU:HD21 | 62:lr:19:LYS:HG3  | 1.95                     | 0.49              |
| 63:lz:93:LEU:O    | 63:lz:102:LYS:NZ  | 2.32                     | 0.49              |
| 65:sD:127:MET:HA  | 65:sD:127:MET:CE  | 2.40                     | 0.49              |
| 69:sQ:30:GLY:N    | 69:sQ:64:ALA:O    | 2.41                     | 0.49              |
| 70:sS:88:LYS:O    | 70:sS:88:LYS:HG3  | 2.11                     | 0.49              |
| 75:sg:32:LEU:HD23 | 75:sg:32:LEU:N    | 2.20                     | 0.49              |
| 79:s2:124:U:H2'   | 79:s2:125:C:C6    | 2.47                     | 0.49              |
| 79:s2:493:A:H2'   | 79:s2:494:C:C6    | 2.48                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 79:s2:746:C:H2'    | 79:s2:747:U:H6     | 1.78                     | 0.49              |
| 79:s2:1389:C:H2'   | 79:s2:1390:U:H6    | 1.77                     | 0.49              |
| 80:cB:176:GLN:CB   | 80:cB:180:ARG:HH22 | 2.21                     | 0.49              |
| 85:l5:74:G:H3'     | 85:l5:75:G:C8      | 2.47                     | 0.49              |
| 85:l5:344:A:H2'    | 85:l5:345:C:O4'    | 2.12                     | 0.49              |
| 85:l5:1383:G:H2'   | 85:l5:1384:C:C6    | 2.48                     | 0.49              |
| 85:l5:1415:G:H2'   | 85:l5:1416:G:C8    | 2.47                     | 0.49              |
| 85:l5:2273:G:H2'   | 85:l5:2274:C:C6    | 2.47                     | 0.49              |
| 85:l5:2481:G:H2'   | 85:l5:2482:C:H6    | 1.78                     | 0.49              |
| 85:l5:2503:G:N2    | 85:l5:4084:G:O5'   | 2.45                     | 0.49              |
| 85:l5:2570:U:H2'   | 85:l5:2571:C:H6    | 1.77                     | 0.49              |
| 85:l5:2846:G:H2'   | 85:l5:2847:G:H8    | 1.78                     | 0.49              |
| 85:l5:2862:G:N3    | 85:l5:3624:A:H2'   | 2.28                     | 0.49              |
| 85:l5:4208:U:H2'   | 85:l5:4209:G:H8    | 1.77                     | 0.49              |
| 85:l5:4460:U:H2'   | 85:l5:4461:C:H6    | 1.78                     | 0.49              |
| 85:l5:4935:C:H2'   | 85:l5:4936:G:H8    | 1.76                     | 0.49              |
| 80:CB:778:GLY:O    | 80:CB:779:THR:OG1  | 2.24                     | 0.49              |
| 18:SW:109:GLY:HA2  | 79:S2:862:A:H1'    | 1.93                     | 0.49              |
| 85:L5:372:A:H4'    | 55:Lj:45:ARG:NH2   | 2.28                     | 0.49              |
| 85:L5:689:U:H2'    | 85:L5:690:C:C6     | 2.47                     | 0.49              |
| 85:L5:1211:G:H2'   | 85:L5:1212:G:C8    | 2.47                     | 0.49              |
| 85:L5:1441:C:C2    | 85:L5:1442:C:H5    | 2.29                     | 0.49              |
| 85:L5:1558:A:H2'   | 85:L5:1559:G:H8    | 1.78                     | 0.49              |
| 85:L5:1597:G:OP2   | 36:LP:131:ARG:NE   | 2.41                     | 0.49              |
| 85:L5:1672:U:H2'   | 85:L5:1673:U:C6    | 2.47                     | 0.49              |
| 85:L5:2052:G:H2'   | 85:L5:2053:C:C6    | 2.47                     | 0.49              |
| 85:L5:2303:C:OP1   | 50:Le:104:SER:OG   | 2.22                     | 0.49              |
| 85:L5:2578:G:C6    | 85:L5:2584:G:C6    | 3.00                     | 0.49              |
| 85:L5:3772:U:H2'   | 85:L5:3773:U:H5''  | 1.94                     | 0.49              |
| 85:L5:4524:G:H2'   | 85:L5:4525:C:C6    | 2.48                     | 0.49              |
| 85:L5:4715:C:OP2   | 23:LB:31:SER:OG    | 2.25                     | 0.49              |
| 22:LA:78:ALA:O     | 22:LA:170:ALA:HB2  | 2.11                     | 0.49              |
| 22:LA:108:PRO:HG2  | 61:Lp:86:LEU:HD21  | 1.93                     | 0.49              |
| 24:LC:146:GLU:CD   | 24:LC:146:GLU:H    | 2.21                     | 0.49              |
| 29:LH:18:ILE:HG22  | 29:LH:27:VAL:HG12  | 1.93                     | 0.49              |
| 30:LI:61:SER:O     | 30:LI:65:LEU:HD12  | 2.12                     | 0.49              |
| 30:LI:65:LEU:HD12  | 30:LI:65:LEU:H     | 1.77                     | 0.49              |
| 31:LJ:113:ILE:HD11 | 31:LJ:123:ILE:HD11 | 1.94                     | 0.49              |
| 36:LP:139:TYR:H    | 36:LP:140:MET:HE2  | 1.76                     | 0.49              |
| 37:LQ:41:SER:HB2   | 37:LQ:132:LYS:HG2  | 1.94                     | 0.49              |
| 37:LQ:125:GLN:HA   | 37:LQ:128:LEU:HB3  | 1.94                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 63:Lz:209:THR:HG22 | 63:Lz:210:MET:SD   | 2.52                     | 0.49              |
| 65:SD:151:LYS:NZ   | 79:S2:1486:A:OP2   | 2.34                     | 0.49              |
| 67:SK:34:GLU:OE2   | 67:SK:35:LEU:HD22  | 2.13                     | 0.49              |
| 69:SQ:128:GLU:OE1  | 79:S2:1648:G:H3'   | 2.12                     | 0.49              |
| 71:ST:37:VAL:HG13  | 71:ST:39:LEU:HD12  | 1.94                     | 0.49              |
| 73:Sc:14:VAL:HB    | 73:Sc:30:VAL:HG22  | 1.93                     | 0.49              |
| 79:S2:899:U:H3'    | 79:S2:900:C:H4'    | 1.94                     | 0.49              |
| 79:S2:902:G:O2'    | 79:S2:903:A:O4'    | 2.30                     | 0.49              |
| 79:S2:906:U:H2'    | 79:S2:907:G:C8     | 2.46                     | 0.49              |
| 79:S2:1112:U:O2'   | 79:S2:1113:A:H5'   | 2.12                     | 0.49              |
| 82:PE:41:U:H2'     | 82:PE:42:G:C8      | 2.42                     | 0.49              |
| 1:cH:27:LEU:H      | 1:cH:27:LEU:HD12   | 1.76                     | 0.49              |
| 2:sE:18:TRP:CH2    | 2:sE:39:ARG:HA     | 2.45                     | 0.49              |
| 2:sE:77:ARG:NH2    | 79:s2:122:G:OP1    | 2.45                     | 0.49              |
| 2:sE:86:PHE:O      | 2:sE:87:MET:SD     | 2.71                     | 0.49              |
| 3:sI:177:SER:HB3   | 3:sI:186:ASP:H     | 1.77                     | 0.49              |
| 5:sX:48:LYS:NZ     | 79:s2:483:C:H5''   | 2.27                     | 0.49              |
| 6:sG:159:ARG:HG2   | 6:sG:173:ALA:HB2   | 1.94                     | 0.49              |
| 6:sG:160:LYS:HZ1   | 6:sG:174:PRO:HD3   | 1.77                     | 0.49              |
| 6:sG:170:ARG:HA    | 79:s2:72:C:N4      | 2.28                     | 0.49              |
| 8:sY:18:LEU:HD12   | 8:sY:85:ASN:ND2    | 2.26                     | 0.49              |
| 10:sA:63:ARG:HD2   | 13:sV:37:ALA:H     | 1.78                     | 0.49              |
| 18:sW:68:ARG:O     | 18:sW:68:ARG:HG3   | 2.11                     | 0.49              |
| 20:l7:37:G:C2      | 20:l7:41:G:C2      | 3.01                     | 0.49              |
| 21:l8:67:U:H2'     | 21:l8:68:G:C8      | 2.41                     | 0.49              |
| 22:lA:30:ARG:NH1   | 22:lA:36:GLU:OE2   | 2.38                     | 0.49              |
| 23:lB:127:LYS:HD3  | 23:lB:127:LYS:N    | 2.27                     | 0.49              |
| 23:lB:175:GLN:HG2  | 23:lB:177:LYS:H    | 1.77                     | 0.49              |
| 26:lE:66:LYS:HE2   | 85:l5:979:C:P      | 2.52                     | 0.49              |
| 29:lH:113:GLU:CD   | 29:lH:125:ARG:HG2  | 2.36                     | 0.49              |
| 30:lI:4:ARG:CZ     | 30:lI:99:ILE:HG13  | 2.43                     | 0.49              |
| 32:lL:50:PRO:O     | 32:lL:52:SER:N     | 2.46                     | 0.49              |
| 34:lN:101:VAL:HA   | 34:lN:104:GLU:OE1  | 2.12                     | 0.49              |
| 34:lN:120:TRP:CH2  | 85:l5:280:G:C8     | 3.00                     | 0.49              |
| 34:lN:135:ILE:HD11 | 34:lN:142:ILE:HD11 | 1.93                     | 0.49              |
| 42:lV:85:ARG:NE    | 85:l5:2847:G:OP1   | 2.43                     | 0.49              |
| 42:lV:111:GLU:H    | 42:lV:111:GLU:CD   | 2.18                     | 0.49              |
| 46:la:41:HIS:HE2   | 85:l5:1681:G:HO2'  | 1.60                     | 0.49              |
| 46:la:79:TRP:CE3   | 46:la:87:ARG:NE    | 2.80                     | 0.49              |
| 49:ld:33:ILE:HD11  | 49:ld:45:ALA:HA    | 1.94                     | 0.49              |
| 64:sR:32:LYS:HD3   | 79:s2:1453:C:C2    | 2.47                     | 0.49              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 65:sD:14:ASP:OD2  | 65:sD:18:LYS:NZ    | 2.46                     | 0.49              |
| 65:sD:67:ARG:HD2  | 67:sK:93:THR:O     | 2.12                     | 0.49              |
| 69:sQ:53:GLU:O    | 69:sQ:56:LEU:HG    | 2.13                     | 0.49              |
| 70:sS:24:ARG:NE   | 70:sS:28:PHE:O     | 2.45                     | 0.49              |
| 70:sS:88:LYS:HE2  | 79:s2:1612:G:H5'   | 1.93                     | 0.49              |
| 75:sg:84:ASP:HB2  | 75:sg:86:THR:HG22  | 1.94                     | 0.49              |
| 75:sg:218:LEU:O   | 75:sg:227:LEU:HD23 | 2.12                     | 0.49              |
| 79:s2:1009:A:H2'  | 79:s2:1010:G:C8    | 2.47                     | 0.49              |
| 79:s2:1740:C:H2'  | 79:s2:1741:U:C6    | 2.46                     | 0.49              |
| 82:pE:70:G:H2'    | 82:pE:71:G:H8      | 1.76                     | 0.49              |
| 83:ls:40:MET:HE1  | 83:ls:41:GLN:HG3   | 1.94                     | 0.49              |
| 84:lt:142:ASN:OD1 | 84:lt:143:VAL:N    | 2.36                     | 0.49              |
| 85:l5:334:A:H2'   | 85:l5:335:A:C8     | 2.47                     | 0.49              |
| 85:l5:468:U:N3    | 85:l5:686:A:N1     | 2.61                     | 0.49              |
| 85:l5:2730:U:H2'  | 85:l5:2731:C:C6    | 2.48                     | 0.49              |
| 85:l5:4079:C:H2'  | 85:l5:4080:C:C6    | 2.47                     | 0.49              |
| 85:l5:4638:U:H2'  | 85:l5:4639:G:N3    | 2.27                     | 0.49              |
| 85:l5:4743:G:H2'  | 85:l5:4744:A:C8    | 2.48                     | 0.49              |
| 80:CB:846:GLU:CD  | 80:CB:846:GLU:H    | 2.19                     | 0.49              |
| 4:SL:16:ILE:HD11  | 4:SL:36:TYR:HB2    | 1.93                     | 0.49              |
| 4:SL:130:GLU:HA   | 4:SL:140:PHE:HD1   | 1.78                     | 0.49              |
| 6:SG:170:ARG:HA   | 79:S2:72:C:H42     | 1.77                     | 0.49              |
| 7:SJ:93:LYS:HB3   | 7:SJ:96:TYR:CE2    | 2.47                     | 0.49              |
| 10:SA:108:PHE:HE2 | 10:SA:119:PRO:HD3  | 1.77                     | 0.49              |
| 16:SN:98:VAL:HG13 | 16:SN:115:LEU:HD12 | 1.94                     | 0.49              |
| 85:L5:80:C:H2'    | 85:L5:81:C:C6      | 2.47                     | 0.49              |
| 85:L5:260:C:H2'   | 85:L5:261:G:H8     | 1.77                     | 0.49              |
| 85:L5:280:G:N2    | 85:L5:306:A:OP2    | 2.39                     | 0.49              |
| 85:L5:937:U:H2'   | 85:L5:938:C:C6     | 2.48                     | 0.49              |
| 85:L5:1502:G:O5'  | 37:LQ:91:ARG:NH2   | 2.46                     | 0.49              |
| 85:L5:1558:A:O2'  | 38:LR:126:LYS:NZ   | 2.46                     | 0.49              |
| 85:L5:1692:C:H2'  | 85:L5:1693:U:C6    | 2.48                     | 0.49              |
| 85:L5:1733:G:N3   | 85:L5:4214:A:H2'   | 2.28                     | 0.49              |
| 85:L5:1917:A:H5'  | 51:Lf:78:HIS:CE1   | 2.47                     | 0.49              |
| 85:L5:1979:A:C5   | 85:L5:1980:U:H5    | 2.31                     | 0.49              |
| 85:L5:2765:A:H2'  | 85:L5:2766:A:C8    | 2.47                     | 0.49              |
| 85:L5:3733:A:H2'  | 85:L5:3734:U:O4'   | 2.12                     | 0.49              |
| 85:L5:3851:U:H3'  | 85:L5:3852:A:H8    | 1.76                     | 0.49              |
| 85:L5:4072:C:C2   | 85:L5:4073:A:C8    | 3.01                     | 0.49              |
| 85:L5:4102:C:C2'  | 85:L5:4106:G:H2'   | 2.42                     | 0.49              |
| 85:L5:4348:A:C6   | 85:L5:4350:C:C4    | 3.01                     | 0.49              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 21:L8:127:U:O2'   | 21:L8:128:C:O4'    | 2.31                     | 0.49              |
| 25:LD:244:HIS:O   | 25:LD:248:ARG:HG2  | 2.13                     | 0.49              |
| 29:LH:66:GLU:N    | 29:LH:66:GLU:OE1   | 2.45                     | 0.49              |
| 36:LP:10:ASN:OD1  | 36:LP:13:LYS:N     | 2.40                     | 0.49              |
| 38:LR:90:PRO:O    | 38:LR:94:THR:HG23  | 2.12                     | 0.49              |
| 38:LR:172:ARG:O   | 38:LR:175:GLU:HG3  | 2.12                     | 0.49              |
| 63:Lz:198:TRP:CZ2 | 63:Lz:202:ARG:HD3  | 2.47                     | 0.49              |
| 64:SR:105:MET:HA  | 64:SR:108:LEU:HD23 | 1.95                     | 0.49              |
| 65:SD:24:PHE:HZ   | 67:SK:68:TYR:CG    | 2.30                     | 0.49              |
| 66:SF:76:MET:HE1  | 66:SF:155:CYS:HA   | 1.93                     | 0.49              |
| 67:SK:3:MET:HE1   | 67:SK:4:PRO:O      | 2.11                     | 0.49              |
| 69:SQ:11:GLN:OE1  | 79:S2:1442:U:H1'   | 2.12                     | 0.49              |
| 70:SS:14:ARG:NH1  | 70:SS:16:LEU:O     | 2.30                     | 0.49              |
| 71:ST:62:ARG:NH1  | 79:S2:1542:C:OP1   | 2.46                     | 0.49              |
| 76:SM:63:LYS:HD2  | 76:SM:64:LEU:N     | 2.27                     | 0.49              |
| 79:S2:1567:G:H2'  | 79:S2:1568:C:C6    | 2.47                     | 0.49              |
| 79:S2:1858:G:H2'  | 79:S2:1859:A:H8    | 1.78                     | 0.49              |
| 83:Ls:20:LEU:HG   | 83:Ls:90:PHE:CD2   | 2.48                     | 0.49              |
| 84:Lt:14:TYR:OH   | 84:Lt:32:ILE:O     | 2.22                     | 0.49              |
| 1:cH:76:GLU:O     | 1:cH:80:VAL:HG23   | 2.12                     | 0.49              |
| 7:sJ:79:ARG:HH22  | 79:s2:820:U:P      | 2.36                     | 0.49              |
| 9:se:8:ARG:O      | 79:s2:616:A:H4'    | 2.12                     | 0.49              |
| 10:sA:136:GLU:HA  | 10:sA:139:TYR:HD1  | 1.77                     | 0.49              |
| 11:sB:150:ILE:H   | 64:sR:132:ARG:N    | 2.11                     | 0.49              |
| 12:sH:15:LYS:HD2  | 12:sH:15:LYS:H     | 1.76                     | 0.49              |
| 14:sa:5:ARG:HB2   | 14:sa:7:ASN:O      | 2.12                     | 0.49              |
| 15:sC:78:LEU:HD11 | 15:sC:94:ILE:HG22  | 1.94                     | 0.49              |
| 15:sC:133:TYR:CD2 | 15:sC:216:MET:HA   | 2.47                     | 0.49              |
| 18:sW:36:ARG:HD3  | 18:sW:110:ILE:HG12 | 1.95                     | 0.49              |
| 19:sb:22:LYS:HA   | 79:s2:921:G:C6     | 2.48                     | 0.49              |
| 23:IB:383:GLU:CD  | 23:IB:383:GLU:H    | 2.20                     | 0.49              |
| 25:ID:110:LEU:HB3 | 25:ID:116:ASP:HA   | 1.95                     | 0.49              |
| 27:IF:225:THR:HB  | 27:IF:229:GLU:OE1  | 2.13                     | 0.49              |
| 32:IL:178:ALA:N   | 46:la:134:GLU:OE1  | 2.46                     | 0.49              |
| 38:IR:44:LEU:HD22 | 38:IR:49:LEU:HD12  | 1.95                     | 0.49              |
| 45:IZ:95:VAL:HG13 | 45:IZ:96:VAL:HG23  | 1.95                     | 0.49              |
| 51:lf:74:VAL:CG1  | 51:lf:84:VAL:HG11  | 2.42                     | 0.49              |
| 56:lk:31:ASN:OD1  | 56:lk:31:ASN:C     | 2.56                     | 0.49              |
| 56:lk:34:PHE:HE2  | 56:lk:47:ILE:HD11  | 1.78                     | 0.49              |
| 65:sD:74:GLN:HA   | 65:sD:79:PHE:HD2   | 1.76                     | 0.49              |
| 69:sQ:123:ASP:OD1 | 69:sQ:125:ARG:HG2  | 2.12                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 76:sM:71:GLU:OE2   | 76:sM:72:HIS:NE2   | 2.46                     | 0.49              |
| 78:sf:99:LYS:NZ    | 79:s2:1288:U:OP2   | 2.41                     | 0.49              |
| 79:s2:953:C:H2'    | 79:s2:954:U:C2     | 2.48                     | 0.49              |
| 79:s2:1723:G:H22   | 79:s2:1810:U:H3    | 1.59                     | 0.49              |
| 83:ls:100:ASP:OD1  | 83:ls:101:MET:N    | 2.45                     | 0.49              |
| 85:l5:487:G:C6     | 85:l5:670:G:C6     | 3.00                     | 0.49              |
| 85:l5:964:A:H2'    | 85:l5:965:G:H4'    | 1.94                     | 0.49              |
| 85:l5:1207:C:H2'   | 85:l5:1208:G:C8    | 2.45                     | 0.49              |
| 85:l5:1324:A:N1    | 85:l5:3875:G:O2'   | 2.39                     | 0.49              |
| 85:l5:2710:C:N3    | 85:l5:2712:G:C8    | 2.79                     | 0.49              |
| 85:l5:2728:U:H2'   | 85:l5:2729:C:C6    | 2.47                     | 0.49              |
| 85:l5:3952:A:H2'   | 85:l5:3953:G:C8    | 2.48                     | 0.49              |
| 85:l5:3971:G:C2    | 85:l5:4051:C:H1'   | 2.48                     | 0.49              |
| 85:l5:4953:G:H2'   | 85:l5:4954:G:H8    | 1.77                     | 0.49              |
| 80:CB:228:PHE:O    | 80:CB:232:TYR:HB2  | 2.12                     | 0.49              |
| 80:CB:398:ILE:HG22 | 80:CB:483:GLY:O    | 2.12                     | 0.49              |
| 80:CB:421:VAL:HG22 | 80:CB:464:VAL:O    | 2.11                     | 0.49              |
| 10:SA:185:MET:C    | 13:SV:45:ARG:HH22  | 2.19                     | 0.49              |
| 11:SB:48:LEU:HD23  | 11:SB:48:LEU:H     | 1.77                     | 0.49              |
| 12:SH:188:GLU:N    | 12:SH:188:GLU:OE1  | 2.45                     | 0.49              |
| 16:SN:119:GLU:O    | 16:SN:122:ILE:HG22 | 2.13                     | 0.49              |
| 85:L5:1341:U:H2'   | 85:L5:1342:A:C8    | 2.47                     | 0.49              |
| 85:L5:1601:A:N7    | 85:L5:3643:A:C4    | 2.81                     | 0.49              |
| 85:L5:1982:G:H8    | 85:L5:1982:G:OP2   | 1.95                     | 0.49              |
| 85:L5:2299:G:O6    | 24:LC:188:ARG:NH2  | 2.40                     | 0.49              |
| 85:L5:2375:A:H2'   | 85:L5:2376:A:C8    | 2.47                     | 0.49              |
| 85:L5:2415:U:H2'   | 85:L5:2416:G:C8    | 2.48                     | 0.49              |
| 85:L5:3727:A:H8    | 85:L5:3727:A:OP2   | 1.96                     | 0.49              |
| 85:L5:4919:G:H2'   | 85:L5:4920:C:C6    | 2.48                     | 0.49              |
| 85:L5:4959:U:H2'   | 85:L5:4960:G:C8    | 2.48                     | 0.49              |
| 28:LG:108:GLN:O    | 28:LG:111:LYS:HG2  | 2.12                     | 0.49              |
| 37:LQ:15:ARG:NH1   | 37:LQ:52:PHE:O     | 2.46                     | 0.49              |
| 39:LS:83:ARG:HD3   | 39:LS:125:GLN:HE21 | 1.78                     | 0.49              |
| 44:LY:43:ASN:OD1   | 44:LY:126:ARG:NH1  | 2.46                     | 0.49              |
| 50:Le:79:VAL:HG21  | 50:Le:85:LEU:HD11  | 1.94                     | 0.49              |
| 62:Lr:63:VAL:HG23  | 62:Lr:79:ARG:HB3   | 1.94                     | 0.49              |
| 70:SS:73:ASN:OD1   | 70:SS:73:ASN:N     | 2.46                     | 0.49              |
| 71:ST:56:ARG:HD3   | 79:S2:1541:G:OP1   | 2.11                     | 0.49              |
| 74:Sd:40:ARG:NH1   | 79:S2:1256:G:O4'   | 2.45                     | 0.49              |
| 75:Sg:219:TRP:HD1  | 75:Sg:226:HIS:HA   | 1.78                     | 0.49              |
| 76:SM:84:LYS:HG3   | 76:SM:88:TRP:HZ2   | 1.72                     | 0.49              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 79:S2:691:G:N2    | 79:S2:691:G:OP2    | 2.45                     | 0.49              |
| 79:S2:1273:C:H4'  | 79:S2:1274:G:N2    | 2.27                     | 0.49              |
| 79:S2:1287:A:C5   | 79:S2:1288:U:H1'   | 2.48                     | 0.49              |
| 79:S2:1714:U:H2'  | 79:S2:1715:A:C8    | 2.47                     | 0.49              |
| 87:1W:7:SER:OG    | 87:1W:30:GLN:O     | 2.30                     | 0.49              |
| 1:CH:131:LYS:HB3  | 1:CH:139:LYS:HB3   | 1.93                     | 0.49              |
| 1:cH:48:GLN:HB2   | 9:se:54:GLY:HA2    | 1.94                     | 0.49              |
| 4:sL:41:GLY:HA3   | 79:s2:291:G:H1'    | 1.93                     | 0.49              |
| 6:sG:24:LEU:HD23  | 6:sG:27:PHE:HE2    | 1.76                     | 0.49              |
| 7:sJ:169:ARG:HH21 | 7:sJ:175:ARG:NH1   | 2.10                     | 0.49              |
| 11:sB:159:GLN:CD  | 11:sB:159:GLN:H    | 2.21                     | 0.49              |
| 17:sO:57:THR:HG22 | 17:sO:59:GLY:H     | 1.77                     | 0.49              |
| 21:l8:92:U:H2'    | 21:l8:93:C:O4'     | 2.12                     | 0.49              |
| 22:lA:201:GLY:HA2 | 22:lA:204:MET:HB2  | 1.94                     | 0.49              |
| 23:lB:47:LEU:H    | 23:lB:84:MET:CE    | 2.26                     | 0.49              |
| 23:lB:268:ARG:NH2 | 85:l5:3896:C:O2'   | 2.26                     | 0.49              |
| 25:lD:69:ILE:H    | 25:lD:69:ILE:HD12  | 1.77                     | 0.49              |
| 25:lD:196:ARG:HA  | 25:lD:199:ILE:HD12 | 1.95                     | 0.49              |
| 26:lE:264:ILE:O   | 26:lE:267:LEU:HD23 | 2.12                     | 0.49              |
| 26:lE:272:ARG:NH2 | 85:l5:4884:G:O6    | 2.46                     | 0.49              |
| 27:lF:32:ARG:NH2  | 85:l5:1701:A:N1    | 2.60                     | 0.49              |
| 31:lJ:95:ARG:HH11 | 31:lJ:96:LYS:H     | 1.60                     | 0.49              |
| 31:lJ:119:TYR:HD2 | 70:sS:105:ASN:HB3  | 1.78                     | 0.49              |
| 32:lL:183:ARG:NH1 | 85:l5:1395:U:OP1   | 2.44                     | 0.49              |
| 40:lT:65:TYR:N    | 40:lT:73:GLY:O     | 2.34                     | 0.49              |
| 42:lV:48:ARG:NE   | 85:l5:4621:C:OP1   | 2.45                     | 0.49              |
| 44:lY:54:GLU:HB2  | 44:lY:108:ARG:HB2  | 1.95                     | 0.49              |
| 56:lk:54:GLU:OE2  | 56:lk:54:GLU:HA    | 2.12                     | 0.49              |
| 58:lm:100:TYR:OH  | 85:l5:4425:G:OP1   | 2.26                     | 0.49              |
| 64:sR:11:LYS:HZ3  | 79:s2:1371:U:C3'   | 2.24                     | 0.49              |
| 65:sD:124:ARG:O   | 65:sD:128:GLU:HG2  | 2.12                     | 0.49              |
| 67:sK:75:GLY:O    | 67:sK:78:TYR:N     | 2.45                     | 0.49              |
| 69:sQ:11:GLN:NE2  | 79:s2:1442:U:H1'   | 2.27                     | 0.49              |
| 69:sQ:13:PHE:CE2  | 79:s2:1442:U:O2'   | 2.63                     | 0.49              |
| 75:sg:5:MET:HA    | 75:sg:5:MET:HE3    | 1.95                     | 0.49              |
| 77:sZ:59:CYS:HB2  | 77:sZ:60:LYS:HZ2   | 1.77                     | 0.49              |
| 79:s2:215:G:H2'   | 79:s2:216:C:H6     | 1.77                     | 0.49              |
| 79:s2:673:G:H2'   | 79:s2:674:C:C6     | 2.48                     | 0.49              |
| 79:s2:963:A:H2'   | 79:s2:964:A:C8     | 2.48                     | 0.49              |
| 79:s2:1401:A:H2'  | 79:s2:1402:A:H8    | 1.77                     | 0.49              |
| 80:cB:349:ALA:O   | 80:cB:352:GLN:HG2  | 2.12                     | 0.49              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 85:L5:221:C:H2'   | 85:L5:222:C:H6     | 1.77                     | 0.49              |
| 85:L5:300:A:H2'   | 85:L5:301:G:C8     | 2.46                     | 0.49              |
| 85:L5:1759:G:H3'  | 85:L5:1760:G:C8    | 2.47                     | 0.49              |
| 85:L5:1800:U:H2'  | 85:L5:1801:A:C8    | 2.47                     | 0.49              |
| 80:CB:426:LYS:HD3 | 80:CB:426:LYS:N    | 2.28                     | 0.49              |
| 2:SE:16:LYS:NZ    | 79:S2:813:A:OP1    | 2.45                     | 0.49              |
| 2:SE:87:MET:HA    | 2:SE:101:LEU:O     | 2.12                     | 0.49              |
| 6:SG:133:LEU:HD13 | 79:S2:65:C:C5      | 2.47                     | 0.49              |
| 15:SC:206:SER:OG  | 15:SC:207:ALA:O    | 2.26                     | 0.49              |
| 15:SC:211:LYS:O   | 15:SC:215:MET:HG3  | 2.13                     | 0.49              |
| 16:SN:64:ARG:NH2  | 79:S2:919:A:OP1    | 2.46                     | 0.49              |
| 17:SO:20:GLN:NE2  | 17:SO:21:VAL:O     | 2.46                     | 0.49              |
| 17:SO:66:ARG:HG3  | 79:S2:962:A:H5''   | 1.95                     | 0.49              |
| 85:L5:151:G:OP2   | 34:LN:4:TYR:OH     | 2.21                     | 0.49              |
| 85:L5:251:C:H2'   | 85:L5:252:C:C6     | 2.47                     | 0.49              |
| 85:L5:654:C:C4    | 85:L5:655:C:N4     | 2.80                     | 0.49              |
| 85:L5:1455:G:H2'  | 85:L5:1456:C:C6    | 2.47                     | 0.49              |
| 85:L5:1460:C:H2'  | 85:L5:1461:C:C6    | 2.48                     | 0.49              |
| 85:L5:1632:A:O2'  | 85:L5:1634:A:OP1   | 2.26                     | 0.49              |
| 85:L5:1993:C:H2'  | 85:L5:1994:C:C6    | 2.48                     | 0.49              |
| 85:L5:2003:G:N2   | 85:L5:2004:U:O4    | 2.46                     | 0.49              |
| 85:L5:2272:C:H2'  | 85:L5:2273:G:H8    | 1.78                     | 0.49              |
| 85:L5:2273:G:H2'  | 85:L5:2274:C:C6    | 2.48                     | 0.49              |
| 85:L5:2289:C:O2'  | 62:Lr:22:LYS:NZ    | 2.42                     | 0.49              |
| 85:L5:2413:U:H2'  | 85:L5:2414:G:C8    | 2.46                     | 0.49              |
| 85:L5:2491:C:H2'  | 85:L5:2492:C:C6    | 2.47                     | 0.49              |
| 85:L5:3832:U:H2'  | 85:L5:3833:C:H6    | 1.77                     | 0.49              |
| 85:L5:3910:C:H2'  | 85:L5:3911:C:C6    | 2.48                     | 0.49              |
| 85:L5:4622:A:H2'  | 85:L5:4623:G:H8    | 1.77                     | 0.49              |
| 85:L5:4986:G:H2'  | 85:L5:4987:C:C6    | 2.48                     | 0.49              |
| 21:L8:7:U:H2'     | 21:L8:8:U:C6       | 2.48                     | 0.49              |
| 24:LC:111:TRP:CD1 | 24:LC:111:TRP:H    | 2.31                     | 0.49              |
| 24:LC:325:MET:CE  | 24:LC:328:LEU:HD12 | 2.42                     | 0.49              |
| 24:LC:331:TYR:HA  | 27:LF:51:TYR:CE1   | 2.46                     | 0.49              |
| 28:LG:32:PHE:HE1  | 45:LZ:53:VAL:HG12  | 1.78                     | 0.49              |
| 31:LJ:26:VAL:HG11 | 31:LJ:32:ARG:HH12  | 1.77                     | 0.49              |
| 31:LJ:95:ARG:HG2  | 31:LJ:96:LYS:N     | 2.27                     | 0.49              |
| 36:LP:40:HIS:HE2  | 36:LP:110:ASP:C    | 2.20                     | 0.49              |
| 38:LR:25:ASP:OD1  | 38:LR:28:GLU:N     | 2.29                     | 0.49              |
| 50:Le:69:MET:HE2  | 50:Le:69:MET:HA    | 1.94                     | 0.49              |
| 54:Li:85:ARG:O    | 54:Li:89:GLU:HG2   | 2.13                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 60:Lo:70:LEU:N     | 60:Lo:81:ARG:O     | 2.43                     | 0.49              |
| 75:Sg:60:ARG:NH1   | 79:S2:1397:U:OP2   | 2.46                     | 0.49              |
| 79:S2:562:U:H2'    | 79:S2:563:G:C8     | 2.48                     | 0.49              |
| 79:S2:861:A:O2'    | 79:S2:862:A:N7     | 2.42                     | 0.49              |
| 79:S2:1024:A:H2'   | 79:S2:1025:U:C6    | 2.47                     | 0.49              |
| 4:sL:28:THR:N      | 4:sL:29:GLY:HA2    | 2.27                     | 0.49              |
| 6:sG:164:LYS:NZ    | 79:s2:67:C:H2'     | 2.27                     | 0.49              |
| 7:sJ:26:ASP:O      | 7:sJ:30:LYS:HG3    | 2.12                     | 0.49              |
| 7:sJ:174:LYS:HG2   | 79:s2:561:A:P      | 2.53                     | 0.49              |
| 12:sH:45:ILE:HD11  | 12:sH:64:VAL:HG22  | 1.94                     | 0.49              |
| 16:sN:142:GLU:HB3  | 16:sN:145:THR:HG22 | 1.93                     | 0.49              |
| 21:l8:144:U:H2'    | 21:l8:145:C:H6     | 1.77                     | 0.49              |
| 23:lB:378:ARG:HE   | 87:lW:11:TYR:HE2   | 1.61                     | 0.49              |
| 26:lE:222:LEU:HB3  | 26:lE:237:LYS:HD2  | 1.95                     | 0.49              |
| 26:lE:254:ASP:HA   | 26:lE:257:ILE:HG12 | 1.93                     | 0.49              |
| 27:lF:213:LEU:O    | 85:l5:2073:C:H5'   | 2.13                     | 0.49              |
| 27:lF:227:PHE:HA   | 27:lF:231:GLY:C    | 2.38                     | 0.49              |
| 29:lH:165:THR:HG21 | 29:lH:179:ILE:HG12 | 1.95                     | 0.49              |
| 31:lJ:113:ILE:HG21 | 31:lJ:119:TYR:HB2  | 1.94                     | 0.49              |
| 33:lM:37:LEU:HD12  | 39:lS:75:VAL:HG23  | 1.94                     | 0.49              |
| 33:lM:39:ASP:OD1   | 33:lM:47:ARG:HB2   | 2.12                     | 0.49              |
| 34:lN:169:ARG:NH2  | 85:l5:63:G:P       | 2.76                     | 0.49              |
| 37:lQ:23:ILE:HD11  | 62:lr:8:MET:CB     | 2.43                     | 0.49              |
| 37:lQ:42:THR:HA    | 37:lQ:45:GLN:HG3   | 1.95                     | 0.49              |
| 44:lY:89:LYS:NZ    | 85:l5:386:A:OP2    | 2.30                     | 0.49              |
| 48:lc:47:ILE:CD1   | 48:lc:72:HIS:HB3   | 2.42                     | 0.49              |
| 51:lf:4:ARG:HD3    | 85:l5:4753:U:H3'   | 1.95                     | 0.49              |
| 52:lg:69:LYS:O     | 52:lg:73:HIS:ND1   | 2.33                     | 0.49              |
| 63:lz:54:ARG:HH22  | 63:lz:156:LYS:HG3  | 1.76                     | 0.49              |
| 65:sD:28:GLU:HB3   | 65:sD:29:LEU:HD12  | 1.94                     | 0.49              |
| 66:sF:123:GLU:HA   | 66:sF:123:GLU:OE1  | 2.12                     | 0.49              |
| 68:sP:61:ARG:O     | 68:sP:65:LYS:HG2   | 2.13                     | 0.49              |
| 70:sS:124:ARG:NH2  | 70:sS:129:LEU:HD23 | 2.28                     | 0.49              |
| 75:sg:147:HIS:ND1  | 75:sg:151:VAL:HG12 | 2.27                     | 0.49              |
| 76:sM:48:HIS:HB2   | 76:sM:111:VAL:O    | 2.13                     | 0.49              |
| 77:sZ:85:ARG:HH12  | 79:s2:1597:C:H5    | 1.60                     | 0.49              |
| 79:s2:1053:C:H2'   | 79:s2:1054:G:H8    | 1.77                     | 0.49              |
| 79:s2:1297:U:H1'   | 79:s2:1301:A:N1    | 2.27                     | 0.49              |
| 79:s2:1442:U:H2'   | 79:s2:1443:C:C6    | 2.48                     | 0.49              |
| 79:s2:1491:G:H2'   | 79:s2:1492:U:C6    | 2.48                     | 0.49              |
| 80:cB:182:VAL:HA   | 80:cB:185:VAL:CG2  | 2.43                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 80:cB:439:LYS:O    | 80:cB:442:LEU:HB3  | 2.13                     | 0.49              |
| 80:cB:609:PHE:CD1  | 80:cB:613:LEU:HD13 | 2.48                     | 0.49              |
| 81:aP:3:C:H2'      | 81:aP:4:U:H6       | 1.77                     | 0.49              |
| 81:aP:9:A:H3'      | 81:aP:11:U:H5      | 1.78                     | 0.49              |
| 84:lt:19:GLY:HA3   | 84:lt:59:THR:HB    | 1.93                     | 0.49              |
| 84:lt:57:ARG:HG2   | 84:lt:58:ILE:H     | 1.77                     | 0.49              |
| 85:l5:302:C:H2'    | 85:l5:303:C:H6     | 1.78                     | 0.49              |
| 85:l5:1458:C:C2    | 85:l5:1459:A:C8    | 3.00                     | 0.49              |
| 85:l5:1567:U:H2'   | 85:l5:1568:C:H6    | 1.77                     | 0.49              |
| 85:l5:1755:C:H42   | 85:l5:1775:A:N6    | 2.10                     | 0.49              |
| 85:l5:1989:G:H2'   | 85:l5:1990:A:H8    | 1.77                     | 0.49              |
| 85:l5:2539:C:H2'   | 85:l5:2540:C:H6    | 1.78                     | 0.49              |
| 85:l5:2758:G:O2'   | 85:l5:2765:A:N3    | 2.40                     | 0.49              |
| 85:l5:4232:U:H1'   | 85:l5:4233:A:C2    | 2.48                     | 0.49              |
| 85:l5:4864:U:H3'   | 85:l5:4865:C:H6    | 1.77                     | 0.49              |
| 85:l5:4889:G:N2    | 85:l5:4931:G:H1'   | 2.28                     | 0.49              |
| 80:CB:755:VAL:HG21 | 80:CB:804:THR:HA   | 1.95                     | 0.49              |
| 6:SG:151:ASP:HA    | 87:LW:105:ARG:HD2  | 1.94                     | 0.49              |
| 10:SA:6:ASP:O      | 10:SA:9:GLN:HG2    | 2.12                     | 0.49              |
| 10:SA:89:LYS:HD3   | 10:SA:201:LEU:HD23 | 1.95                     | 0.49              |
| 11:SB:90:ASP:OD1   | 11:SB:91:VAL:N     | 2.45                     | 0.49              |
| 16:SN:64:ARG:HH22  | 79:S2:918:U:H5''   | 1.78                     | 0.49              |
| 17:SO:147:ARG:HB2  | 17:SO:150:ARG:NH2  | 2.27                     | 0.49              |
| 85:L5:666:G:N7     | 85:L5:668:C:N4     | 2.61                     | 0.49              |
| 85:L5:1280:C:OP2   | 26:LE:52:ARG:NH2   | 2.42                     | 0.49              |
| 85:L5:1398:A:OP1   | 46:La:136:LYS:NZ   | 2.42                     | 0.49              |
| 85:L5:1749:A:H2'   | 85:L5:1750:G:C8    | 2.47                     | 0.49              |
| 85:L5:1843:A:H2'   | 85:L5:1844:G:C8    | 2.47                     | 0.49              |
| 85:L5:1888:A:N7    | 85:L5:2049:G:H5'   | 2.27                     | 0.49              |
| 85:L5:2362:U:H2'   | 85:L5:2363:A:C8    | 2.47                     | 0.49              |
| 85:L5:2598:A:H2'   | 85:L5:2599:G:O4'   | 2.13                     | 0.49              |
| 85:L5:2602:G:H2'   | 85:L5:2603:C:C6    | 2.48                     | 0.49              |
| 85:L5:2648:G:H2'   | 85:L5:2649:G:H8    | 1.77                     | 0.49              |
| 85:L5:2749:C:H5'   | 52:Lg:65:MET:HE1   | 1.94                     | 0.49              |
| 85:L5:2817:C:H2'   | 85:L5:2818:C:C6    | 2.47                     | 0.49              |
| 85:L5:2877:G:H2'   | 85:L5:2878:G:O4'   | 2.12                     | 0.49              |
| 85:L5:3834:C:H2'   | 85:L5:3835:C:H6    | 1.77                     | 0.49              |
| 85:L5:4411:G:H2'   | 85:L5:4412:C:C6    | 2.47                     | 0.49              |
| 85:L5:4935:C:H5    | 26:LE:180:VAL:HG23 | 1.78                     | 0.49              |
| 85:L5:5037:U:H2'   | 85:L5:5038:A:H8    | 1.76                     | 0.49              |
| 21:L8:28:C:H2'     | 21:L8:29:G:C8      | 2.47                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 21:L8:38:U:N3      | 53:Lh:84:ARG:HG3   | 2.28                     | 0.49              |
| 23:LB:62:ARG:CZ    | 23:LB:358:ARG:HH22 | 2.26                     | 0.49              |
| 23:LB:92:TYR:CE1   | 23:LB:161:ARG:HD2  | 2.47                     | 0.49              |
| 23:LB:305:THR:OG1  | 23:LB:305:THR:O    | 2.30                     | 0.49              |
| 25:LD:262:LYS:HG2  | 25:LD:263:LYS:H    | 1.78                     | 0.49              |
| 27:LF:226:HIS:HD2  | 27:LF:228:VAL:HG22 | 1.78                     | 0.49              |
| 31:LJ:96:LYS:HD2   | 31:LJ:175:LEU:HD12 | 1.94                     | 0.49              |
| 32:LL:154:VAL:HG22 | 32:LL:155:MET:HE3  | 1.94                     | 0.49              |
| 36:LP:107:LEU:HD12 | 36:LP:152:GLU:CD   | 2.38                     | 0.49              |
| 37:LQ:25:LEU:O     | 37:LQ:29:VAL:HG23  | 2.13                     | 0.49              |
| 37:LQ:64:SER:HA    | 37:LQ:67:ILE:HG22  | 1.95                     | 0.49              |
| 44:LY:114:ASP:OD1  | 44:LY:114:ASP:N    | 2.41                     | 0.49              |
| 45:LZ:10:VAL:HG11  | 45:LZ:85:TYR:HB2   | 1.95                     | 0.49              |
| 51:Lf:76:ARG:HE    | 51:Lf:85:ARG:HH11  | 1.61                     | 0.49              |
| 63:Lz:106:LYS:HG3  | 63:Lz:107:TYR:HD1  | 1.77                     | 0.49              |
| 66:SF:92:ILE:HG13  | 66:SF:93:VAL:N     | 2.28                     | 0.49              |
| 66:SF:124:ASP:CG   | 73:Sc:47:LYS:HZ2   | 2.19                     | 0.49              |
| 66:SF:127:ARG:HH22 | 73:Sc:66:ARG:NH1   | 2.09                     | 0.49              |
| 66:SF:168:THR:OG1  | 79:S2:1535:U:OP2   | 2.28                     | 0.49              |
| 68:SP:41:GLN:N     | 68:SP:41:GLN:OE1   | 2.45                     | 0.49              |
| 71:ST:42:HIS:HB3   | 71:ST:93:SER:HB3   | 1.95                     | 0.49              |
| 71:ST:104:LEU:HG   | 71:ST:121:ARG:NH2  | 2.26                     | 0.49              |
| 72:SU:18:HIS:CE1   | 72:SU:95:SER:H     | 2.31                     | 0.49              |
| 75:Sg:167:SER:OG   | 75:Sg:175:LYS:O    | 2.29                     | 0.49              |
| 75:Sg:194:TYR:CZ   | 75:Sg:212:LYS:HG2  | 2.48                     | 0.49              |
| 76:SM:79:VAL:HG21  | 76:SM:88:TRP:CZ3   | 2.47                     | 0.49              |
| 79:S2:352:U:H2'    | 79:S2:353:C:H6     | 1.78                     | 0.49              |
| 79:S2:1253:A:H4'   | 79:S2:1254:C:H5''  | 1.95                     | 0.49              |
| 79:S2:1387:G:C2    | 79:S2:1388:A:H1'   | 2.48                     | 0.49              |
| 84:Lt:60:VAL:HG22  | 84:Lt:80:LEU:HD13  | 1.95                     | 0.49              |
| 1:cH:44:TRP:CZ2    | 9:se:49:PHE:HA     | 2.48                     | 0.49              |
| 2:sE:49:ARG:HH22   | 79:s2:496:C:P      | 2.36                     | 0.49              |
| 2:sE:66:MET:HE1    | 79:s2:502:C:N1     | 2.28                     | 0.49              |
| 3:sI:7:ASN:ND2     | 79:s2:351:G:OP1    | 2.46                     | 0.49              |
| 6:sG:7:PHE:HE1     | 6:sG:113:ILE:HD13  | 1.75                     | 0.49              |
| 11:sB:149:GLN:N    | 64:sR:131:PRO:HB3  | 2.28                     | 0.49              |
| 11:sB:151:ARG:HB3  | 64:sR:132:ARG:HD2  | 1.94                     | 0.49              |
| 12:sH:31:GLU:HG3   | 12:sH:37:LYS:HD2   | 1.94                     | 0.49              |
| 14:sa:6:ARG:HE     | 79:s2:1134:G:P     | 2.36                     | 0.49              |
| 14:sa:24:THR:HG21  | 14:sa:71:LEU:CD1   | 2.43                     | 0.49              |
| 15:sC:207:ALA:HB2  | 79:s2:4:C:H4'      | 1.95                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 17:sO:33:ILE:HD12  | 17:sO:42:VAL:HA    | 1.94                     | 0.49              |
| 22:1A:35:ALA:O     | 22:1A:91:GLY:HA3   | 2.12                     | 0.49              |
| 23:1B:50:LYS:NZ    | 23:1B:337:VAL:O    | 2.46                     | 0.49              |
| 26:1E:123:ARG:HG2  | 85:l5:959:G:C8     | 2.48                     | 0.49              |
| 27:1F:66:ARG:HA    | 27:1F:69:ILE:HD12  | 1.94                     | 0.49              |
| 27:1F:151:ASN:ND2  | 85:l5:943:A:H62    | 2.05                     | 0.49              |
| 30:1I:3:ARG:NH2    | 85:l5:4431:U:OP2   | 2.36                     | 0.49              |
| 31:1J:174:ILE:HG12 | 31:1J:175:LEU:HD22 | 1.94                     | 0.49              |
| 37:1Q:32:TYR:HE2   | 37:1Q:44:ASN:OD1   | 1.96                     | 0.49              |
| 41:1U:18:VAL:HG21  | 41:1U:77:PRO:HA    | 1.93                     | 0.49              |
| 42:1V:139:ILE:HD12 | 42:1V:140:ALA:N    | 2.27                     | 0.49              |
| 43:1X:80:PRO:HA    | 43:1X:98:PHE:HA    | 1.95                     | 0.49              |
| 57:1l:16:LYS:HB3   | 57:1l:42:ARG:HH21  | 1.76                     | 0.49              |
| 61:lp:59:SER:OG    | 61:lp:60:CYS:N     | 2.44                     | 0.49              |
| 66:sF:55:ARG:HG3   | 66:sF:58:ALA:HB2   | 1.95                     | 0.49              |
| 67:sK:28:HIS:CG    | 74:sd:8:TRP:NE1    | 2.76                     | 0.49              |
| 71:sT:41:LYS:HZ3   | 79:s2:1569:A:P     | 2.35                     | 0.49              |
| 75:sg:110:SER:HB3  | 75:sg:153:CYS:HA   | 1.95                     | 0.49              |
| 77:sZ:96:LEU:O     | 77:sZ:97:ILE:HD13  | 2.13                     | 0.49              |
| 79:s2:455:A:O2'    | 79:s2:1735:A:N3    | 2.39                     | 0.49              |
| 79:s2:1222:G:H2'   | 79:s2:1223:A:C8    | 2.48                     | 0.49              |
| 79:s2:1355:C:N3    | 79:s2:1356:G:N2    | 2.61                     | 0.49              |
| 79:s2:1751:C:H1'   | 79:s2:1784:G:N2    | 2.28                     | 0.49              |
| 80:cB:113:SER:O    | 80:cB:116:THR:OG1  | 2.21                     | 0.49              |
| 81:aP:15:G:H21     | 81:aP:21:A:H1'     | 1.78                     | 0.49              |
| 85:l5:129:C:H2'    | 85:l5:130:C:C6     | 2.48                     | 0.49              |
| 85:l5:703:G:H2'    | 85:l5:704:C:H4'    | 1.95                     | 0.49              |
| 85:l5:1858:A:H2'   | 85:l5:1859:C:C6    | 2.48                     | 0.49              |
| 85:l5:3807:A:H2'   | 85:l5:3808:C:C6    | 2.48                     | 0.49              |
| 85:l5:4039:G:N2    | 85:l5:4050:A:O2'   | 2.41                     | 0.49              |
| 85:l5:4094:G:H2'   | 85:l5:4095:G:H5'   | 1.95                     | 0.49              |
| 85:l5:4151:G:H2'   | 85:l5:4152:G:C8    | 2.48                     | 0.49              |
| 85:l5:4414:A:N3    | 85:l5:4427:G:N2    | 2.61                     | 0.49              |
| 85:l5:4571:A:H2'   | 85:l5:4572:U:H6    | 1.77                     | 0.49              |
| 80:CB:538:ILE:HD11 | 80:CB:544:HIS:CE1  | 2.47                     | 0.49              |
| 80:CB:604:MET:HE2  | 80:CB:604:MET:HA   | 1.94                     | 0.49              |
| 80:CB:604:MET:SD   | 80:CB:702:PHE:HD2  | 2.35                     | 0.49              |
| 80:CB:684:GLN:HA   | 80:CB:687:THR:HG22 | 1.94                     | 0.49              |
| 2:SE:73:ASP:HA     | 2:SE:164:LEU:HD22  | 1.95                     | 0.49              |
| 4:SL:22:ARG:HA     | 4:SL:22:ARG:HH11   | 1.78                     | 0.49              |
| 4:SL:82:MET:HE3    | 79:S2:395:G:H5'    | 1.94                     | 0.49              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 6:SG:200:LYS:NZ   | 6:SG:204:GLU:HG2   | 2.28                     | 0.49              |
| 11:SB:144:LYS:HD2 | 11:SB:208:HIS:HB3  | 1.94                     | 0.49              |
| 18:SW:24:GLN:CD   | 18:SW:64:ASN:HD22  | 2.17                     | 0.49              |
| 85:L5:123:C:H2'   | 85:L5:124:C:H6     | 1.77                     | 0.49              |
| 85:L5:509:A:N1    | 46:La:102:ASP:HB2  | 2.28                     | 0.49              |
| 85:L5:654:C:H2'   | 85:L5:655:C:C6     | 2.48                     | 0.49              |
| 85:L5:1336:G:H21  | 85:L5:2349:A:N6    | 2.10                     | 0.49              |
| 85:L5:1460:C:H2'  | 85:L5:1461:C:H6    | 1.78                     | 0.49              |
| 85:L5:1628:C:H3'  | 22:LA:9:ARG:NH2    | 2.28                     | 0.49              |
| 85:L5:1760:G:N2   | 85:L5:1761:G:O6    | 2.39                     | 0.49              |
| 85:L5:2258:C:N4   | 26:LE:88:VAL:HG12  | 2.28                     | 0.49              |
| 85:L5:2832:A:H2'  | 85:L5:2833:A:H8    | 1.78                     | 0.49              |
| 85:L5:3883:U:H2'  | 85:L5:3884:U:H6    | 1.77                     | 0.49              |
| 85:L5:4063:U:H2'  | 85:L5:4064:C:C2    | 2.47                     | 0.49              |
| 85:L5:4093:G:N1   | 85:L5:4114:C:C2    | 2.80                     | 0.49              |
| 85:L5:4592:C:H2'  | 85:L5:4593:C:C6    | 2.47                     | 0.49              |
| 85:L5:5004:C:H2'  | 85:L5:5005:G:O4'   | 2.12                     | 0.49              |
| 21:L8:28:C:H2'    | 21:L8:29:G:H8      | 1.77                     | 0.49              |
| 21:L8:130:C:H4'   | 43:LX:107:HIS:ND1  | 2.27                     | 0.49              |
| 28:LG:173:LEU:HA  | 54:Li:43:MET:CE    | 2.37                     | 0.49              |
| 30:LI:36:LEU:HD11 | 30:LI:69:ARG:HH11  | 1.77                     | 0.49              |
| 30:LI:205:PRO:HD2 | 30:LI:208:LYS:HE3  | 1.95                     | 0.49              |
| 38:LR:170:ARG:O   | 38:LR:174:GLU:HG2  | 2.13                     | 0.49              |
| 40:LT:147:GLU:OE1 | 40:LT:147:GLU:N    | 2.33                     | 0.49              |
| 47:Lb:66:SER:O    | 47:Lb:70:GLU:HG3   | 2.13                     | 0.49              |
| 52:Lg:70:THR:HA   | 52:Lg:73:HIS:CE1   | 2.48                     | 0.49              |
| 62:Lr:14:SER:OG   | 62:Lr:17:LEU:N     | 2.46                     | 0.49              |
| 65:SD:154:ASP:OD2 | 65:SD:154:ASP:C    | 2.55                     | 0.49              |
| 75:Sg:107:ASP:OD1 | 75:Sg:125:ARG:HB2  | 2.13                     | 0.49              |
| 75:Sg:292:SER:OG  | 75:Sg:294:ASP:OD1  | 2.30                     | 0.49              |
| 76:SM:48:HIS:ND1  | 76:SM:112:LYS:HA   | 2.28                     | 0.49              |
| 79:S2:52:G:H2'    | 79:S2:53:C:C6      | 2.48                     | 0.49              |
| 79:S2:185:G:O6    | 79:S2:214:U:C4     | 2.66                     | 0.49              |
| 79:S2:185:G:H2'   | 79:S2:186:C:H6     | 1.78                     | 0.49              |
| 79:S2:949:G:H2'   | 79:S2:950:C:H6     | 1.77                     | 0.49              |
| 79:S2:1361:G:H1'  | 79:S2:1379:A:N7    | 2.28                     | 0.49              |
| 79:S2:1439:A:H2'  | 79:S2:1440:C:C6    | 2.47                     | 0.49              |
| 82:PE:18:U:O2'    | 82:PE:57:A:N3      | 2.40                     | 0.49              |
| 84:Lt:107:ASP:O   | 84:Lt:110:VAL:HG22 | 2.13                     | 0.49              |
| 5:sX:46:HIS:CE1   | 79:s2:648:A:H1'    | 2.47                     | 0.49              |
| 6:sG:23:LYS:CD    | 6:sG:41:LEU:HB2    | 2.40                     | 0.49              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 6:sG:44:GLU:OE2   | 6:sG:45:TRP:HZ3    | 1.96                     | 0.49              |
| 6:sG:140:ARG:HA   | 6:sG:143:LYS:HE3   | 1.94                     | 0.49              |
| 10:sA:210:ILE:HA  | 10:sA:214:GLU:OE2  | 2.13                     | 0.49              |
| 11:sB:65:ARG:NH2  | 17:sO:51:GLU:OE2   | 2.46                     | 0.49              |
| 12:sH:127:ASP:OD1 | 12:sH:127:ASP:N    | 2.46                     | 0.49              |
| 22:lA:183:GLY:HA2 | 85:l5:1613:A:H5''  | 1.94                     | 0.49              |
| 23:lB:315:ASN:OD1 | 23:lB:326:VAL:N    | 2.44                     | 0.49              |
| 32:lL:93:THR:OG1  | 53:lh:116:LEU:HA   | 2.12                     | 0.49              |
| 40:lT:14:MET:HG3  | 40:lT:15:PHE:CD1   | 2.47                     | 0.49              |
| 41:lU:80:LYS:HE2  | 41:lU:110:TYR:HD2  | 1.75                     | 0.49              |
| 48:lc:38:ILE:HG13 | 48:lc:39:ARG:N     | 2.27                     | 0.49              |
| 50:le:91:CYS:O    | 50:le:93:LYS:N     | 2.46                     | 0.49              |
| 51:lf:106:TYR:HB3 | 51:lf:107:PRO:CD   | 2.43                     | 0.49              |
| 55:lj:33:THR:HG23 | 55:lj:40:PRO:HD3   | 1.94                     | 0.49              |
| 55:lj:67:LEU:O    | 55:lj:70:VAL:HG22  | 2.12                     | 0.49              |
| 60:lo:51:GLN:HB3  | 85:l5:3925:U:H4'   | 1.95                     | 0.49              |
| 60:lo:99:ARG:HH22 | 60:lo:102:GLN:CG   | 2.26                     | 0.49              |
| 65:sD:98:ALA:HB1  | 65:sD:186:VAL:HG23 | 1.95                     | 0.49              |
| 68:sP:89:MET:H    | 68:sP:89:MET:CE    | 2.23                     | 0.49              |
| 69:sQ:25:CYS:SG   | 69:sQ:68:ILE:HG22  | 2.53                     | 0.49              |
| 72:sU:24:LEU:HD11 | 72:sU:87:ARG:HB2   | 1.93                     | 0.49              |
| 79:s2:1221:G:H2'  | 79:s2:1222:G:H8    | 1.75                     | 0.49              |
| 79:s2:1466:G:H2'  | 79:s2:1467:C:O4'   | 2.12                     | 0.49              |
| 79:s2:1627:C:H2'  | 79:s2:1628:C:C6    | 2.47                     | 0.49              |
| 79:s2:1801:A:H2'  | 79:s2:1802:C:C6    | 2.48                     | 0.49              |
| 80:cB:176:GLN:HB3 | 80:cB:180:ARG:CZ   | 2.43                     | 0.49              |
| 80:cB:214:PHE:HE1 | 80:cB:289:PHE:HZ   | 1.60                     | 0.49              |
| 80:cB:600:ASN:ND2 | 80:cB:716:ARG:HG2  | 2.23                     | 0.49              |
| 83:ls:66:ARG:NH2  | 83:ls:79:LEU:HD21  | 2.27                     | 0.49              |
| 84:lt:122:ALA:O   | 85:l5:1995:G:O2'   | 2.28                     | 0.49              |
| 85:l5:408:A:O2'   | 85:l5:411:G:OP2    | 2.20                     | 0.49              |
| 85:l5:1709:C:C2   | 85:l5:1716:G:N1    | 2.80                     | 0.49              |
| 85:l5:2038:U:H2'  | 85:l5:2039:G:O4'   | 2.13                     | 0.49              |
| 85:l5:2703:G:C6   | 85:l5:2714:G:C6    | 3.01                     | 0.49              |
| 85:l5:3829:G:C2   | 85:l5:3830:A:C8    | 3.01                     | 0.49              |
| 85:l5:4079:C:H2'  | 85:l5:4080:C:H6    | 1.78                     | 0.49              |
| 85:l5:5053:U:H3'  | 85:l5:5054:C:C6    | 2.48                     | 0.49              |
| 2:SE:248:ILE:O    | 2:SE:251:GLU:HG3   | 2.13                     | 0.49              |
| 3:SI:69:SER:HB3   | 4:SL:21:LYS:HG2    | 1.95                     | 0.49              |
| 3:SI:182:CYS:SG   | 3:SI:184:ARG:HG2   | 2.53                     | 0.49              |
| 5:SX:61:GLN:HE22  | 79:S2:1824:A:P     | 2.36                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 6:SG:217:MET:HA    | 6:SG:217:MET:HE2   | 1.95                     | 0.49              |
| 10:SA:33:GLN:O     | 10:SA:36:GLN:NE2   | 2.45                     | 0.49              |
| 10:SA:48:ILE:O     | 10:SA:48:ILE:HG13  | 2.12                     | 0.49              |
| 16:SN:47:PRO:O     | 16:SN:50:ILE:HG13  | 2.13                     | 0.49              |
| 85:L5:224:U:OP1    | 24:LC:163:LYS:NZ   | 2.46                     | 0.49              |
| 85:L5:372:A:N3     | 85:L5:1531:U:H1'   | 2.28                     | 0.49              |
| 85:L5:947:C:H2'    | 85:L5:948:C:C6     | 2.48                     | 0.49              |
| 85:L5:965:G:N2     | 85:L5:2092:G:H1'   | 2.28                     | 0.49              |
| 85:L5:1510:G:H2'   | 85:L5:1511:U:C6    | 2.48                     | 0.49              |
| 85:L5:1535:C:H5'   | 55:Lj:11:ARG:CD    | 2.43                     | 0.49              |
| 85:L5:1836:G:O2'   | 40:LT:108:ARG:NH2  | 2.46                     | 0.49              |
| 85:L5:1852:U:OP1   | 46:La:23:GLY:N     | 2.37                     | 0.49              |
| 85:L5:2073:C:C2    | 85:L5:2074:C:C5    | 3.01                     | 0.49              |
| 85:L5:2283:G:H2'   | 85:L5:2284:G:C8    | 2.47                     | 0.49              |
| 85:L5:2641:A:H3'   | 85:L5:2642:A:H8    | 1.77                     | 0.49              |
| 85:L5:2864:A:H2'   | 85:L5:2865:U:H6    | 1.77                     | 0.49              |
| 85:L5:4120:U:C4    | 52:Lg:97:ILE:HG22  | 2.48                     | 0.49              |
| 85:L5:4347:G:H2'   | 85:L5:4348:A:C8    | 2.47                     | 0.49              |
| 85:L5:4603:C:OP2   | 29:LH:98:HIS:ND1   | 2.40                     | 0.49              |
| 85:L5:4998:G:H2'   | 85:L5:4999:G:C8    | 2.48                     | 0.49              |
| 23:LB:36:ASP:OD1   | 23:LB:39:LYS:HE2   | 2.12                     | 0.49              |
| 23:LB:257:TRP:C    | 23:LB:257:TRP:CD1  | 2.91                     | 0.49              |
| 24:LC:74:ALA:O     | 24:LC:78:ARG:NH1   | 2.46                     | 0.49              |
| 26:LE:172:LEU:HD13 | 26:LE:188:ARG:HE   | 1.77                     | 0.49              |
| 26:LE:224:LYS:HG2  | 26:LE:227:HIS:HB2  | 1.95                     | 0.49              |
| 28:LG:29:ASN:ND2   | 28:LG:31:LEU:HB3   | 2.22                     | 0.49              |
| 32:LL:48:PRO:HG3   | 53:Lh:118:LYS:HE3  | 1.94                     | 0.49              |
| 34:LN:63:ARG:NE    | 34:LN:131:GLU:OE1  | 2.46                     | 0.49              |
| 35:LO:118:MET:HE1  | 39:LS:168:THR:C    | 2.38                     | 0.49              |
| 36:LP:147:GLU:OE2  | 36:LP:147:GLU:N    | 2.46                     | 0.49              |
| 40:LT:29:THR:HG23  | 40:LT:30:TYR:HD1   | 1.77                     | 0.49              |
| 44:LY:67:ILE:HD12  | 44:LY:107:THR:HG21 | 1.94                     | 0.49              |
| 46:La:37:GLY:O     | 46:La:38:LEU:HD23  | 2.12                     | 0.49              |
| 48:Lc:74:TYR:CD2   | 48:Lc:81:LEU:HB2   | 2.48                     | 0.49              |
| 63:Lz:61:PRO:C     | 63:Lz:62:LYS:HD2   | 2.38                     | 0.49              |
| 65:SD:157:MET:HA   | 65:SD:189:MET:CE   | 2.42                     | 0.49              |
| 66:SF:103:LEU:HB3  | 66:SF:104:THR:HG23 | 1.94                     | 0.49              |
| 75:Sg:178:ASN:O    | 75:Sg:182:CYS:HA   | 2.12                     | 0.49              |
| 79:S2:31:U:H2'     | 79:S2:32:U:C6      | 2.48                     | 0.49              |
| 79:S2:653:A:H2'    | 79:S2:654:A:O4'    | 2.13                     | 0.49              |
| 79:S2:1355:C:H2'   | 79:S2:1356:G:O4'   | 2.13                     | 0.49              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 79:S2:1447:G:H2'  | 79:S2:1448:A:H8    | 1.78                     | 0.49              |
| 79:S2:1780:G:H3'  | 79:S2:1781:A:C8    | 2.47                     | 0.49              |
| 79:S2:1795:G:H2'  | 79:S2:1796:G:H8    | 1.78                     | 0.49              |
| 83:Ls:137:PHE:HZ  | 83:Ls:174:LEU:HB2  | 1.78                     | 0.49              |
| 87:IW:101:ARG:HB2 | 87:IW:102:LYS:HZ2  | 1.77                     | 0.49              |
| 1:CH:132:LEU:HA   | 1:CH:137:ILE:O     | 2.13                     | 0.48              |
| 1:cH:42:LYS:HG3   | 9:se:42:PHE:CE1    | 2.48                     | 0.48              |
| 3:sI:141:ARG:CZ   | 79:s2:191:A:H5''   | 2.43                     | 0.48              |
| 6:sG:20:ASP:O     | 6:sG:24:LEU:HD12   | 2.13                     | 0.48              |
| 8:sY:23:MET:HE1   | 8:sY:75:ILE:HG22   | 1.95                     | 0.48              |
| 9:se:35:ARG:HH22  | 79:s2:526:A:H5''   | 1.77                     | 0.48              |
| 12:sH:21:SER:O    | 12:sH:25:GLN:HB2   | 2.13                     | 0.48              |
| 12:sH:95:ILE:HD12 | 12:sH:96:ALA:H     | 1.77                     | 0.48              |
| 14:sa:99:PRO:O    | 14:sa:100:ARG:NH1  | 2.46                     | 0.48              |
| 15:sC:91:SER:O    | 15:sC:94:ILE:HG13  | 2.13                     | 0.48              |
| 19:sb:7:LEU:HD12  | 19:sb:7:LEU:H      | 1.78                     | 0.48              |
| 20:l7:15:C:H1'    | 25:lD:13:PHE:CE1   | 2.47                     | 0.48              |
| 20:l7:45:U:H2'    | 20:l7:46:C:C6      | 2.47                     | 0.48              |
| 25:lD:64:ILE:O    | 25:lD:74:ILE:HD12  | 2.13                     | 0.48              |
| 25:lD:289:ARG:HA  | 25:lD:292:GLU:OE1  | 2.13                     | 0.48              |
| 31:lJ:36:ALA:O    | 31:lJ:39:VAL:HG22  | 2.13                     | 0.48              |
| 35:lO:175:MET:SD  | 35:lO:175:MET:C    | 2.96                     | 0.48              |
| 35:lO:194:GLU:O   | 35:lO:198:THR:HG23 | 2.12                     | 0.48              |
| 41:lU:48:LYS:HA   | 41:lU:52:LYS:O     | 2.13                     | 0.48              |
| 43:lX:79:PHE:CG   | 53:lh:32:ARG:CZ    | 2.96                     | 0.48              |
| 47:lb:90:SER:OG   | 47:lb:91:ARG:N     | 2.45                     | 0.48              |
| 49:ld:32:ARG:HB3  | 49:ld:48:GLU:HG2   | 1.94                     | 0.48              |
| 55:lj:22:CYS:HB3  | 55:lj:37:CYS:HB3   | 1.94                     | 0.48              |
| 63:lz:139:THR:HA  | 63:lz:156:LYS:HG2  | 1.94                     | 0.48              |
| 64:sR:28:PHE:H    | 79:s2:1455:A:C3'   | 2.23                     | 0.48              |
| 65:sD:23:GLU:OE2  | 65:sD:27:ARG:NE    | 2.41                     | 0.48              |
| 69:sQ:71:ARG:CZ   | 79:s2:1407:U:H4'   | 2.43                     | 0.48              |
| 70:sS:26:ILE:HG13 | 70:sS:27:ALA:H     | 1.77                     | 0.48              |
| 72:sU:27:ARG:HH11 | 72:sU:27:ARG:HB3   | 1.78                     | 0.48              |
| 72:sU:56:MET:CE   | 79:s2:1580:A:H5'   | 2.43                     | 0.48              |
| 75:sg:167:SER:OG  | 75:sg:175:LYS:HB2  | 2.13                     | 0.48              |
| 79:s2:145:G:H2'   | 79:s2:146:G:H8     | 1.77                     | 0.48              |
| 79:s2:1134:G:H2'  | 79:s2:1135:C:C6    | 2.47                     | 0.48              |
| 79:s2:1627:C:H2'  | 79:s2:1628:C:H6    | 1.78                     | 0.48              |
| 82:pE:10:G:H1     | 82:pE:26:A:H1'     | 1.78                     | 0.48              |
| 82:pE:58:A:O2'    | 82:pE:60:U:OP2     | 2.24                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 85:l5:229:G:H2'    | 85:l5:230:G:H8     | 1.78                     | 0.48              |
| 85:l5:714:G:H2'    | 85:l5:715:G:H8     | 1.77                     | 0.48              |
| 85:l5:1847:C:H2'   | 85:l5:1848:C:H6    | 1.77                     | 0.48              |
| 85:l5:2037:C:H2'   | 85:l5:2038:U:C6    | 2.48                     | 0.48              |
| 85:l5:2067:C:H2'   | 85:l5:2068:C:C6    | 2.48                     | 0.48              |
| 85:l5:2335:C:H2'   | 85:l5:2336:G:H8    | 1.77                     | 0.48              |
| 85:l5:2552:G:N2    | 85:l5:2767:U:C4    | 2.82                     | 0.48              |
| 85:l5:3765:G:O2'   | 85:l5:3767:C:N4    | 2.46                     | 0.48              |
| 85:l5:4188:U:H2'   | 85:l5:4189:U:C6    | 2.48                     | 0.48              |
| 85:l5:4459:U:H2'   | 85:l5:4460:U:H6    | 1.77                     | 0.48              |
| 85:l5:4649:G:H2'   | 85:l5:4650:G:O4'   | 2.13                     | 0.48              |
| 85:l5:4964:C:H2'   | 85:l5:4965:U:C6    | 2.47                     | 0.48              |
| 85:l5:5010:U:H2'   | 85:l5:5011:A:C8    | 2.48                     | 0.48              |
| 80:CB:78:PHE:HD1   | 80:CB:79:TYR:H     | 1.61                     | 0.48              |
| 80:CB:749:ILE:HG13 | 80:CB:784:VAL:HB   | 1.95                     | 0.48              |
| 5:SX:75:ILE:HG13   | 5:SX:76:LYS:H      | 1.77                     | 0.48              |
| 7:SJ:78:LEU:O      | 7:SJ:82:VAL:HG12   | 2.13                     | 0.48              |
| 16:SN:47:PRO:HB3   | 16:SN:71:ILE:HD12  | 1.94                     | 0.48              |
| 16:SN:108:ASP:OD1  | 16:SN:111:ALA:N    | 2.32                     | 0.48              |
| 17:SO:34:PHE:O     | 17:SO:41:PHE:N     | 2.37                     | 0.48              |
| 17:SO:101:GLY:HA3  | 17:SO:134:PRO:HD2  | 1.95                     | 0.48              |
| 85:L5:432:U:H4'    | 85:L5:433:A:H5''   | 1.93                     | 0.48              |
| 85:L5:1788:A:H2'   | 30:LI:22:PHE:CZ    | 2.48                     | 0.48              |
| 85:L5:1881:C:H5'   | 85:L5:2281:U:H1'   | 1.95                     | 0.48              |
| 85:L5:2270:G:H2'   | 85:L5:2271:C:H6    | 1.77                     | 0.48              |
| 85:L5:2373:C:H4'   | 49:Ld:64:ILE:HD11  | 1.95                     | 0.48              |
| 85:L5:2659:A:N7    | 85:L5:2673:G:C5    | 2.81                     | 0.48              |
| 85:L5:2757:A:H2'   | 85:L5:2758:G:C8    | 2.48                     | 0.48              |
| 85:L5:3722:G:H2'   | 85:L5:3723:A:H8    | 1.78                     | 0.48              |
| 85:L5:3951:G:H2'   | 85:L5:3952:A:C8    | 2.47                     | 0.48              |
| 85:L5:4075:U:O2    | 85:L5:4076:G:O2'   | 2.24                     | 0.48              |
| 85:L5:4194:U:H5'   | 47:Lb:3:LYS:HE3    | 1.94                     | 0.48              |
| 85:L5:4651:A:H2'   | 85:L5:4652:G:O4'   | 2.11                     | 0.48              |
| 85:L5:4888:U:H2'   | 85:L5:4889:G:C8    | 2.48                     | 0.48              |
| 85:L5:4895:C:H3'   | 85:L5:4895:C:OP2   | 2.12                     | 0.48              |
| 24:LC:107:THR:O    | 24:LC:111:TRP:NE1  | 2.30                     | 0.48              |
| 25:LD:287:PHE:CZ   | 25:LD:291:GLN:NE2  | 2.81                     | 0.48              |
| 35:LO:135:PHE:HE2  | 35:LO:137:TYR:CZ   | 2.30                     | 0.48              |
| 40:LT:118:GLU:HA   | 40:LT:121:GLU:HG3  | 1.94                     | 0.48              |
| 43:LX:76:ILE:HG21  | 43:LX:109:ILE:HG22 | 1.95                     | 0.48              |
| 46:La:126:ALA:HB3  | 46:La:129:PHE:CZ   | 2.48                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 52:Lg:103:VAL:O    | 52:Lg:107:LEU:HG   | 2.12                     | 0.48              |
| 53:Lh:27:GLU:HA    | 53:Lh:30:GLN:HG3   | 1.95                     | 0.48              |
| 54:Li:26:HIS:NE2   | 54:Li:29:ARG:HD3   | 2.28                     | 0.48              |
| 64:SR:77:GLU:HA    | 64:SR:80:ARG:NE    | 2.28                     | 0.48              |
| 64:SR:77:GLU:HA    | 64:SR:80:ARG:HE    | 1.77                     | 0.48              |
| 72:SU:25:THR:HG23  | 72:SU:86:LYS:HB3   | 1.94                     | 0.48              |
| 76:SM:73:GLN:HG2   | 76:SM:74:ILE:HD13  | 1.94                     | 0.48              |
| 77:SZ:72:VAL:O     | 77:SZ:76:ARG:HB2   | 2.13                     | 0.48              |
| 79:S2:5:U:HO2'     | 79:S2:602:G:HO2'   | 1.54                     | 0.48              |
| 79:S2:14:C:O2'     | 79:S2:668:A:N1     | 2.34                     | 0.48              |
| 79:S2:179:C:H3'    | 79:S2:180:G:H8     | 1.78                     | 0.48              |
| 79:S2:218:U:H2'    | 79:S2:219:U:H6     | 1.76                     | 0.48              |
| 79:S2:1688:C:H2'   | 79:S2:1689:C:C6    | 2.47                     | 0.48              |
| 82:PE:39:U:H2'     | 82:PE:40:C:C6      | 2.48                     | 0.48              |
| 1:cH:104:GLN:HG3   | 79:s2:1501:C:OP1   | 2.13                     | 0.48              |
| 4:sL:77:VAL:HA     | 4:sL:88:ILE:HG22   | 1.95                     | 0.48              |
| 5:sX:129:SER:O     | 5:sX:133:LEU:HD12  | 2.12                     | 0.48              |
| 6:sG:32:MET:SD     | 6:sG:63:MET:CE     | 3.01                     | 0.48              |
| 10:sA:222:VAL:HG13 | 10:sA:223:THR:HG23 | 1.95                     | 0.48              |
| 13:sV:8:PHE:CD2    | 13:sV:10:ASP:OD2   | 2.66                     | 0.48              |
| 15:sC:60:TRP:NE1   | 15:sC:62:PRO:HA    | 2.28                     | 0.48              |
| 20:l7:19:C:H2'     | 20:l7:20:U:C6      | 2.48                     | 0.48              |
| 20:l7:24:C:H2'     | 20:l7:25:G:O4'     | 2.13                     | 0.48              |
| 20:l7:85:G:H2'     | 20:l7:86:G:H8      | 1.78                     | 0.48              |
| 22:lA:181:LYS:NZ   | 61:lp:18:TYR:OH    | 2.43                     | 0.48              |
| 28:lG:33:GLU:N     | 28:lG:33:GLU:OE1   | 2.46                     | 0.48              |
| 28:lG:219:VAL:HA   | 28:lG:222:ILE:HG12 | 1.94                     | 0.48              |
| 29:lH:106:GLN:HG3  | 29:lH:107:GLU:H    | 1.77                     | 0.48              |
| 32:lL:52:SER:OG    | 32:lL:152:GLY:O    | 2.18                     | 0.48              |
| 33:lM:24:LEU:HD11  | 33:lM:86:TRP:CD1   | 2.49                     | 0.48              |
| 39:lS:128:LYS:HE3  | 39:lS:130:GLU:OE1  | 2.12                     | 0.48              |
| 39:lS:157:ARG:N    | 39:lS:174:THR:OG1  | 2.46                     | 0.48              |
| 40:lT:115:LYS:HD2  | 40:lT:126:VAL:HG21 | 1.96                     | 0.48              |
| 42:lV:109:LYS:HB3  | 42:lV:111:GLU:OE1  | 2.12                     | 0.48              |
| 49:ld:85:ARG:NH1   | 49:ld:117:LEU:HB3  | 2.28                     | 0.48              |
| 52:lg:60:ARG:O     | 52:lg:63:VAL:HG12  | 2.13                     | 0.48              |
| 54:li:60:LEU:HD23  | 54:li:69:ALA:HA    | 1.95                     | 0.48              |
| 63:lz:143:ASN:ND2  | 63:lz:150:GLU:OE1  | 2.46                     | 0.48              |
| 63:lz:145:VAL:HG23 | 63:lz:146:ALA:H    | 1.78                     | 0.48              |
| 75:sg:242:SER:HB2  | 75:sg:245:ARG:O    | 2.13                     | 0.48              |
| 77:sZ:66:LYS:C     | 77:sZ:66:LYS:HD2   | 2.39                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 77:sZ:91:LEU:HD22  | 77:sZ:96:LEU:HD21  | 1.95                     | 0.48              |
| 79:s2:363:A:N1     | 79:s2:397:G:O2'    | 2.37                     | 0.48              |
| 79:s2:804:U:H2'    | 79:s2:805:U:H6     | 1.77                     | 0.48              |
| 79:s2:839:C:C4     | 79:s2:841:G:C6     | 3.02                     | 0.48              |
| 79:s2:1051:G:H2'   | 79:s2:1052:A:H8    | 1.79                     | 0.48              |
| 79:s2:1067:C:H2'   | 79:s2:1068:G:O4'   | 2.12                     | 0.48              |
| 79:s2:1192:U:H2'   | 79:s2:1193:U:C6    | 2.49                     | 0.48              |
| 79:s2:1671:G:C4    | 79:s2:1672:U:C5    | 3.01                     | 0.48              |
| 80:cB:8:GLN:HE22   | 80:cB:45:ILE:HD11  | 1.77                     | 0.48              |
| 80:cB:19:ILE:HG21  | 80:cB:468:ASN:ND2  | 2.27                     | 0.48              |
| 80:cB:26:ALA:HB2   | 80:cB:128:VAL:HB   | 1.94                     | 0.48              |
| 80:cB:427:VAL:HG21 | 80:cB:485:ILE:HG23 | 1.94                     | 0.48              |
| 82:pE:9:A:O2'      | 82:pE:45:G:N3      | 2.41                     | 0.48              |
| 84:lt:53:TRP:CZ3   | 84:lt:56:LEU:HD11  | 2.48                     | 0.48              |
| 85:l5:690:C:H2'    | 85:l5:691:C:H6     | 1.77                     | 0.48              |
| 85:l5:966:A:C2     | 85:l5:2093:A:H2    | 2.31                     | 0.48              |
| 85:l5:1643:A:H2'   | 85:l5:1644:C:C6    | 2.46                     | 0.48              |
| 85:l5:1709:C:C4    | 85:l5:1716:G:N2    | 2.76                     | 0.48              |
| 85:l5:1831:G:H2'   | 85:l5:1832:C:O4'   | 2.13                     | 0.48              |
| 85:l5:1982:G:H2'   | 85:l5:1983:A:O4'   | 2.12                     | 0.48              |
| 85:l5:2372:U:H2'   | 85:l5:2373:C:H6    | 1.79                     | 0.48              |
| 85:l5:3951:G:H2'   | 85:l5:3952:A:C8    | 2.48                     | 0.48              |
| 85:l5:4989:U:O2'   | 85:l5:4991:U:O4'   | 2.28                     | 0.48              |
| 85:l5:5055:G:H2'   | 85:l5:5056:A:C8    | 2.48                     | 0.48              |
| 80:CB:71:LYS:HD3   | 80:CB:114:GLU:OE2  | 2.13                     | 0.48              |
| 3:SI:75:LYS:HE3    | 79:S2:303:C:H4'    | 1.94                     | 0.48              |
| 5:SX:11:ARG:O      | 5:SX:15:SER:OG     | 2.21                     | 0.48              |
| 11:SB:103:MET:HB3  | 11:SB:215:VAL:HG12 | 1.94                     | 0.48              |
| 85:L5:84:A:OP1     | 85:L5:86:U:H1'     | 2.13                     | 0.48              |
| 85:L5:350:C:H3'    | 24:LC:197:ARG:NH1  | 2.28                     | 0.48              |
| 85:L5:452:A:N6     | 85:L5:1293:G:H5''  | 2.29                     | 0.48              |
| 85:L5:1273:G:O2'   | 85:L5:1274:A:H5'   | 2.13                     | 0.48              |
| 85:L5:1800:U:H2'   | 85:L5:1801:A:H8    | 1.77                     | 0.48              |
| 85:L5:1846:G:H2'   | 85:L5:1847:C:H6    | 1.77                     | 0.48              |
| 85:L5:2475:G:C6    | 43:LX:50:LYS:HG2   | 2.48                     | 0.48              |
| 85:L5:2616:C:OP1   | 38:LR:64:ARG:NE    | 2.46                     | 0.48              |
| 85:L5:2659:A:N1    | 85:L5:2672:C:O2'   | 2.44                     | 0.48              |
| 85:L5:2745:A:H2'   | 85:L5:2746:A:C8    | 2.48                     | 0.48              |
| 85:L5:2876:G:C8    | 61:Lp:16:THR:HG22  | 2.48                     | 0.48              |
| 85:L5:3664:G:H2'   | 85:L5:3665:G:C8    | 2.46                     | 0.48              |
| 85:L5:3796:U:H2'   | 85:L5:3797:C:C6    | 2.48                     | 0.48              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 85:L5:4080:C:H2'  | 85:L5:4081:G:C8    | 2.48                     | 0.48              |
| 85:L5:4084:G:O6   | 22:LA:70:LYS:NZ    | 2.41                     | 0.48              |
| 85:L5:4101:C:O2   | 85:L5:4104:G:O5'   | 2.31                     | 0.48              |
| 85:L5:4251:A:H2'  | 85:L5:4252:C:C6    | 2.48                     | 0.48              |
| 85:L5:4481:U:H2'  | 85:L5:4482:U:C6    | 2.48                     | 0.48              |
| 85:L5:4619:U:H2'  | 85:L5:4620:U:H6    | 1.78                     | 0.48              |
| 85:L5:5024:C:C5   | 85:L5:5025:C:H1'   | 2.48                     | 0.48              |
| 85:L5:5036:C:H2'  | 85:L5:5037:U:C6    | 2.48                     | 0.48              |
| 85:L5:5048:A:N3   | 49:Ld:31:LYS:HA    | 2.27                     | 0.48              |
| 21:L8:67:U:H2'    | 21:L8:68:G:H8      | 1.78                     | 0.48              |
| 23:LB:302:ASN:HB2 | 23:LB:313:SER:HA   | 1.95                     | 0.48              |
| 23:LB:340:THR:OG1 | 23:LB:341:LYS:N    | 2.46                     | 0.48              |
| 26:LE:281:ILE:HB  | 26:LE:286:LEU:HD21 | 1.94                     | 0.48              |
| 29:LH:36:ARG:HB3  | 29:LH:80:MET:HE3   | 1.95                     | 0.48              |
| 30:LI:36:LEU:HD22 | 30:LI:73:ASN:ND2   | 2.28                     | 0.48              |
| 35:LO:42:ASN:ND2  | 35:LO:135:PHE:HD2  | 2.07                     | 0.48              |
| 35:LO:150:GLN:HG3 | 35:LO:151:ALA:N    | 2.27                     | 0.48              |
| 36:LP:69:ARG:HG3  | 36:LP:80:GLN:HB3   | 1.95                     | 0.48              |
| 38:LR:173:ARG:NH2 | 79:S2:909:G:OP1    | 2.45                     | 0.48              |
| 49:Ld:23:ARG:HD2  | 49:Ld:25:TYR:OH    | 2.12                     | 0.48              |
| 49:Ld:65:ASP:OD1  | 49:Ld:66:THR:N     | 2.46                     | 0.48              |
| 49:Ld:72:VAL:HG23 | 49:Ld:73:TRP:CD1   | 2.48                     | 0.48              |
| 60:Lo:11:PHE:CD1  | 60:Lo:11:PHE:C     | 2.89                     | 0.48              |
| 63:Lz:60:ARG:CZ   | 63:Lz:61:PRO:HG3   | 2.43                     | 0.48              |
| 70:SS:87:GLN:HA   | 70:SS:95:TYR:HA    | 1.94                     | 0.48              |
| 74:Sd:42:CYS:SG   | 79:S2:1495:G:N2    | 2.69                     | 0.48              |
| 75:Sg:67:SER:HB3  | 75:Sg:83:TRP:CD1   | 2.49                     | 0.48              |
| 79:S2:57:U:O2     | 79:S2:499:G:O2'    | 2.32                     | 0.48              |
| 79:S2:72:C:N4     | 79:S2:74:G:H1      | 2.10                     | 0.48              |
| 79:S2:146:G:H1    | 79:S2:173:A:H61    | 1.61                     | 0.48              |
| 79:S2:1171:G:H1'  | 79:S2:1172:U:H5    | 1.78                     | 0.48              |
| 79:S2:1428:G:N1   | 79:S2:1585:U:O4'   | 2.46                     | 0.48              |
| 79:S2:1617:G:N2   | 79:S2:1619:A:H3'   | 2.28                     | 0.48              |
| 2:sE:120:LYS:O    | 2:sE:164:LEU:HD23  | 2.13                     | 0.48              |
| 4:sL:73:LEU:HD21  | 4:sL:90:ARG:CZ     | 2.44                     | 0.48              |
| 7:sJ:3:VAL:HG12   | 7:sJ:5:ARG:H       | 1.77                     | 0.48              |
| 7:sJ:77:LEU:HA    | 7:sJ:80:ARG:HE     | 1.78                     | 0.48              |
| 17:sO:33:ILE:HG21 | 17:sO:97:LEU:HD22  | 1.94                     | 0.48              |
| 18:sW:106:THR:OG1 | 18:sW:107:SER:N    | 2.46                     | 0.48              |
| 19:sb:72:ARG:NH1  | 79:s2:1119:A:O3'   | 2.43                     | 0.48              |
| 22:lA:173:GLY:O   | 61:lp:69:TRP:NE1   | 2.31                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:1B:215:GLU:HB2  | 23:1B:284:ILE:HD13 | 1.94                     | 0.48              |
| 24:1C:111:TRP:CD1  | 24:1C:111:TRP:H    | 2.31                     | 0.48              |
| 26:1E:250:GLN:O    | 26:1E:254:ASP:OD1  | 2.31                     | 0.48              |
| 30:1I:4:ARG:NH1    | 85:15:1866:U:OP1   | 2.36                     | 0.48              |
| 30:1I:45:GLU:OE1   | 30:1I:45:GLU:N     | 2.45                     | 0.48              |
| 33:1M:124:LYS:HA   | 33:1M:127:VAL:HG22 | 1.95                     | 0.48              |
| 34:1N:99:GLN:HB2   | 34:1N:130:PHE:CZ   | 2.48                     | 0.48              |
| 36:1P:101:ASN:HD21 | 85:15:400:A:H4'    | 1.78                     | 0.48              |
| 46:1a:10:LYS:NZ    | 85:15:2287:G:O6    | 2.38                     | 0.48              |
| 50:1e:91:CYS:C     | 50:1e:93:LYS:H     | 2.22                     | 0.48              |
| 60:1o:43:ARG:NH2   | 85:15:291:U:O4     | 2.46                     | 0.48              |
| 64:sR:4:VAL:HG11   | 79:s2:1212:G:H5''  | 1.96                     | 0.48              |
| 67:sK:77:GLN:N     | 67:sK:77:GLN:OE1   | 2.46                     | 0.48              |
| 67:sK:95:ARG:NH2   | 67:sK:98:ARG:HA    | 2.28                     | 0.48              |
| 68:sP:37:TYR:OH    | 68:sP:112:ILE:O    | 2.24                     | 0.48              |
| 78:sf:138:ARG:HG2  | 78:sf:149:CYS:SG   | 2.53                     | 0.48              |
| 79:s2:289:G:N2     | 79:s2:293:C:C2     | 2.81                     | 0.48              |
| 79:s2:403:G:H2'    | 79:s2:404:G:H8     | 1.79                     | 0.48              |
| 79:s2:863:U:H2'    | 79:s2:864:A:C8     | 2.47                     | 0.48              |
| 80:cB:88:PHE:HB3   | 80:cB:356:ILE:HD12 | 1.95                     | 0.48              |
| 80:cB:109:VAL:HG11 | 85:15:4605:A:HO2'  | 1.78                     | 0.48              |
| 81:aP:51:C:H2'     | 81:aP:52:G:C8      | 2.44                     | 0.48              |
| 85:15:25:A:H61     | 85:15:58:G:H1      | 1.61                     | 0.48              |
| 85:15:318:A:H2'    | 85:15:319:A:H8     | 1.77                     | 0.48              |
| 85:15:452:A:N6     | 85:15:1293:G:H5''  | 2.27                     | 0.48              |
| 85:15:461:G:H2'    | 85:15:462:G:C8     | 2.48                     | 0.48              |
| 85:15:1624:G:C5    | 85:15:1643:A:C8    | 3.01                     | 0.48              |
| 85:15:4058:U:H4'   | 85:15:4059:C:H5    | 1.78                     | 0.48              |
| 85:15:4089:G:H2'   | 85:15:4090:G:C8    | 2.47                     | 0.48              |
| 80:CB:368:ARG:NH1  | 80:CB:371:LEU:HD11 | 2.28                     | 0.48              |
| 3:SI:70:GLU:N      | 3:SI:70:GLU:OE1    | 2.46                     | 0.48              |
| 6:SG:7:PHE:CE1     | 6:SG:113:ILE:HB    | 2.48                     | 0.48              |
| 11:SB:107:ARG:HH12 | 17:SO:133:THR:N    | 2.11                     | 0.48              |
| 12:SH:163:GLN:HG3  | 12:SH:189:PHE:CD1  | 2.49                     | 0.48              |
| 14:Sa:38:LYS:HG3   | 79:S2:1868:U:OP2   | 2.13                     | 0.48              |
| 18:SW:28:ARG:HB3   | 18:SW:29:PRO:HD3   | 1.94                     | 0.48              |
| 85:L5:50:C:H2'     | 85:L5:51:A:O4'     | 2.13                     | 0.48              |
| 85:L5:247:G:H2'    | 85:L5:248:C:H6     | 1.78                     | 0.48              |
| 85:L5:1815:G:C2    | 47:Lb:45:PHE:HE2   | 2.31                     | 0.48              |
| 85:L5:1856:C:H2'   | 85:L5:1857:C:C6    | 2.48                     | 0.48              |
| 85:L5:2286:G:H2'   | 85:L5:2287:G:H8    | 1.77                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 85:L5:2352:U:H1'   | 24:LC:96:CYS:HA    | 1.95                     | 0.48              |
| 85:L5:2898:G:H5''  | 38:LR:104:ARG:HH12 | 1.77                     | 0.48              |
| 85:L5:3637:U:O4    | 85:L5:3651:A:H2    | 1.95                     | 0.48              |
| 85:L5:4101:C:H5''  | 85:L5:4102:C:OP2   | 2.13                     | 0.48              |
| 85:L5:4627:U:H2'   | 85:L5:4628:U:C6    | 2.48                     | 0.48              |
| 85:L5:4637:G:H2'   | 85:L5:4638:U:H6    | 1.78                     | 0.48              |
| 85:L5:4754:G:N1    | 85:L5:4880:C:N3    | 2.62                     | 0.48              |
| 26:LE:223:ARG:NH2  | 26:LE:234:ASP:HB2  | 2.28                     | 0.48              |
| 28:LG:154:LEU:O    | 28:LG:204:PHE:N    | 2.47                     | 0.48              |
| 30:LI:59:GLN:HA    | 30:LI:128:ARG:HA   | 1.95                     | 0.48              |
| 34:LN:53:TYR:HD2   | 34:LN:54:LYS:N     | 2.11                     | 0.48              |
| 37:LQ:172:ARG:HA   | 37:LQ:176:ARG:HG3  | 1.95                     | 0.48              |
| 48:Lc:15:ASN:O     | 48:Lc:18:LEU:HD12  | 2.13                     | 0.48              |
| 53:Lh:27:GLU:OE1   | 53:Lh:50:VAL:HG11  | 2.13                     | 0.48              |
| 63:Lz:95:LYS:HE2   | 63:Lz:127:GLY:HA3  | 1.96                     | 0.48              |
| 64:SR:95:ILE:HD12  | 64:SR:118:GLN:OE1  | 2.13                     | 0.48              |
| 75:Sg:217:MET:HE1  | 75:Sg:219:TRP:CD1  | 2.48                     | 0.48              |
| 77:SZ:50:PHE:CZ    | 77:SZ:58:LEU:HD11  | 2.48                     | 0.48              |
| 79:S2:165:G:H2'    | 79:S2:166:A:H8     | 1.79                     | 0.48              |
| 79:S2:350:C:O2'    | 79:S2:383:G:N1     | 2.41                     | 0.48              |
| 79:S2:408:A:O2'    | 79:S2:410:G:OP1    | 2.30                     | 0.48              |
| 79:S2:629:A:O2'    | 79:S2:631:U:OP1    | 2.30                     | 0.48              |
| 79:S2:1598:G:N2    | 79:S2:1599:U:O4    | 2.29                     | 0.48              |
| 79:S2:1610:G:C6    | 79:S2:1630:A:C5    | 3.00                     | 0.48              |
| 79:S2:1804:U:H2'   | 79:S2:1805:G:C8    | 2.49                     | 0.48              |
| 83:Ls:28:PHE:HE2   | 83:Ls:95:LEU:HB2   | 1.78                     | 0.48              |
| 87:IW:119:LYS:O    | 87:IW:123:LYS:HG2  | 2.13                     | 0.48              |
| 2:sE:87:MET:SD     | 2:sE:142:HIS:CE1   | 3.07                     | 0.48              |
| 2:sE:95:THR:OG1    | 2:sE:97:GLU:OE1    | 2.29                     | 0.48              |
| 2:sE:192:ILE:HD11  | 2:sE:242:LYS:O     | 2.13                     | 0.48              |
| 11:sB:125:VAL:HG11 | 11:sB:172:MET:CE   | 2.43                     | 0.48              |
| 16:sN:48:SER:OG    | 79:s2:926:A:H1'    | 2.13                     | 0.48              |
| 21:l8:131:G:O3'    | 43:IX:108:GLN:NE2  | 2.47                     | 0.48              |
| 23:lB:144:LYS:C    | 23:lB:148:LYS:HZ3  | 2.21                     | 0.48              |
| 23:lB:150:PHE:HB3  | 23:lB:198:ARG:NH2  | 2.28                     | 0.48              |
| 25:lD:23:ARG:O     | 25:lD:23:ARG:HD2   | 2.14                     | 0.48              |
| 25:lD:284:LYS:HE2  | 30:lI:209:TRP:CE2  | 2.49                     | 0.48              |
| 26:lE:124:LYS:HB3  | 85:l5:958:G:N2     | 2.29                     | 0.48              |
| 30:lI:15:LYS:HB2   | 85:l5:1863:U:OP1   | 2.13                     | 0.48              |
| 37:lQ:97:LYS:NZ    | 37:lQ:118:GLY:HA2  | 2.28                     | 0.48              |
| 38:lR:39:GLN:HB3   | 38:lR:42:ARG:HH11  | 1.78                     | 0.48              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 40:IT:110:LYS:HD3 | 40:IT:110:LYS:HA   | 1.68                     | 0.48              |
| 43:IX:131:ASP:O   | 57:IL:14:ALA:HB1   | 2.13                     | 0.48              |
| 61:lp:42:CYS:HB3  | 61:lp:60:CYS:SG    | 2.53                     | 0.48              |
| 64:sR:11:LYS:CD   | 79:s2:1372:U:H3'   | 2.43                     | 0.48              |
| 75:sg:37:ASP:C    | 75:sg:38:LYS:HG2   | 2.39                     | 0.48              |
| 75:sg:201:SER:OG  | 75:sg:203:ASP:OD1  | 2.31                     | 0.48              |
| 75:sg:287:THR:OG1 | 75:sg:288:SER:N    | 2.45                     | 0.48              |
| 79:s2:29:G:C6     | 79:s2:646:G:C6     | 3.02                     | 0.48              |
| 79:s2:634:A:H2'   | 79:s2:635:G:H8     | 1.78                     | 0.48              |
| 79:s2:1855:G:H2'  | 79:s2:1856:C:H6    | 1.78                     | 0.48              |
| 83:ls:7:ALA:HA    | 83:ls:10:LYS:HE3   | 1.95                     | 0.48              |
| 85:l5:73:A:H5'    | 85:l5:74:G:OP2     | 2.13                     | 0.48              |
| 85:l5:1908:A:H2'  | 85:l5:1909:G:O4'   | 2.13                     | 0.48              |
| 85:l5:2360:A:N1   | 85:l5:3860:A:H5''  | 2.28                     | 0.48              |
| 85:l5:2648:G:H2'  | 85:l5:2649:G:C8    | 2.48                     | 0.48              |
| 85:l5:2895:A:H2'  | 85:l5:2896:G:C8    | 2.48                     | 0.48              |
| 85:l5:3795:A:C6   | 85:l5:3806:G:C6    | 3.01                     | 0.48              |
| 85:l5:3871:A:H2'  | 85:l5:3872:A:H8    | 1.75                     | 0.48              |
| 85:l5:3880:G:H2'  | 85:l5:3881:G:C8    | 2.48                     | 0.48              |
| 85:l5:4129:G:H2'  | 85:l5:4130:C:C6    | 2.49                     | 0.48              |
| 80:CB:135:VAL:N   | 80:CB:181:ILE:HD11 | 2.29                     | 0.48              |
| 6:SG:58:LYS:NZ    | 6:SG:105:ASN:HA    | 2.27                     | 0.48              |
| 6:SG:198:ARG:NH1  | 79:S2:126:G:OP2    | 2.37                     | 0.48              |
| 10:SA:174:MET:HA  | 10:SA:177:MET:HG2  | 1.95                     | 0.48              |
| 10:SA:176:TRP:CE3 | 10:SA:199:PRO:HB3  | 2.49                     | 0.48              |
| 14:Sa:7:ASN:ND2   | 14:Sa:7:ASN:O      | 2.46                     | 0.48              |
| 85:L5:6:C:H2'     | 85:L5:7:C:H6       | 1.78                     | 0.48              |
| 85:L5:116:G:OP2   | 34:LN:2:GLY:N      | 2.46                     | 0.48              |
| 85:L5:121:A:H62   | 85:L5:152:U:H3     | 1.61                     | 0.48              |
| 85:L5:159:C:OP2   | 54:Li:25:ARG:HB3   | 2.14                     | 0.48              |
| 85:L5:266:C:O2'   | 85:L5:267:G:H8     | 1.96                     | 0.48              |
| 85:L5:1671:U:O4   | 85:L5:1853:G:H1'   | 2.14                     | 0.48              |
| 85:L5:1998:A:H4'  | 83:Ls:9:TRP:HZ2    | 1.79                     | 0.48              |
| 85:L5:2264:C:H2'  | 85:L5:2265:G:O4'   | 2.13                     | 0.48              |
| 85:L5:3758:U:H2'  | 85:L5:3765:G:N2    | 2.27                     | 0.48              |
| 85:L5:3882:C:C2   | 85:L5:3883:U:C5    | 3.01                     | 0.48              |
| 85:L5:4194:U:O3'  | 30:LI:116:ARG:NH2  | 2.37                     | 0.48              |
| 85:L5:4763:U:O2'  | 39:LS:174:THR:OG1  | 2.27                     | 0.48              |
| 20:L7:75:G:H1'    | 20:L7:76:U:H5      | 1.78                     | 0.48              |
| 23:LB:59:GLU:OE1  | 23:LB:60:VAL:N     | 2.39                     | 0.48              |
| 25:LD:117:LYS:O   | 25:LD:117:LYS:NZ   | 2.30                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 29:LH:48:LEU:HB2   | 29:LH:54:ARG:HG3   | 1.96                     | 0.48              |
| 37:LQ:25:LEU:HA    | 37:LQ:28:LEU:HD23  | 1.94                     | 0.48              |
| 50:Le:108:ARG:HD3  | 50:Le:127:ALA:HB3  | 1.95                     | 0.48              |
| 51:Lf:106:TYR:HB3  | 51:Lf:107:PRO:CD   | 2.44                     | 0.48              |
| 53:Lh:40:ALA:HB3   | 53:Lh:43:LYS:HG2   | 1.96                     | 0.48              |
| 66:SF:77:MET:HE1   | 79:S2:1674:G:H4'   | 1.94                     | 0.48              |
| 68:SP:37:TYR:CE1   | 68:SP:112:ILE:HG22 | 2.48                     | 0.48              |
| 69:SQ:52:LEU:O     | 69:SQ:55:VAL:HG12  | 2.13                     | 0.48              |
| 70:SS:4:VAL:HG22   | 70:SS:5:ILE:H      | 1.79                     | 0.48              |
| 76:SM:29:ASP:HB2   | 76:SM:113:ASP:HB2  | 1.94                     | 0.48              |
| 87:IW:80:ARG:HH11  | 87:IW:80:ARG:HB3   | 1.78                     | 0.48              |
| 1:cH:44:TRP:CD1    | 9:se:52:LYS:H      | 2.32                     | 0.48              |
| 4:sL:10:TYR:CD2    | 4:sL:12:LYS:HB3    | 2.48                     | 0.48              |
| 7:sJ:2:PRO:HD2     | 79:s2:428:U:O3'    | 2.14                     | 0.48              |
| 8:sY:119:GLY:HA2   | 79:s2:85:A:C5'     | 2.43                     | 0.48              |
| 10:sA:50:ASN:HB3   | 10:sA:53:ARG:HD2   | 1.96                     | 0.48              |
| 11:sB:179:ASN:OD1  | 11:sB:179:ASN:N    | 2.44                     | 0.48              |
| 13:sV:66:ASP:O     | 13:sV:69:ILE:HD12  | 2.12                     | 0.48              |
| 22:lA:140:ASN:ND2  | 22:lA:142:GLU:O    | 2.47                     | 0.48              |
| 25:ID:216:GLU:HG3  | 25:ID:220:LYS:HE2  | 1.95                     | 0.48              |
| 28:lG:51:LEU:HD21  | 85:l5:4086:G:C4    | 2.48                     | 0.48              |
| 33:IM:37:LEU:HD21  | 33:IM:47:ARG:HD3   | 1.95                     | 0.48              |
| 34:lN:176:LYS:NZ   | 85:l5:65:A:N3      | 2.52                     | 0.48              |
| 37:lQ:53:MET:HB2   | 37:lQ:57:ASN:HB2   | 1.95                     | 0.48              |
| 44:lY:1:MET:HB2    | 44:lY:3:PHE:CZ     | 2.49                     | 0.48              |
| 51:lf:28:LEU:HD22  | 51:lf:101:ILE:HG21 | 1.96                     | 0.48              |
| 52:lg:64:LEU:HD13  | 85:l5:2749:C:H4'   | 1.94                     | 0.48              |
| 55:lj:43:ARG:HH22  | 85:l5:55:G:P       | 2.37                     | 0.48              |
| 58:lm:92:ASP:OD2   | 58:lm:105:PRO:HG3  | 2.13                     | 0.48              |
| 63:lz:16:GLU:HG2   | 63:lz:18:LEU:HD13  | 1.94                     | 0.48              |
| 64:sR:7:LYS:NZ     | 79:s2:1367:U:O4    | 2.37                     | 0.48              |
| 65:sD:67:ARG:O     | 65:sD:70:THR:OG1   | 2.28                     | 0.48              |
| 66:sF:123:GLU:OE2  | 66:sF:138:ALA:HB1  | 2.14                     | 0.48              |
| 67:sK:51:SER:O     | 67:sK:55:ARG:HG2   | 2.13                     | 0.48              |
| 69:sQ:41:MET:HE1   | 71:sT:9:VAL:CA     | 2.43                     | 0.48              |
| 75:sg:114:SER:HB3  | 75:sg:119:GLN:HB2  | 1.95                     | 0.48              |
| 75:sg:164:ILE:HG21 | 75:sg:221:LEU:HD13 | 1.95                     | 0.48              |
| 76:sM:58:GLU:HG3   | 76:sM:60:MET:SD    | 2.54                     | 0.48              |
| 79:s2:508:A:H3'    | 79:s2:509:G:C8     | 2.48                     | 0.48              |
| 79:s2:651:U:H2'    | 79:s2:652:U:H6     | 1.78                     | 0.48              |
| 79:s2:880:G:C8     | 79:s2:907:G:C2     | 3.02                     | 0.48              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 79:s2:1420:G:O2'  | 79:s2:1421:A:O5'   | 2.31                     | 0.48              |
| 79:s2:1601:A:H61  | 79:s2:1635:C:H3'   | 1.78                     | 0.48              |
| 79:s2:1745:A:H2'  | 79:s2:1746:U:O4'   | 2.12                     | 0.48              |
| 80:cB:219:HIS:CD2 | 80:cB:337:LYS:HG2  | 2.48                     | 0.48              |
| 80:cB:664:ASP:OD1 | 80:cB:664:ASP:N    | 2.42                     | 0.48              |
| 80:cB:676:LYS:HA  | 80:cB:679:VAL:HG12 | 1.95                     | 0.48              |
| 84:lt:127:GLY:O   | 84:lt:131:GLU:HG3  | 2.13                     | 0.48              |
| 85:l5:958:G:N2    | 85:l5:1285:U:OP1   | 2.38                     | 0.48              |
| 85:l5:1211:G:H2'  | 85:l5:1212:G:H8    | 1.78                     | 0.48              |
| 85:l5:1550:G:H1   | 85:l5:1578:U:H3    | 1.60                     | 0.48              |
| 85:l5:1566:C:H2'  | 85:l5:1567:U:C6    | 2.48                     | 0.48              |
| 85:l5:1763:C:H2'  | 85:l5:1764:G:H5'   | 1.94                     | 0.48              |
| 85:l5:1951:G:H1   | 85:l5:2032:U:H3    | 1.60                     | 0.48              |
| 85:l5:2081:C:H2'  | 85:l5:2082:G:C8    | 2.48                     | 0.48              |
| 85:l5:2684:C:H2'  | 85:l5:2685:C:C6    | 2.48                     | 0.48              |
| 85:l5:2898:G:H2'  | 85:l5:2899:C:H6    | 1.79                     | 0.48              |
| 85:l5:4361:U:H2'  | 85:l5:4362:A:H8    | 1.78                     | 0.48              |
| 85:l5:4538:G:H2'  | 85:l5:4539:U:C6    | 2.48                     | 0.48              |
| 85:l5:4739:C:H2'  | 85:l5:4740:G:H5'   | 1.96                     | 0.48              |
| 85:l5:4759:C:H2'  | 85:l5:4760:G:C8    | 2.48                     | 0.48              |
| 80:CB:79:TYR:CG   | 80:CB:351:LEU:HD13 | 2.48                     | 0.48              |
| 7:SJ:137:VAL:HG22 | 7:SJ:138:ARG:H     | 1.78                     | 0.48              |
| 8:SY:8:ARG:HD3    | 8:SY:8:ARG:HA      | 1.74                     | 0.48              |
| 8:SY:9:THR:HG22   | 8:SY:25:ILE:HG22   | 1.96                     | 0.48              |
| 12:SH:143:ARG:HB3 | 12:SH:145:ARG:HH21 | 1.79                     | 0.48              |
| 14:Sa:33:ASP:OD1  | 14:Sa:34:LYS:N     | 2.40                     | 0.48              |
| 85:L5:52:G:P      | 55:Lj:48:ASN:HD22  | 2.35                     | 0.48              |
| 85:L5:154:G:O3'   | 53:Lh:105:LYS:NZ   | 2.46                     | 0.48              |
| 85:L5:197:A:H2'   | 85:L5:198:A:C8     | 2.48                     | 0.48              |
| 85:L5:256:G:H2'   | 85:L5:257:C:C6     | 2.49                     | 0.48              |
| 85:L5:735:G:O3'   | 33:LM:74:ARG:NH2   | 2.47                     | 0.48              |
| 85:L5:1953:U:H2'  | 85:L5:1954:U:C6    | 2.49                     | 0.48              |
| 85:L5:2057:A:OP1  | 35:LO:18:ARG:NH1   | 2.47                     | 0.48              |
| 85:L5:2323:C:H2'  | 85:L5:2324:C:H6    | 1.77                     | 0.48              |
| 85:L5:2652:G:N2   | 61:Lp:59:SER:O     | 2.46                     | 0.48              |
| 85:L5:2749:C:O3'  | 52:Lg:72:LYS:NZ    | 2.33                     | 0.48              |
| 85:L5:2777:G:H5'' | 85:L5:2778:G:H5'   | 1.94                     | 0.48              |
| 85:L5:3870:C:H2'  | 85:L5:3871:A:H8    | 1.78                     | 0.48              |
| 85:L5:4095:G:H5'' | 85:L5:4110:C:C2    | 2.48                     | 0.48              |
| 85:L5:4102:C:P    | 85:L5:4106:G:O2'   | 2.71                     | 0.48              |
| 85:L5:4608:G:H3'  | 85:L5:4609:G:H8    | 1.77                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 85:L5:4674:C:H2'   | 85:L5:4675:U:C6    | 2.48                     | 0.48              |
| 85:L5:4896:G:O2'   | 85:L5:4897:G:O4'   | 2.31                     | 0.48              |
| 23:LB:63:PRO:HA    | 23:LB:68:ASN:ND2   | 2.28                     | 0.48              |
| 26:LE:242:ILE:HD12 | 26:LE:246:ARG:HD3  | 1.95                     | 0.48              |
| 27:LF:46:ARG:O     | 27:LF:50:ILE:HG12  | 2.13                     | 0.48              |
| 27:LF:85:ALA:H     | 40:LT:138:ALA:HB2  | 1.77                     | 0.48              |
| 27:LF:179:LEU:HD21 | 27:LF:207:PHE:HB2  | 1.95                     | 0.48              |
| 28:LG:88:ASP:OD2   | 28:LG:89:ARG:N     | 2.46                     | 0.48              |
| 37:LQ:172:ARG:NH1  | 46:La:56:VAL:O     | 2.46                     | 0.48              |
| 43:LX:151:ASN:OD1  | 43:LX:156:ILE:HG21 | 2.14                     | 0.48              |
| 46:La:16:SER:OG    | 46:La:20:GLY:N     | 2.47                     | 0.48              |
| 50:Le:70:LEU:HD23  | 50:Le:75:ARG:HA    | 1.95                     | 0.48              |
| 54:Li:7:MET:HE1    | 54:Li:9:VAL:HG23   | 1.94                     | 0.48              |
| 55:Lj:21:ARG:CZ    | 55:Lj:39:TYR:HB2   | 2.43                     | 0.48              |
| 59:Ln:1:MET:SD     | 79:S2:1705:C:O2'   | 2.68                     | 0.48              |
| 65:SD:19:ALA:HA    | 74:Sd:49:ASP:OD1   | 2.14                     | 0.48              |
| 65:SD:214:LYS:HG3  | 65:SD:215:ASP:N    | 2.29                     | 0.48              |
| 66:SF:76:MET:N     | 66:SF:76:MET:SD    | 2.86                     | 0.48              |
| 66:SF:91:ARG:NH2   | 66:SF:92:ILE:HG22  | 2.28                     | 0.48              |
| 67:SK:95:ARG:HD3   | 67:SK:95:ARG:N     | 2.28                     | 0.48              |
| 71:ST:117:GLN:NE2  | 71:ST:118:ASP:OD2  | 2.47                     | 0.48              |
| 75:Sg:44:LYS:O     | 75:Sg:53:GLY:HA2   | 2.14                     | 0.48              |
| 75:Sg:133:ASN:ND2  | 75:Sg:137:VAL:HG22 | 2.28                     | 0.48              |
| 77:SZ:47:LEU:CD2   | 77:SZ:80:ARG:HB2   | 2.43                     | 0.48              |
| 79:S2:952:G:H2'    | 79:S2:953:C:C6     | 2.48                     | 0.48              |
| 79:S2:1114:U:O2'   | 79:S2:1115:U:O5'   | 2.27                     | 0.48              |
| 79:S2:1629:C:H2'   | 79:S2:1630:A:O4'   | 2.14                     | 0.48              |
| 79:S2:1842:C:H2'   | 79:S2:1843:G:H8    | 1.78                     | 0.48              |
| 81:AP:4:U:H2'      | 81:AP:5:C:C6       | 2.48                     | 0.48              |
| 81:AP:25:C:H2'     | 81:AP:26:G:H8      | 1.77                     | 0.48              |
| 87:IW:102:LYS:HA   | 87:IW:105:ARG:HD3  | 1.94                     | 0.48              |
| 87:LW:97:LYS:O     | 87:LW:99:GLU:N     | 2.46                     | 0.48              |
| 2:sE:246:LEU:HD11  | 2:sE:250:GLU:HB2   | 1.95                     | 0.48              |
| 6:sG:3:LEU:N       | 6:sG:16:ILE:O      | 2.33                     | 0.48              |
| 11:sB:89:GLU:HG2   | 11:sB:90:ASP:H     | 1.79                     | 0.48              |
| 11:sB:198:GLU:OE2  | 11:sB:207:LEU:HB2  | 2.14                     | 0.48              |
| 13:sV:4:ASP:HB2    | 15:sC:174:ILE:HG22 | 1.95                     | 0.48              |
| 22:IA:66:PRO:HG2   | 22:IA:67:TYR:CE2   | 2.49                     | 0.48              |
| 22:IA:241:ARG:HG2  | 85:l5:3659:G:OP1   | 2.13                     | 0.48              |
| 24:IC:2:ALA:HB3    | 85:l5:491:G:H5'    | 1.94                     | 0.48              |
| 25:ID:34:LYS:HB2   | 40:IT:27:LEU:CD1   | 2.43                     | 0.48              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:ID:108:ARG:HD3 | 25:ID:112:ARG:NH2  | 2.29                     | 0.48              |
| 28:IG:163:PRO:CD  | 85:I5:150:U:H3     | 2.26                     | 0.48              |
| 30:II:76:MET:CE   | 30:II:80:CYS:HB2   | 2.42                     | 0.48              |
| 32:IL:81:LEU:HB3  | 32:IL:86:ILE:HG23  | 1.95                     | 0.48              |
| 37:IQ:97:LYS:HE2  | 37:IQ:117:GLY:O    | 2.13                     | 0.48              |
| 39:IS:95:ARG:HD2  | 39:IS:97:TYR:OH    | 2.14                     | 0.48              |
| 42:IV:84:GLN:HA   | 42:IV:101:ASN:HA   | 1.95                     | 0.48              |
| 46:la:75:LEU:HG   | 46:la:113:GLY:HA2  | 1.96                     | 0.48              |
| 47:lb:38:LYS:O    | 47:lb:41:ARG:HG2   | 2.14                     | 0.48              |
| 50:le:7:LEU:HB2   | 50:le:93:LYS:HB3   | 1.96                     | 0.48              |
| 52:lg:25:THR:CG2  | 52:lg:29:ARG:HG2   | 2.44                     | 0.48              |
| 52:lg:100:GLN:O   | 52:lg:104:VAL:HG13 | 2.14                     | 0.48              |
| 53:lh:97:LYS:O    | 53:lh:101:ASN:ND2  | 2.46                     | 0.48              |
| 55:lj:21:ARG:NH2  | 55:lj:37:CYS:O     | 2.47                     | 0.48              |
| 62:lr:26:SER:HB2  | 62:lr:28:GLU:OE2   | 2.14                     | 0.48              |
| 63:lz:172:VAL:O   | 63:lz:173:LYS:HG2  | 2.14                     | 0.48              |
| 75:sg:65:PHE:CE1  | 75:sg:83:TRP:CD2   | 3.02                     | 0.48              |
| 79:s2:445:A:H2'   | 79:s2:446:G:C8     | 2.49                     | 0.48              |
| 79:s2:581:U:H3'   | 79:s2:582:U:C6     | 2.49                     | 0.48              |
| 79:s2:610:G:H2'   | 79:s2:611:G:H8     | 1.79                     | 0.48              |
| 79:s2:797:C:O2'   | 79:s2:799:U:OP1    | 2.29                     | 0.48              |
| 79:s2:1563:G:H2'  | 79:s2:1564:C:C6    | 2.48                     | 0.48              |
| 79:s2:1828:C:C2   | 79:s2:1829:G:C8    | 3.02                     | 0.48              |
| 80:cB:430:MET:SD  | 80:cB:430:MET:N    | 2.85                     | 0.48              |
| 80:cB:627:GLU:CD  | 80:cB:628:LEU:N    | 2.71                     | 0.48              |
| 83:ls:13:TYR:O    | 83:ls:17:ILE:HG12  | 2.14                     | 0.48              |
| 84:lt:147:HIS:CD2 | 84:lt:149:HIS:HB2  | 2.49                     | 0.48              |
| 85:l5:1:C:H4'     | 85:l5:2:G:O4'      | 2.14                     | 0.48              |
| 85:l5:273:U:H2'   | 85:l5:274:C:C6     | 2.48                     | 0.48              |
| 85:l5:2481:G:H2'  | 85:l5:2482:C:C6    | 2.48                     | 0.48              |
| 85:l5:3788:C:N4   | 85:l5:3812:C:O4'   | 2.46                     | 0.48              |
| 85:l5:4485:C:H2'  | 85:l5:4486:C:H6    | 1.79                     | 0.48              |
| 85:l5:5058:A:H2'  | 85:l5:5059:C:C6    | 2.48                     | 0.48              |
| 80:CB:256:MET:SD  | 80:CB:260:LEU:HD22 | 2.53                     | 0.48              |
| 80:CB:300:VAL:O   | 80:CB:304:ILE:HG22 | 2.14                     | 0.48              |
| 2:SE:188:ASN:ND2  | 2:SE:218:PHE:HB2   | 2.29                     | 0.48              |
| 10:SA:85:ARG:NH1  | 10:SA:203:PHE:O    | 2.45                     | 0.48              |
| 11:SB:136:ARG:HB3 | 11:SB:216:LYS:HG2  | 1.95                     | 0.48              |
| 14:Sa:2:THR:OG1   | 14:Sa:3:LYS:N      | 2.45                     | 0.48              |
| 85:L5:1081:C:H2'  | 85:L5:1082:C:O4'   | 2.14                     | 0.48              |
| 85:L5:1178:G:H5'' | 85:L5:1180:C:H41   | 1.77                     | 0.48              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 85:L5:1800:U:H2'  | 85:L5:1801:A:C8    | 2.49                     | 0.48              |
| 85:L5:1994:C:O2'  | 84:Lt:131:GLU:HG3  | 2.13                     | 0.48              |
| 85:L5:2461:G:H2'  | 85:L5:2462:C:C6    | 2.49                     | 0.48              |
| 85:L5:2764:A:H2'  | 85:L5:2765:A:C8    | 2.48                     | 0.48              |
| 85:L5:4110:C:H3'  | 85:L5:4111:U:C2'   | 2.33                     | 0.48              |
| 85:L5:4261:C:H2'  | 85:L5:4262:C:C6    | 2.48                     | 0.48              |
| 85:L5:4286:C:H2'  | 85:L5:4287:G:H8    | 1.77                     | 0.48              |
| 85:L5:4517:A:H5'' | 85:L5:4518:A:H5''  | 1.96                     | 0.48              |
| 85:L5:4917:C:H2'  | 85:L5:4918:C:H6    | 1.79                     | 0.48              |
| 85:L5:4938:A:OP1  | 26:LE:183:ARG:NE   | 2.33                     | 0.48              |
| 21:L8:93:C:H3'    | 55:Lj:72:ARG:HH12  | 1.76                     | 0.48              |
| 23:LB:28:LYS:HG2  | 23:LB:30:LYS:HG3   | 1.95                     | 0.48              |
| 23:LB:116:ARG:HA  | 23:LB:122:TRP:CE3  | 2.49                     | 0.48              |
| 26:LE:253:VAL:O   | 26:LE:257:ILE:HG22 | 2.13                     | 0.48              |
| 30:LI:210:ARG:HB2 | 30:LI:210:ARG:HH11 | 1.78                     | 0.48              |
| 31:LJ:38:LYS:HA   | 31:LJ:41:GLU:CD    | 2.37                     | 0.48              |
| 31:LJ:58:ARG:HA   | 31:LJ:61:GLY:HA2   | 1.94                     | 0.48              |
| 31:LJ:120:ASP:O   | 31:LJ:123:ILE:HG12 | 2.14                     | 0.48              |
| 35:LO:186:GLU:N   | 35:LO:186:GLU:OE1  | 2.47                     | 0.48              |
| 36:LP:7:ASP:OD2   | 36:LP:7:ASP:N      | 2.46                     | 0.48              |
| 36:LP:33:ALA:HA   | 36:LP:36:ILE:HG22  | 1.94                     | 0.48              |
| 45:LZ:9:LYS:O     | 45:LZ:25:ILE:HG22  | 2.13                     | 0.48              |
| 45:LZ:81:MET:HE2  | 45:LZ:81:MET:HA    | 1.96                     | 0.48              |
| 65:SD:116:ARG:HD3 | 65:SD:150:MET:HE1  | 1.96                     | 0.48              |
| 65:SD:143:ARG:HD2 | 79:S2:607:U:N3     | 2.29                     | 0.48              |
| 66:SF:88:MET:O    | 66:SF:91:ARG:HG3   | 2.14                     | 0.48              |
| 68:SP:128:HIS:NE2 | 79:S2:1522:A:O4'   | 2.47                     | 0.48              |
| 70:SS:33:ILE:H    | 70:SS:33:ILE:HD12  | 1.77                     | 0.48              |
| 70:SS:113:ARG:HA  | 70:SS:116:LYS:HZ3  | 1.78                     | 0.48              |
| 75:Sg:14:HIS:ND1  | 75:Sg:41:ILE:HD13  | 2.28                     | 0.48              |
| 75:Sg:132:TRP:CE2 | 75:Sg:138:CYS:HB2  | 2.49                     | 0.48              |
| 79:S2:107:A:H2'   | 79:S2:108:G:H8     | 1.76                     | 0.48              |
| 79:S2:656:G:N2    | 79:S2:663:C:H5''   | 2.28                     | 0.48              |
| 79:S2:1846:G:H2'  | 79:S2:1847:G:H8    | 1.77                     | 0.48              |
| 84:Lt:16:ARG:HH12 | 84:Lt:32:ILE:HD13  | 1.78                     | 0.48              |
| 84:Lt:63:THR:HG23 | 84:Lt:70:GLN:HB2   | 1.95                     | 0.48              |
| 1:cH:102:LYS:O    | 1:cH:105:VAL:HG22  | 2.13                     | 0.48              |
| 3:sI:98:LYS:O     | 3:sI:175:ILE:HG23  | 2.14                     | 0.48              |
| 6:sG:217:MET:N    | 6:sG:219:GLU:OE2   | 2.46                     | 0.48              |
| 7:sJ:88:ASP:HB3   | 7:sJ:91:LYS:HG2    | 1.96                     | 0.48              |
| 9:se:38:TYR:C     | 9:se:38:TYR:CD1    | 2.92                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:sA:120:ARG:HE   | 15:sC:65:LYS:HZ1   | 1.59                     | 0.48              |
| 14:sa:13:LYS:NZ    | 79:s2:1132:C:H2'   | 2.28                     | 0.48              |
| 15:sC:66:LEU:HA    | 15:sC:69:LEU:HD12  | 1.94                     | 0.48              |
| 15:sC:167:ARG:HG3  | 15:sC:167:ARG:HH11 | 1.78                     | 0.48              |
| 15:sC:267:GLN:OE1  | 15:sC:267:GLN:N    | 2.37                     | 0.48              |
| 31:IJ:18:ARG:HB3   | 31:IJ:133:VAL:HG23 | 1.95                     | 0.48              |
| 34:IN:135:ILE:HD11 | 34:IN:142:ILE:CD1  | 2.43                     | 0.48              |
| 36:IP:83:TRP:O     | 85:l5:3856:A:H5''  | 2.13                     | 0.48              |
| 36:IP:133:HIS:HA   | 85:l5:1600:A:H5'   | 1.95                     | 0.48              |
| 42:IV:90:ARG:HH12  | 42:IV:123:LYS:CB   | 2.24                     | 0.48              |
| 52:lg:26:PRO:HD2   | 85:l5:2521:G:H4'   | 1.96                     | 0.48              |
| 58:lm:110:CYS:HB3  | 58:lm:115:CYS:SG   | 2.53                     | 0.48              |
| 62:lr:37:SER:HG    | 62:lr:40:TYR:H     | 1.60                     | 0.48              |
| 62:lr:103:ARG:NE   | 62:lr:106:LEU:HD11 | 2.29                     | 0.48              |
| 64:sR:14:ARG:HB2   | 79:s2:1373:C:H4'   | 1.95                     | 0.48              |
| 64:sR:36:GLU:O     | 64:sR:47:ARG:NH2   | 2.46                     | 0.48              |
| 68:sP:108:LYS:HZ3  | 68:sP:110:GLU:H    | 1.62                     | 0.48              |
| 72:sU:18:HIS:CE1   | 72:sU:95:SER:H     | 2.31                     | 0.48              |
| 75:sg:34:ALA:HA    | 75:sg:40:ILE:HD13  | 1.95                     | 0.48              |
| 76:sM:33:ARG:CZ    | 79:s2:1284:A:C8    | 2.97                     | 0.48              |
| 79:s2:2:A:OP2      | 79:s2:418:A:H5'    | 2.14                     | 0.48              |
| 79:s2:494:C:N4     | 79:s2:509:G:H21    | 2.12                     | 0.48              |
| 79:s2:1201:U:H2'   | 79:s2:1202:U:H6    | 1.77                     | 0.48              |
| 79:s2:1461:G:H3'   | 79:s2:1463:U:H3    | 1.78                     | 0.48              |
| 79:s2:1566:G:N2    | 79:s2:1569:A:OP2   | 2.45                     | 0.48              |
| 81:aP:42:A:H2'     | 81:aP:43:A:C8      | 2.46                     | 0.48              |
| 83:ls:84:GLY:HA2   | 85:l5:2022:C:H5'   | 1.95                     | 0.48              |
| 85:l5:1327:C:H2'   | 85:l5:1328:G:C8    | 2.48                     | 0.48              |
| 85:l5:2249:C:H2'   | 85:l5:2250:C:H5    | 1.79                     | 0.48              |
| 85:l5:2402:G:C2    | 85:l5:2403:A:C8    | 3.01                     | 0.48              |
| 85:l5:2479:G:H2'   | 85:l5:2480:G:C8    | 2.48                     | 0.48              |
| 85:l5:2569:G:H2'   | 85:l5:2570:U:H6    | 1.76                     | 0.48              |
| 85:l5:2817:C:H2'   | 85:l5:2818:C:C6    | 2.49                     | 0.48              |
| 85:l5:4095:G:H5''  | 85:l5:4096:C:OP1   | 2.14                     | 0.48              |
| 85:l5:4538:G:H2'   | 85:l5:4539:U:H6    | 1.78                     | 0.48              |
| 85:l5:4974:C:N4    | 85:l5:4975:G:O6    | 2.46                     | 0.48              |
| 80:CB:25:ILE:HB    | 80:CB:142:VAL:HG21 | 1.95                     | 0.48              |
| 80:CB:74:ALA:HB3   | 80:CB:453:MET:SD   | 2.54                     | 0.48              |
| 80:CB:160:MET:O    | 80:CB:164:LEU:HG   | 2.14                     | 0.48              |
| 6:SG:190:ARG:O     | 6:SG:194:LEU:HG    | 2.14                     | 0.48              |
| 7:SJ:126:ALA:O     | 7:SJ:130:ILE:HG13  | 2.12                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:SA:52:LYS:HZ2  | 10:SA:53:ARG:HE   | 1.61                     | 0.48              |
| 12:SH:26:ALA:HB1  | 12:SH:87:PHE:HZ   | 1.78                     | 0.48              |
| 16:SN:4:MET:SD    | 16:SN:5:HIS:CD2   | 3.07                     | 0.48              |
| 85:L5:36:U:H2'    | 85:L5:37:U:C6     | 2.48                     | 0.48              |
| 85:L5:108:A:N1    | 85:L5:333:U:O2'   | 2.43                     | 0.48              |
| 85:L5:204:U:H3    | 85:L5:211:G:H1    | 1.62                     | 0.48              |
| 85:L5:500:G:O5'   | 85:L5:504:G:N2    | 2.47                     | 0.48              |
| 85:L5:513:U:C2    | 85:L5:515:C:H5''  | 2.49                     | 0.48              |
| 85:L5:724:C:H1'   | 24:LC:343:GLN:CD  | 2.39                     | 0.48              |
| 85:L5:978:G:H4'   | 26:LE:45:SER:OG   | 2.14                     | 0.48              |
| 85:L5:1863:U:H2'  | 85:L5:1864:G:C8   | 2.49                     | 0.48              |
| 85:L5:2361:G:H22  | 85:L5:3859:G:H3'  | 1.78                     | 0.48              |
| 85:L5:2528:G:H4'  | 85:L5:2783:A:H4'  | 1.95                     | 0.48              |
| 85:L5:2674:A:N6   | 61:Lp:42:CYS:HA   | 2.28                     | 0.48              |
| 85:L5:3671:G:H2'  | 85:L5:3672:G:N3   | 2.28                     | 0.48              |
| 85:L5:3966:A:N6   | 85:L5:4057:C:O2   | 2.46                     | 0.48              |
| 85:L5:4079:C:H2'  | 85:L5:4080:C:H6   | 1.79                     | 0.48              |
| 85:L5:4503:A:H2'  | 85:L5:4504:C:C6   | 2.48                     | 0.48              |
| 21:L8:71:A:OP2    | 44:LY:50:ARG:NE   | 2.46                     | 0.48              |
| 22:LA:5:ILE:HG12  | 22:LA:8:GLN:OE1   | 2.13                     | 0.48              |
| 24:LC:254:GLU:O   | 24:LC:258:ARG:HG2 | 2.13                     | 0.48              |
| 27:LF:63:GLN:NE2  | 27:LF:67:THR:HG23 | 2.29                     | 0.48              |
| 28:LG:142:THR:O   | 28:LG:146:LEU:HG  | 2.14                     | 0.48              |
| 31:LJ:28:GLU:HG2  | 31:LJ:32:ARG:NH2  | 2.29                     | 0.48              |
| 31:LJ:158:SER:H   | 31:LJ:161:GLU:CD  | 2.21                     | 0.48              |
| 33:LM:31:ILE:HA   | 39:LS:98:ARG:HH21 | 1.79                     | 0.48              |
| 47:Lb:60:ASN:O    | 47:Lb:63:LYS:HG3  | 2.14                     | 0.48              |
| 48:Lc:45:LEU:HD12 | 48:Lc:46:VAL:N    | 2.28                     | 0.48              |
| 49:Ld:19:GLU:O    | 49:Ld:90:ARG:NE   | 2.39                     | 0.48              |
| 56:Lk:8:ILE:HD12  | 56:Lk:11:PHE:HB3  | 1.96                     | 0.48              |
| 66:SF:32:ASP:O    | 66:SF:36:GLN:NE2  | 2.47                     | 0.48              |
| 68:SP:38:SER:OG   | 68:SP:41:GLN:OE1  | 2.31                     | 0.48              |
| 71:ST:34:VAL:HG13 | 71:ST:35:ASP:OD1  | 2.13                     | 0.48              |
| 71:ST:98:SER:OG   | 79:S2:1567:G:O3'  | 2.31                     | 0.48              |
| 76:SM:62:VAL:HA   | 76:SM:65:VAL:HG22 | 1.95                     | 0.48              |
| 76:SM:84:LYS:O    | 76:SM:88:TRP:CD1  | 2.67                     | 0.48              |
| 79:S2:59:U:N3     | 79:S2:62:G:OP1    | 2.38                     | 0.48              |
| 79:S2:558:G:O2'   | 79:S2:559:G:OP2   | 2.26                     | 0.48              |
| 79:S2:1215:C:H5   | 79:S2:1645:C:H2'  | 1.79                     | 0.48              |
| 79:S2:1515:G:H2'  | 79:S2:1516:G:H8   | 1.79                     | 0.48              |
| 79:S2:1547:C:H3'  | 79:S2:1548:G:H8   | 1.79                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 79:S2:1650:A:H1'   | 79:S2:1675:A:N6    | 2.28                     | 0.48              |
| 87:IW:87:LEU:HD13  | 87:IW:90:ILE:HD11  | 1.96                     | 0.48              |
| 1:cH:75:LEU:HG     | 1:cH:79:LYS:HZ3    | 1.78                     | 0.48              |
| 3:sI:120:PRO:O     | 3:sI:121:LEU:HD13  | 2.14                     | 0.48              |
| 7:sJ:97:ILE:O      | 7:sJ:100:LEU:HG    | 2.13                     | 0.48              |
| 14:sa:3:LYS:NZ     | 14:sa:5:ARG:H      | 2.06                     | 0.48              |
| 21:l8:51:U:O3'     | 57:l1:21:ARG:NH2   | 2.43                     | 0.48              |
| 23:lB:144:LYS:C    | 23:lB:148:LYS:NZ   | 2.72                     | 0.48              |
| 23:lB:305:THR:HG21 | 23:lB:367:PHE:HA   | 1.96                     | 0.48              |
| 34:lN:195:ARG:HH12 | 85:l5:98:A:H5'     | 1.78                     | 0.48              |
| 37:lQ:90:VAL:HB    | 46:la:80:THR:HG21  | 1.96                     | 0.48              |
| 41:lU:81:ARG:NH2   | 85:l5:2622:G:O6    | 2.46                     | 0.48              |
| 42:lV:115:SER:C    | 42:lV:135:ASN:HD21 | 2.22                     | 0.48              |
| 43:lX:129:ARG:NH2  | 43:lX:131:ASP:OD2  | 2.46                     | 0.48              |
| 44:lY:126:ARG:HH21 | 85:l5:197:A:P      | 2.36                     | 0.48              |
| 46:la:36:GLY:HA3   | 46:la:40:HIS:CE1   | 2.48                     | 0.48              |
| 49:ld:36:VAL:O     | 49:ld:41:ARG:NH1   | 2.46                     | 0.48              |
| 51:lf:46:ARG:HD2   | 51:lf:106:TYR:HD2  | 1.79                     | 0.48              |
| 53:lh:93:ARG:NH2   | 85:l5:19:G:OP2     | 2.44                     | 0.48              |
| 55:lj:12:ARG:HH11  | 85:l5:2404:A:H1'   | 1.79                     | 0.48              |
| 64:sR:53:TYR:CD2   | 79:s2:1465:A:C8    | 3.02                     | 0.48              |
| 70:sS:55:ARG:NH2   | 77:sZ:47:LEU:O     | 2.46                     | 0.48              |
| 72:sU:44:LYS:HE3   | 72:sU:44:LYS:HB2   | 1.65                     | 0.48              |
| 75:sg:8:ARG:O      | 75:sg:309:VAL:HB   | 2.14                     | 0.48              |
| 76:sM:41:ALA:O     | 76:sM:44:LYS:HG2   | 2.13                     | 0.48              |
| 79:s2:573:U:H1'    | 79:s2:576:A:N7     | 2.29                     | 0.48              |
| 79:s2:678:U:OP2    | 79:s2:1026:C:N4    | 2.44                     | 0.48              |
| 79:s2:1334:G:H2'   | 79:s2:1335:G:C8    | 2.49                     | 0.48              |
| 79:s2:1661:A:C4    | 79:s2:1662:U:C5    | 3.02                     | 0.48              |
| 79:s2:1807:C:H2'   | 79:s2:1808:U:C6    | 2.49                     | 0.48              |
| 80:cB:28:VAL:HG21  | 85:l5:4606:G:H5''  | 1.95                     | 0.48              |
| 80:cB:205:ILE:HD12 | 80:cB:211:THR:HG23 | 1.96                     | 0.48              |
| 80:cB:428:ARG:NH1  | 80:cB:489:GLU:OE1  | 2.46                     | 0.48              |
| 80:cB:665:ILE:HD11 | 80:cB:705:HIS:CE1  | 2.49                     | 0.48              |
| 80:cB:670:GLN:CD   | 80:cB:670:GLN:H    | 2.22                     | 0.48              |
| 80:cB:685:TRP:CD2  | 80:cB:726:ARG:HD3  | 2.49                     | 0.48              |
| 80:cB:761:GLY:O    | 80:cB:765:ARG:NE   | 2.41                     | 0.48              |
| 83:ls:57:LYS:H     | 83:ls:60:MET:HE1   | 1.78                     | 0.48              |
| 83:ls:58:ASN:HD21  | 85:l5:2022:C:P     | 2.34                     | 0.48              |
| 85:l5:500:G:N3     | 85:l5:504:G:H2'    | 2.28                     | 0.48              |
| 85:l5:923:C:H2'    | 85:l5:925:C:H5     | 1.78                     | 0.48              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 85:L5:1079:C:H2'  | 85:L5:1080:C:C6    | 2.49                     | 0.48              |
| 85:L5:1081:C:H2'  | 85:L5:1082:C:O4'   | 2.13                     | 0.48              |
| 85:L5:1441:C:C2   | 85:L5:1442:C:H5    | 2.32                     | 0.48              |
| 85:L5:1893:C:H1'  | 85:L5:1937:C:O2    | 2.13                     | 0.48              |
| 85:L5:2004:U:H2'  | 85:L5:2005:G:C8    | 2.49                     | 0.48              |
| 85:L5:2508:U:H2'  | 85:L5:2509:C:C6    | 2.49                     | 0.48              |
| 85:L5:3711:A:HO2' | 85:L5:3712:A:H8    | 1.61                     | 0.48              |
| 85:L5:3835:C:H2'  | 85:L5:3836:A:C8    | 2.49                     | 0.48              |
| 85:L5:4344:U:H2'  | 85:L5:4345:C:C6    | 2.49                     | 0.48              |
| 85:L5:4458:C:H2'  | 85:L5:4459:U:C6    | 2.49                     | 0.48              |
| 85:L5:4586:G:C6   | 85:L5:4717:A:C6    | 3.02                     | 0.48              |
| 85:L5:5050:C:C2   | 85:L5:5051:C:C5    | 3.02                     | 0.48              |
| 80:CB:111:PHE:CD2 | 80:CB:501:VAL:HG22 | 2.49                     | 0.48              |
| 2:SE:180:LEU:O    | 2:SE:227:VAL:HG23  | 2.14                     | 0.48              |
| 2:SE:241:GLY:O    | 2:SE:244:ILE:HG22  | 2.14                     | 0.48              |
| 7:SJ:65:GLU:OE1   | 7:SJ:70:ARG:NE     | 2.46                     | 0.48              |
| 11:SB:60:ASP:HA   | 11:SB:63:LYS:HG2   | 1.95                     | 0.48              |
| 11:SB:66:VAL:HG13 | 11:SB:85:LYS:HB3   | 1.95                     | 0.48              |
| 14:Sa:12:LYS:HB2  | 14:Sa:33:ASP:OD2   | 2.13                     | 0.48              |
| 85:L5:6:C:H2'     | 85:L5:7:C:C6       | 2.48                     | 0.48              |
| 85:L5:294:G:OP2   | 85:L5:296:A:O2'    | 2.26                     | 0.48              |
| 85:L5:655:C:H2'   | 85:L5:656:C:C2     | 2.49                     | 0.48              |
| 85:L5:739:G:O2'   | 85:L5:740:G:H5''   | 2.14                     | 0.48              |
| 85:L5:1316:G:H2'  | 85:L5:1317:U:C6    | 2.49                     | 0.48              |
| 85:L5:1602:U:H2'  | 85:L5:1603:C:H6    | 1.79                     | 0.48              |
| 85:L5:2074:C:C2   | 85:L5:2075:G:C8    | 3.02                     | 0.48              |
| 85:L5:2483:G:H1   | 85:L5:2495:U:H3    | 1.61                     | 0.48              |
| 85:L5:2501:C:H2'  | 85:L5:2502:G:C8    | 2.49                     | 0.48              |
| 85:L5:2518:G:H1'  | 85:L5:2539:C:H1'   | 1.94                     | 0.48              |
| 85:L5:2705:G:H1   | 85:L5:2710:C:N4    | 2.11                     | 0.48              |
| 85:L5:2727:C:H2'  | 85:L5:2728:U:C6    | 2.49                     | 0.48              |
| 85:L5:2824:C:H2'  | 85:L5:2825:A:C8    | 2.48                     | 0.48              |
| 85:L5:2852:U:N3   | 85:L5:2855:G:OP2   | 2.32                     | 0.48              |
| 85:L5:3911:C:H2'  | 85:L5:3912:U:C6    | 2.49                     | 0.48              |
| 85:L5:3951:G:N2   | 85:L5:4062:A:C6    | 2.82                     | 0.48              |
| 85:L5:4122:G:C6   | 85:L5:4123:C:C4    | 3.02                     | 0.48              |
| 85:L5:4254:G:H2'  | 85:L5:4254:G:N3    | 2.29                     | 0.48              |
| 85:L5:4390:A:H2'  | 85:L5:4391:G:O4'   | 2.13                     | 0.48              |
| 85:L5:4425:G:OP1  | 58:Lm:100:TYR:OH   | 2.22                     | 0.48              |
| 85:L5:5051:C:H4'  | 23:LB:324:GLY:HA2  | 1.96                     | 0.48              |
| 23:LB:80:GLU:HG3  | 23:LB:82:PRO:HD3   | 1.96                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:LD:224:SER:O    | 25:LD:227:ILE:HG12 | 2.13                     | 0.48              |
| 30:LI:97:ILE:C     | 30:LI:97:ILE:HD12  | 2.39                     | 0.48              |
| 31:LJ:135:GLY:HA2  | 31:LJ:139:PHE:CE1  | 2.49                     | 0.48              |
| 32:LL:186:ARG:O    | 32:LL:190:ARG:HG2  | 2.14                     | 0.48              |
| 35:LO:187:LYS:HD3  | 35:LO:187:LYS:H    | 1.77                     | 0.48              |
| 37:LQ:130:SER:OG   | 37:LQ:134:CYS:N    | 2.45                     | 0.48              |
| 39:LS:83:ARG:HD3   | 39:LS:125:GLN:NE2  | 2.29                     | 0.48              |
| 49:Ld:51:LYS:HG2   | 49:Ld:55:LYS:HE3   | 1.95                     | 0.48              |
| 50:Le:107:ASN:O    | 50:Le:111:ILE:HG12 | 2.14                     | 0.48              |
| 53:Lh:88:THR:HB    | 53:Lh:91:MET:CG    | 2.44                     | 0.48              |
| 60:Lo:7:THR:OG1    | 60:Lo:21:HIS:O     | 2.27                     | 0.48              |
| 63:Lz:68:LEU:HB3   | 63:Lz:116:LEU:CD2  | 2.44                     | 0.48              |
| 63:Lz:120:ILE:HB   | 63:Lz:121:PRO:HD3  | 1.94                     | 0.48              |
| 63:Lz:205:TYR:HA   | 63:Lz:215:ARG:NH1  | 2.29                     | 0.48              |
| 64:SR:75:GLU:HG2   | 64:SR:76:GLU:N     | 2.29                     | 0.48              |
| 66:SF:82:ASN:OD1   | 66:SF:82:ASN:N     | 2.47                     | 0.48              |
| 72:SU:107:GLU:HG3  | 72:SU:110:VAL:HG22 | 1.94                     | 0.48              |
| 78:Sf:102:VAL:HG23 | 78:Sf:104:LYS:HZ2  | 1.78                     | 0.48              |
| 79:S2:422:U:H2'    | 79:S2:423:U:C6     | 2.49                     | 0.48              |
| 79:S2:644:G:H2'    | 79:S2:645:C:H6     | 1.78                     | 0.48              |
| 79:S2:806:U:H2'    | 79:S2:807:G:C8     | 2.48                     | 0.48              |
| 79:S2:815:U:C2     | 79:S2:816:A:C8     | 3.02                     | 0.48              |
| 79:S2:1523:C:H2'   | 79:S2:1524:G:C8    | 2.45                     | 0.48              |
| 79:S2:1617:G:H2'   | 79:S2:1619:A:OP2   | 2.14                     | 0.48              |
| 87:LW:45:ASN:HD21  | 87:LW:47:ARG:HD3   | 1.79                     | 0.48              |
| 1:CH:119:GLN:HG3   | 1:CH:120:VAL:N     | 2.28                     | 0.48              |
| 1:cH:50:LYS:HA     | 79:s2:607:U:OP1    | 2.14                     | 0.48              |
| 2:sE:15:PRO:CD     | 2:sE:18:TRP:CZ3    | 2.96                     | 0.48              |
| 4:sL:104:LYS:HE3   | 79:s2:399:C:C4     | 2.48                     | 0.48              |
| 6:sG:6:SER:HB3     | 6:sG:112:VAL:HG12  | 1.96                     | 0.48              |
| 7:sJ:12:THR:HG22   | 79:s2:520:A:OP1    | 2.14                     | 0.48              |
| 8:sY:4:THR:O       | 8:sY:32:LYS:NZ     | 2.45                     | 0.48              |
| 14:sa:3:LYS:HE3    | 14:sa:5:ARG:O      | 2.13                     | 0.48              |
| 17:sO:138:ASP:O    | 79:s2:984:C:O2'    | 2.32                     | 0.48              |
| 21:l8:55:U:C2      | 21:l8:56:G:C8      | 3.02                     | 0.48              |
| 25:ID:132:VAL:HG11 | 25:ID:170:GLY:HA2  | 1.94                     | 0.48              |
| 30:II:8:CYS:C      | 30:II:9:TYR:HD1    | 2.22                     | 0.48              |
| 31:IJ:94:LEU:HD23  | 31:IJ:94:LEU:C     | 2.39                     | 0.48              |
| 33:IM:39:ASP:OD1   | 33:IM:47:ARG:NE    | 2.39                     | 0.48              |
| 46:la:118:PRO:HG2  | 46:la:120:GLN:HE22 | 1.78                     | 0.48              |
| 48:lc:45:LEU:HB3   | 48:lc:96:ILE:HD11  | 1.96                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 49:ld:46:LEU:O     | 49:ld:49:ILE:HG12  | 2.14                     | 0.48              |
| 60:lo:2:VAL:N      | 60:lo:90:HIS:O     | 2.47                     | 0.48              |
| 63:lz:24:LYS:HE3   | 63:lz:173:LYS:HA   | 1.96                     | 0.48              |
| 64:sR:10:LYS:HG2   | 79:s2:1366:G:C2    | 2.49                     | 0.48              |
| 66:sF:194:ASP:N    | 66:sF:194:ASP:OD2  | 2.46                     | 0.48              |
| 67:sK:29:MET:HG3   | 67:sK:42:ASN:ND2   | 2.27                     | 0.48              |
| 67:sK:60:GLU:HB2   | 67:sK:69:TRP:CD1   | 2.48                     | 0.48              |
| 68:sP:87:PRO:HD3   | 68:sP:112:ILE:HG23 | 1.95                     | 0.48              |
| 70:sS:5:ILE:HG23   | 70:sS:9:PHE:CD2    | 2.49                     | 0.48              |
| 71:sT:31:PRO:HD2   | 71:sT:53:PHE:CE2   | 2.44                     | 0.48              |
| 72:sU:36:CYS:O     | 72:sU:40:ILE:HG23  | 2.14                     | 0.48              |
| 73:sc:13:ARG:HH21  | 73:sc:54:ASP:C     | 2.22                     | 0.48              |
| 75:sg:121:VAL:HG12 | 75:sg:131:LEU:HD13 | 1.96                     | 0.48              |
| 79:s2:28:U:H2'     | 79:s2:29:G:H8      | 1.78                     | 0.48              |
| 79:s2:1097:G:H2'   | 79:s2:1098:C:C6    | 2.48                     | 0.48              |
| 79:s2:1808:U:C2    | 79:s2:1809:A:N7    | 2.82                     | 0.48              |
| 80:cB:10:ARG:O     | 80:cB:14:ASP:OD1   | 2.32                     | 0.48              |
| 80:cB:123:ASP:CG   | 80:cB:415:ARG:HH12 | 2.22                     | 0.48              |
| 80:cB:607:ARG:HH21 | 80:cB:701:ARG:NH1  | 2.11                     | 0.48              |
| 82:pE:43:A:H2'     | 82:pE:44:G:C8      | 2.49                     | 0.48              |
| 83:ls:118:PRO:HA   | 83:ls:164:GLY:N    | 2.29                     | 0.48              |
| 85:l5:197:A:N6     | 85:l5:242:U:H3     | 2.11                     | 0.48              |
| 85:l5:281:U:H2'    | 85:l5:282:C:H6     | 1.79                     | 0.48              |
| 85:l5:324:A:H2'    | 85:l5:325:U:C6     | 2.48                     | 0.48              |
| 85:l5:1566:C:H2'   | 85:l5:1567:U:H6    | 1.79                     | 0.48              |
| 85:l5:2072:C:C2    | 85:l5:2073:C:C5    | 3.02                     | 0.48              |
| 85:l5:2576:G:C6    | 85:l5:2588:C:C4    | 3.02                     | 0.48              |
| 85:l5:2747:U:H2'   | 85:l5:2748:C:C6    | 2.49                     | 0.48              |
| 85:l5:3702:A:C6    | 85:l5:3703:G:C8    | 3.02                     | 0.48              |
| 85:l5:3951:G:N2    | 85:l5:4062:A:C6    | 2.82                     | 0.48              |
| 85:l5:4592:C:H2'   | 85:l5:4593:C:H6    | 1.79                     | 0.48              |
| 85:l5:4723:A:H2'   | 85:l5:4724:A:H8    | 1.79                     | 0.48              |
| 85:l5:4926:C:H3'   | 85:l5:4927:G:N3    | 2.29                     | 0.48              |
| 80:CB:353:MET:SD   | 80:CB:354:ILE:N    | 2.87                     | 0.48              |
| 80:CB:400:LYS:HG2  | 80:CB:402:VAL:CG1  | 2.44                     | 0.48              |
| 80:CB:838:THR:HG22 | 80:CB:842:LYS:HD2  | 1.95                     | 0.48              |
| 2:SE:255:ARG:HH21  | 2:SE:256:LEU:HD23  | 1.79                     | 0.48              |
| 6:SG:146:ASN:OD1   | 87:LW:94:ARG:NH1   | 2.46                     | 0.48              |
| 11:SB:146:ARG:NH2  | 79:S2:1122:A:N3    | 2.62                     | 0.48              |
| 14:Sa:74:CYS:SG    | 14:Sa:77:CYS:CB    | 2.81                     | 0.48              |
| 15:SC:209:VAL:HG21 | 15:SC:233:LEU:HD13 | 1.95                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 19:Sb:36:LYS:O     | 19:Sb:77:CYS:HB3   | 2.14                     | 0.48              |
| 85:L5:151:G:H3'    | 34:LN:49:ARG:HH12  | 1.79                     | 0.48              |
| 85:L5:154:G:H2'    | 85:L5:155:C:H6     | 1.79                     | 0.48              |
| 85:L5:240:G:H5'    | 44:LY:31:SER:OG    | 2.14                     | 0.48              |
| 85:L5:341:G:C2     | 85:L5:342:G:C8     | 3.02                     | 0.48              |
| 85:L5:451:C:O2'    | 85:L5:1293:G:H2'   | 2.14                     | 0.48              |
| 85:L5:920:C:H5''   | 39:LS:74:ARG:NH1   | 2.29                     | 0.48              |
| 85:L5:1196:G:H2'   | 85:L5:1197:C:C6    | 2.49                     | 0.48              |
| 85:L5:1322:A:O2'   | 85:L5:1324:A:OP2   | 2.31                     | 0.48              |
| 85:L5:1407:C:O2'   | 85:L5:1408:G:H5'   | 2.14                     | 0.48              |
| 85:L5:2540:C:H2'   | 85:L5:2541:G:H8    | 1.78                     | 0.48              |
| 85:L5:3906:A:O2'   | 85:L5:3907:G:OP2   | 2.31                     | 0.48              |
| 85:L5:3923:A:H2'   | 85:L5:3924:C:H6    | 1.79                     | 0.48              |
| 85:L5:4540:C:H2'   | 85:L5:4541:G:C8    | 2.49                     | 0.48              |
| 20:L7:1:G:H2'      | 20:L7:2:U:O4'      | 2.13                     | 0.48              |
| 22:LA:201:GLY:O    | 22:LA:204:MET:HB2  | 2.14                     | 0.48              |
| 23:LB:125:SER:OG   | 23:LB:126:LYS:N    | 2.47                     | 0.48              |
| 25:LD:235:MET:O    | 25:LD:235:MET:HE2  | 2.14                     | 0.48              |
| 31:LJ:52:LYS:NZ    | 60:Lo:101:GLY:O    | 2.47                     | 0.48              |
| 37:LQ:121:LEU:HD13 | 37:LQ:125:GLN:HG3  | 1.95                     | 0.48              |
| 39:LS:15:ARG:HD2   | 39:LS:25:PRO:HG2   | 1.96                     | 0.48              |
| 51:Lf:83:MET:HA    | 51:Lf:83:MET:HE3   | 1.96                     | 0.48              |
| 64:SR:117:LEU:HA   | 64:SR:117:LEU:HD12 | 1.44                     | 0.48              |
| 65:SD:54:ARG:O     | 65:SD:58:VAL:HG23  | 2.13                     | 0.48              |
| 66:SF:99:ILE:O     | 66:SF:102:LEU:HD12 | 2.14                     | 0.48              |
| 68:SP:17:TYR:CD1   | 68:SP:112:ILE:HD13 | 2.49                     | 0.48              |
| 74:Sd:21:CYS:HA    | 74:Sd:38:MET:HA    | 1.96                     | 0.48              |
| 75:Sg:126:ASP:O    | 75:Sg:128:THR:HG22 | 2.13                     | 0.48              |
| 79:S2:149:A:C2     | 79:S2:150:A:H1'    | 2.48                     | 0.48              |
| 79:S2:363:A:N1     | 79:S2:397:G:O2'    | 2.47                     | 0.48              |
| 79:S2:441:C:H2'    | 79:S2:442:C:C6     | 2.49                     | 0.48              |
| 79:S2:1035:A:C4    | 79:S2:1036:A:C8    | 3.02                     | 0.48              |
| 6:sG:159:ARG:CZ    | 79:s2:76:U:H2'     | 2.43                     | 0.48              |
| 7:sJ:49:THR:O      | 7:sJ:53:ILE:HG23   | 2.13                     | 0.48              |
| 8:sY:53:ASP:OD2    | 28:LG:232:GLU:HG3  | 2.14                     | 0.48              |
| 8:sY:94:HIS:ND1    | 8:sY:94:HIS:O      | 2.47                     | 0.48              |
| 10:sA:26:GLY:O     | 10:sA:150:THR:OG1  | 2.19                     | 0.48              |
| 11:sB:185:VAL:HA   | 11:sB:188:LEU:HB3  | 1.96                     | 0.48              |
| 12:sH:43:LEU:HB3   | 12:sH:72:PHE:CE1   | 2.48                     | 0.48              |
| 12:sH:145:ARG:NH1  | 12:sH:145:ARG:HA   | 2.29                     | 0.48              |
| 15:sC:216:MET:SD   | 15:sC:216:MET:C    | 2.97                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 21:l8:52:A:O4'     | 57:l1:21:ARG:NH2   | 2.45                     | 0.48              |
| 23:lB:173:LEU:HD21 | 23:lB:175:GLN:HB3  | 1.96                     | 0.48              |
| 25:lD:164:LYS:HA   | 25:lD:167:VAL:HG22 | 1.95                     | 0.48              |
| 25:lD:259:LYS:HD3  | 25:lD:259:LYS:N    | 2.27                     | 0.48              |
| 26:lE:211:HIS:HE2  | 26:lE:249:ASP:CG   | 2.21                     | 0.48              |
| 26:lE:270:TYR:HD1  | 33:lM:110:PHE:CD1  | 2.31                     | 0.48              |
| 28:lG:197:LYS:NZ   | 85:l5:148:C:OP2    | 2.47                     | 0.48              |
| 31:lJ:31:ASP:O     | 31:lJ:34:THR:OG1   | 2.26                     | 0.48              |
| 31:lJ:98:ASN:HD21  | 31:lJ:107:PHE:HB3  | 1.78                     | 0.48              |
| 34:lN:34:SER:OG    | 34:lN:35:ALA:N     | 2.45                     | 0.48              |
| 36:lP:107:LEU:HD12 | 36:lP:108:ASP:H    | 1.78                     | 0.48              |
| 37:lQ:37:ARG:NE    | 85:l5:2087:C:OP2   | 2.43                     | 0.48              |
| 37:lQ:106:THR:HG23 | 37:lQ:109:ALA:H    | 1.79                     | 0.48              |
| 44:lY:84:ARG:HH21  | 44:lY:86:GLN:HE22  | 1.61                     | 0.48              |
| 48:lc:50:ASN:HD21  | 48:lc:75:SER:HA    | 1.78                     | 0.48              |
| 63:lz:107:TYR:CE1  | 63:lz:110:PHE:CD1  | 3.01                     | 0.48              |
| 64:sR:29:HIS:H     | 79:s2:1455:A:C4'   | 2.27                     | 0.48              |
| 64:sR:65:PRO:HB3   | 64:sR:73:LEU:HD22  | 1.96                     | 0.48              |
| 74:sd:6:LEU:HD21   | 79:s2:1301:A:H4'   | 1.95                     | 0.48              |
| 74:sd:32:ARG:NH1   | 79:s2:1661:A:OP2   | 2.44                     | 0.48              |
| 75:sg:22:ALA:O     | 75:sg:32:LEU:HD21  | 2.14                     | 0.48              |
| 75:sg:72:SER:OG    | 75:sg:77:PHE:HB2   | 2.14                     | 0.48              |
| 79:s2:42:A:H2'     | 79:s2:43:U:C6      | 2.49                     | 0.48              |
| 79:s2:498:C:N4     | 79:s2:499:G:O6     | 2.46                     | 0.48              |
| 79:s2:557:U:H2'    | 79:s2:558:G:N9     | 2.29                     | 0.48              |
| 79:s2:925:G:C2     | 79:s2:1018:U:C2    | 3.02                     | 0.48              |
| 79:s2:1280:G:H2'   | 79:s2:1281:G:H8    | 1.79                     | 0.48              |
| 79:s2:1723:G:H1    | 79:s2:1810:U:H3    | 1.62                     | 0.48              |
| 80:cB:83:GLU:HA    | 80:cB:86:LEU:HD13  | 1.96                     | 0.48              |
| 80:cB:406:ASP:OD1  | 80:cB:407:LYS:N    | 2.41                     | 0.48              |
| 83:ls:47:LEU:HD12  | 83:ls:51:ALA:HB3   | 1.95                     | 0.48              |
| 85:l5:180:C:H2'    | 85:l5:181:C:H4'    | 1.96                     | 0.48              |
| 85:l5:490:C:H2'    | 85:l5:491:G:C8     | 2.49                     | 0.48              |
| 85:l5:499:G:H2'    | 85:l5:504:G:H22    | 1.78                     | 0.48              |
| 85:l5:1752:G:H2'   | 85:l5:1753:G:C8    | 2.48                     | 0.48              |
| 85:l5:1976:G:OP1   | 85:l5:1984:A:H4'   | 2.14                     | 0.48              |
| 85:l5:2021:G:H2'   | 85:l5:2022:C:C6    | 2.49                     | 0.48              |
| 85:l5:2379:A:H2'   | 85:l5:2380:G:O4'   | 2.14                     | 0.48              |
| 85:l5:2558:C:H2'   | 85:l5:2559:G:H8    | 1.78                     | 0.48              |
| 85:l5:3816:A:OP1   | 85:l5:3818:U:H5    | 1.97                     | 0.48              |
| 85:l5:4523:A:H5''  | 85:l5:4524:G:H5'   | 1.96                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 85:L5:4585:U:H2'   | 85:L5:4586:G:H8    | 1.78                     | 0.48              |
| 80:CB:56:PHE:HD2   | 80:CB:456:ARG:N    | 2.08                     | 0.48              |
| 80:CB:127:VAL:N    | 80:CB:154:VAL:O    | 2.47                     | 0.48              |
| 80:CB:279:SER:HB3  | 80:CB:285:LEU:HD23 | 1.96                     | 0.48              |
| 2:SE:47:PHE:O      | 2:SE:51:ARG:HB2    | 2.14                     | 0.48              |
| 6:SG:137:ARG:HH11  | 6:SG:178:ARG:NH2   | 2.12                     | 0.48              |
| 7:SJ:37:LEU:HA     | 7:SJ:127:ARG:HH12  | 1.78                     | 0.48              |
| 8:SY:12:PHE:HE2    | 8:SY:48:TYR:HH     | 1.59                     | 0.48              |
| 11:SB:82:ARG:CB    | 11:SB:103:MET:HE1  | 2.39                     | 0.48              |
| 11:SB:145:LYS:NZ   | 11:SB:152:LYS:O    | 2.44                     | 0.48              |
| 16:SN:11:LEU:HD23  | 16:SN:11:LEU:H     | 1.77                     | 0.48              |
| 18:SW:51:GLU:HB2   | 18:SW:62:VAL:CG1   | 2.42                     | 0.48              |
| 85:L5:25:A:C8      | 85:L5:341:G:C8     | 3.02                     | 0.48              |
| 85:L5:39:A:N7      | 85:L5:1654:G:C5    | 2.82                     | 0.48              |
| 85:L5:119:G:N7     | 28:LG:132:ARG:NH2  | 2.61                     | 0.48              |
| 85:L5:1293:G:OP2   | 85:L5:1293:G:N2    | 2.40                     | 0.48              |
| 85:L5:1315:C:H2'   | 85:L5:1316:G:H8    | 1.78                     | 0.48              |
| 85:L5:1361:G:H2'   | 85:L5:1362:G:H8    | 1.78                     | 0.48              |
| 85:L5:1568:C:H2'   | 85:L5:1569:U:H6    | 1.78                     | 0.48              |
| 85:L5:1600:A:H5'   | 36:LP:133:HIS:HA   | 1.96                     | 0.48              |
| 85:L5:2012:A:C2    | 85:L5:2013:A:H1'   | 2.49                     | 0.48              |
| 85:L5:2309:G:O6    | 85:L5:2330:G:N2    | 2.47                     | 0.48              |
| 85:L5:2538:U:H2'   | 85:L5:2539:C:C6    | 2.49                     | 0.48              |
| 85:L5:2726:G:H2'   | 85:L5:2727:C:C6    | 2.49                     | 0.48              |
| 85:L5:4208:U:H2'   | 85:L5:4209:G:C8    | 2.48                     | 0.48              |
| 85:L5:4758:U:H5''  | 35:LO:116:LYS:HE3  | 1.96                     | 0.48              |
| 20:L7:46:C:O5'     | 25:LD:158:LYS:NZ   | 2.47                     | 0.48              |
| 21:L8:14:U:H2'     | 21:L8:15:G:C8      | 2.48                     | 0.48              |
| 21:L8:38:U:H3      | 53:Lh:84:ARG:HG3   | 1.78                     | 0.48              |
| 23:LB:228:TYR:CE1  | 23:LB:270:GLY:HA2  | 2.49                     | 0.48              |
| 23:LB:302:ASN:O    | 23:LB:304:SER:N    | 2.44                     | 0.48              |
| 24:LC:62:THR:HB    | 24:LC:92:PHE:CE1   | 2.49                     | 0.48              |
| 24:LC:68:GLY:HA3   | 24:LC:71:ARG:HH21  | 1.79                     | 0.48              |
| 24:LC:236:ASN:OD1  | 24:LC:239:LYS:N    | 2.46                     | 0.48              |
| 29:LH:48:LEU:HD21  | 29:LH:56:ARG:HD2   | 1.95                     | 0.48              |
| 29:LH:50:LYS:HD3   | 29:LH:50:LYS:H     | 1.78                     | 0.48              |
| 35:LO:111:PRO:HG2  | 35:LO:112:TYR:CD2  | 2.49                     | 0.48              |
| 35:LO:147:TRP:NE1  | 35:LO:149:TYR:HB2  | 2.29                     | 0.48              |
| 41:LU:76:VAL:HG23  | 41:LU:78:PHE:H     | 1.77                     | 0.48              |
| 58:Lm:96:CYS:HA    | 58:Lm:121:LEU:HD13 | 1.96                     | 0.48              |
| 65:SD:126:ILE:HG21 | 65:SD:134:CYS:HB2  | 1.96                     | 0.48              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 66:SF:59:LYS:HG3  | 66:SF:60:ARG:O     | 2.14                     | 0.48              |
| 71:ST:111:LYS:HG3 | 71:ST:111:LYS:O    | 2.13                     | 0.48              |
| 72:SU:48:LEU:HD23 | 72:SU:48:LEU:H     | 1.78                     | 0.48              |
| 73:Sc:15:THR:OG1  | 73:Sc:31:ARG:HG3   | 2.13                     | 0.48              |
| 73:Sc:44:ARG:HD2  | 73:Sc:63:ARG:CZ    | 2.44                     | 0.48              |
| 73:Sc:44:ARG:HD2  | 73:Sc:63:ARG:NH2   | 2.28                     | 0.48              |
| 76:SM:61:TYR:O    | 76:SM:64:LEU:HG    | 2.13                     | 0.48              |
| 79:S2:17:C:H4'    | 79:S2:1166:G:C8    | 2.49                     | 0.48              |
| 79:S2:29:G:H2'    | 79:S2:30:C:C6      | 2.49                     | 0.48              |
| 79:S2:52:G:H2'    | 79:S2:53:C:H6      | 1.79                     | 0.48              |
| 79:S2:824:C:H2'   | 79:S2:825:A:C8     | 2.49                     | 0.48              |
| 79:S2:1424:G:H2'  | 79:S2:1425:G:C8    | 2.49                     | 0.48              |
| 79:S2:1590:C:H3'  | 79:S2:1591:C:H6    | 1.79                     | 0.48              |
| 1:CH:77:VAL:HG13  | 1:CH:132:LEU:HD11  | 1.95                     | 0.47              |
| 1:cH:58:THR:HA    | 65:sD:113:LEU:HD21 | 1.95                     | 0.47              |
| 1:cH:84:GLY:O     | 1:cH:88:LYS:NZ     | 2.46                     | 0.47              |
| 2:sE:11:ARG:HG3   | 2:sE:20:LEU:HD23   | 1.96                     | 0.47              |
| 3:sI:97:VAL:HG13  | 3:sI:99:ASN:H      | 1.78                     | 0.47              |
| 3:sI:141:ARG:NH1  | 79:s2:191:A:H5''   | 2.28                     | 0.47              |
| 7:sJ:125:HIS:O    | 7:sJ:128:VAL:HG12  | 2.14                     | 0.47              |
| 9:se:35:ARG:NH2   | 79:s2:526:A:H5''   | 2.29                     | 0.47              |
| 10:sA:109:THR:O   | 79:s2:1351:G:H4'   | 2.13                     | 0.47              |
| 11:sB:103:MET:SD  | 11:sB:215:VAL:HG13 | 2.54                     | 0.47              |
| 12:sH:162:GLN:N   | 12:sH:162:GLN:OE1  | 2.47                     | 0.47              |
| 13:sV:2:GLN:H     | 13:sV:8:PHE:HA     | 1.79                     | 0.47              |
| 19:sb:67:THR:OG1  | 19:sb:68:GLY:N     | 2.47                     | 0.47              |
| 27:lF:76:ARG:HH21 | 85:l5:730:G:P      | 2.37                     | 0.47              |
| 27:lF:91:PHE:HE1  | 27:lF:244:ILE:HD11 | 1.79                     | 0.47              |
| 28:lG:134:PRO:HB3 | 28:lG:206:GLN:CD   | 2.38                     | 0.47              |
| 28:lG:216:ALA:HA  | 28:lG:219:VAL:HG22 | 1.96                     | 0.47              |
| 32:lL:178:ALA:HB3 | 46:la:134:GLU:OE1  | 2.14                     | 0.47              |
| 33:lM:57:LEU:HD23 | 33:lM:57:LEU:HA    | 1.74                     | 0.47              |
| 34:lN:38:ARG:HA   | 34:lN:62:TYR:HA    | 1.95                     | 0.47              |
| 35:lO:7:LEU:HD23  | 35:lO:33:VAL:HG22  | 1.95                     | 0.47              |
| 35:lO:113:ASP:OD1 | 35:lO:113:ASP:C    | 2.56                     | 0.47              |
| 36:lP:22:LEU:HB3  | 36:lP:90:PHE:CE2   | 2.49                     | 0.47              |
| 37:lQ:133:GLY:O   | 37:lQ:136:THR:HG22 | 2.14                     | 0.47              |
| 41:lU:105:ASN:ND2 | 41:lU:111:GLU:HB3  | 2.28                     | 0.47              |
| 46:la:72:THR:HG23 | 46:la:110:LYS:HB3  | 1.96                     | 0.47              |
| 48:lc:81:LEU:HD21 | 48:lc:94:LEU:HD22  | 1.96                     | 0.47              |
| 49:ld:22:THR:OG1  | 49:ld:88:LEU:O     | 2.32                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 60:lo:63:THR:OG1   | 60:lo:64:LYS:N     | 2.47                     | 0.47              |
| 62:lr:39:ARG:HD3   | 62:lr:105:ASP:OD2  | 2.14                     | 0.47              |
| 64:sR:41:ILE:HG22  | 79:s2:1387:G:C2'   | 2.43                     | 0.47              |
| 69:sQ:104:SER:HA   | 69:sQ:107:GLU:CD   | 2.38                     | 0.47              |
| 74:sd:19:ARG:HH12  | 79:s2:1660:C:P     | 2.37                     | 0.47              |
| 77:sZ:82:SER:O     | 77:sZ:85:ARG:HG2   | 2.14                     | 0.47              |
| 79:s2:124:U:H2'    | 79:s2:125:C:H6     | 1.79                     | 0.47              |
| 79:s2:350:C:H1'    | 79:s2:383:G:H1     | 1.78                     | 0.47              |
| 79:s2:378:U:H2'    | 79:s2:379:C:C6     | 2.49                     | 0.47              |
| 79:s2:1309:C:H2'   | 79:s2:1310:U:C6    | 2.49                     | 0.47              |
| 79:s2:1817:G:H2'   | 79:s2:1818:A:C8    | 2.49                     | 0.47              |
| 80:cB:130:ASP:OD1  | 80:cB:132:VAL:N    | 2.47                     | 0.47              |
| 80:cB:225:LEU:O    | 80:cB:225:LEU:HD23 | 2.14                     | 0.47              |
| 83:ls:61:MET:SD    | 83:ls:61:MET:N     | 2.82                     | 0.47              |
| 83:ls:82:ILE:HG21  | 83:ls:88:PHE:CZ    | 2.48                     | 0.47              |
| 85:l5:7:C:H2'      | 85:l5:8:U:C6       | 2.48                     | 0.47              |
| 85:l5:111:C:C2     | 85:l5:331:G:C2     | 3.02                     | 0.47              |
| 85:l5:444:G:H2'    | 85:l5:445:U:H6     | 1.79                     | 0.47              |
| 85:l5:676:C:H2'    | 85:l5:677:G:H8     | 1.79                     | 0.47              |
| 85:l5:2443:G:P     | 85:l5:2516:G:H22   | 2.35                     | 0.47              |
| 85:l5:4075:U:O2    | 85:l5:4076:G:O2'   | 2.16                     | 0.47              |
| 85:l5:4507:A:H2'   | 85:l5:4508:C:C6    | 2.48                     | 0.47              |
| 85:l5:4750:G:H2'   | 85:l5:4751:G:H8    | 1.79                     | 0.47              |
| 80:CB:9:ILE:HA     | 80:CB:12:ILE:HD12  | 1.95                     | 0.47              |
| 80:CB:112:SER:O    | 80:CB:115:VAL:HG12 | 2.14                     | 0.47              |
| 80:CB:176:GLN:HE21 | 80:CB:180:ARG:NH1  | 2.11                     | 0.47              |
| 3:SI:6:ASP:OD1     | 3:SI:8:TRP:N       | 2.45                     | 0.47              |
| 3:SI:23:LYS:NZ     | 79:S2:449:A:OP1    | 2.36                     | 0.47              |
| 10:SA:169:HIS:HA   | 10:SA:203:PHE:CE2  | 2.49                     | 0.47              |
| 16:SN:55:ARG:HH21  | 19:Sb:51:GLN:HB2   | 1.79                     | 0.47              |
| 17:SO:117:ARG:HH22 | 73:Sc:62:GLU:HG3   | 1.79                     | 0.47              |
| 85:L5:340:C:H42    | 32:LL:20:ARG:HH21  | 1.60                     | 0.47              |
| 85:L5:497:G:H22    | 85:L5:658:C:H42    | 1.61                     | 0.47              |
| 85:L5:1291:G:H2'   | 85:L5:1292:C:C6    | 2.49                     | 0.47              |
| 85:L5:1925:G:H2'   | 85:L5:1926:C:C6    | 2.48                     | 0.47              |
| 85:L5:2743:A:H2'   | 85:L5:2744:A:C8    | 2.49                     | 0.47              |
| 85:L5:2870:A:P     | 85:L5:2879:A:H61   | 2.35                     | 0.47              |
| 85:L5:3667:C:H4'   | 22:LA:8:GLN:HA     | 1.96                     | 0.47              |
| 85:L5:4357:G:H2'   | 85:L5:4358:U:C6    | 2.49                     | 0.47              |
| 85:L5:4705:A:H2'   | 85:L5:4706:G:O4'   | 2.14                     | 0.47              |
| 85:L5:4926:C:H5'   | 85:L5:4927:G:H21   | 1.79                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 85:L5:4991:U:H2'   | 85:L5:4992:G:C8    | 2.49                     | 0.47              |
| 21:L8:26:C:O3'     | 24:LC:55:SER:OG    | 2.31                     | 0.47              |
| 21:L8:141:C:C2     | 21:L8:142:U:C5     | 3.01                     | 0.47              |
| 22:LA:136:VAL:HG11 | 22:LA:139:HIS:HE1  | 1.79                     | 0.47              |
| 22:LA:224:THR:HA   | 22:LA:237:LEU:HB3  | 1.95                     | 0.47              |
| 24:LC:211:TYR:HE1  | 24:LC:229:LEU:HB3  | 1.79                     | 0.47              |
| 25:LD:23:ARG:O     | 25:LD:23:ARG:HD2   | 2.14                     | 0.47              |
| 26:LE:264:ILE:HD11 | 26:LE:267:LEU:HD13 | 1.94                     | 0.47              |
| 28:LG:55:VAL:HB    | 28:LG:57:TRP:CE2   | 2.49                     | 0.47              |
| 30:LI:45:GLU:O     | 30:LI:141:LYS:HD3  | 2.14                     | 0.47              |
| 31:LJ:3:GLN:N      | 31:LJ:5:GLN:OE1    | 2.47                     | 0.47              |
| 34:LN:80:THR:HG23  | 34:LN:87:HIS:HD2   | 1.79                     | 0.47              |
| 37:LQ:187:LYS:C    | 37:LQ:188:ASN:ND2  | 2.71                     | 0.47              |
| 38:LR:23:TRP:CH2   | 38:LR:25:ASP:HA    | 2.49                     | 0.47              |
| 38:LR:103:ARG:HG2  | 38:LR:124:TYR:CE2  | 2.49                     | 0.47              |
| 41:LU:72:VAL:HG22  | 41:LU:72:VAL:O     | 2.13                     | 0.47              |
| 46:La:116:LYS:C    | 46:La:117:LEU:HD22 | 2.38                     | 0.47              |
| 59:Ln:1:MET:HE2    | 59:Ln:1:MET:H1     | 1.78                     | 0.47              |
| 60:Lo:10:THR:OG1   | 60:Lo:11:PHE:N     | 2.47                     | 0.47              |
| 65:SD:34:TYR:OH    | 65:SD:37:VAL:HB    | 2.13                     | 0.47              |
| 67:SK:43:LEU:O     | 67:SK:46:MET:SD    | 2.72                     | 0.47              |
| 71:ST:7:LYS:HD2    | 79:S2:1426:U:H4'   | 1.96                     | 0.47              |
| 71:ST:65:TYR:HD2   | 71:ST:66:LEU:HD22  | 1.78                     | 0.47              |
| 76:SM:84:LYS:HD2   | 76:SM:88:TRP:NE1   | 2.26                     | 0.47              |
| 77:SZ:47:LEU:HD11  | 77:SZ:83:LEU:HD11  | 1.95                     | 0.47              |
| 79:S2:64:A:N6      | 79:S2:83:A:OP2     | 2.47                     | 0.47              |
| 79:S2:1842:C:H2'   | 79:S2:1843:G:C8    | 2.49                     | 0.47              |
| 82:PE:19:G:N2      | 82:PE:57:A:H1'     | 2.29                     | 0.47              |
| 84:Lt:64:ILE:HB    | 84:Lt:71:ILE:HB    | 1.96                     | 0.47              |
| 1:cH:100:ASN:HD21  | 79:s2:635:G:N2     | 2.12                     | 0.47              |
| 2:sE:86:PHE:O      | 2:sE:88:ASP:N      | 2.47                     | 0.47              |
| 5:sX:46:HIS:HE1    | 79:s2:648:A:H1'    | 1.79                     | 0.47              |
| 10:sA:9:GLN:C      | 10:sA:55:TRP:CH2   | 2.88                     | 0.47              |
| 10:sA:42:LYS:HG3   | 10:sA:44:ASP:H     | 1.79                     | 0.47              |
| 11:sB:149:GLN:HB3  | 64:sR:133:GLY:O    | 2.14                     | 0.47              |
| 12:sH:170:VAL:HA   | 12:sH:173:PHE:CD2  | 2.48                     | 0.47              |
| 14:sa:79:ILE:HG22  | 14:sa:84:VAL:HG23  | 1.94                     | 0.47              |
| 16:sN:46:THR:O     | 16:sN:50:ILE:HG12  | 2.13                     | 0.47              |
| 18:sW:52:ILE:HD13  | 18:sW:54:ASP:OD2   | 2.14                     | 0.47              |
| 22:lA:10:LYS:NZ    | 85:l5:3687:A:OP2   | 2.47                     | 0.47              |
| 22:lA:66:PRO:HG2   | 22:lA:67:TYR:CD2   | 2.49                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:1B:246:ARG:NH1  | 85:15:4525:C:OP1   | 2.47                     | 0.47              |
| 26:1E:88:VAL:HA    | 26:1E:89:LEU:HA    | 1.57                     | 0.47              |
| 26:1E:179:LEU:HD11 | 85:15:4938:A:C5    | 2.50                     | 0.47              |
| 33:1M:70:GLN:OE1   | 33:1M:71:LYS:N     | 2.47                     | 0.47              |
| 36:1P:25:HIS:CD2   | 85:15:2361:G:C6    | 3.02                     | 0.47              |
| 36:1P:140:MET:HB2  | 85:15:3860:A:OP1   | 2.14                     | 0.47              |
| 37:1Q:54:SER:HG    | 37:1Q:56:THR:HG1   | 1.61                     | 0.47              |
| 38:1R:116:ASP:CG   | 38:1R:117:ARG:H    | 2.19                     | 0.47              |
| 39:1S:27:LEU:HD12  | 40:1T:148:PRO:HB3  | 1.95                     | 0.47              |
| 40:1T:12:ARG:NH1   | 85:15:4275:G:H4'   | 2.29                     | 0.47              |
| 42:1V:89:ARG:HB3   | 42:1V:95:PHE:CZ    | 2.49                     | 0.47              |
| 43:1X:119:ILE:HG23 | 43:1X:144:TYR:CE2  | 2.48                     | 0.47              |
| 46:1a:72:THR:HG22  | 46:1a:112:LEU:HG   | 1.96                     | 0.47              |
| 65:sD:217:ILE:HG12 | 65:sD:219:PRO:HD3  | 1.96                     | 0.47              |
| 66:sF:113:VAL:O    | 66:sF:117:ILE:HG22 | 2.13                     | 0.47              |
| 66:sF:166:ILE:HA   | 79:s2:1599:U:C4    | 2.48                     | 0.47              |
| 72:sU:27:ARG:NH1   | 72:sU:82:MET:SD    | 2.87                     | 0.47              |
| 72:sU:61:LEU:HD12  | 74:sd:34:TYR:CE2   | 2.49                     | 0.47              |
| 75:sg:210:GLY:HA3  | 75:sg:236:ILE:HD11 | 1.96                     | 0.47              |
| 79:s2:109:U:H2'    | 79:s2:110:U:C6     | 2.48                     | 0.47              |
| 79:s2:508:A:H5'    | 79:s2:509:G:OP2    | 2.14                     | 0.47              |
| 79:s2:885:U:O2     | 79:s2:901:G:O6     | 2.31                     | 0.47              |
| 79:s2:946:U:H2'    | 79:s2:947:G:H8     | 1.79                     | 0.47              |
| 79:s2:1264:C:O2    | 79:s2:1517:G:N1    | 2.47                     | 0.47              |
| 79:s2:1552:G:H1'   | 79:s2:1557:C:H41   | 1.79                     | 0.47              |
| 79:s2:1702:G:H2'   | 79:s2:1703:C:O4'   | 2.14                     | 0.47              |
| 79:s2:1802:C:C2    | 79:s2:1803:U:C5    | 3.03                     | 0.47              |
| 80:cB:520:LEU:O    | 80:cB:524:LEU:HG   | 2.14                     | 0.47              |
| 85:15:169:G:H2'    | 85:15:171:U:O2     | 2.13                     | 0.47              |
| 85:15:222:C:H2'    | 85:15:223:G:O4'    | 2.13                     | 0.47              |
| 85:15:733:A:C2     | 85:15:734:G:H1'    | 2.48                     | 0.47              |
| 85:15:1328:G:O2'   | 85:15:2349:A:OP1   | 2.30                     | 0.47              |
| 85:15:1662:C:H2'   | 85:15:1663:C:H6    | 1.79                     | 0.47              |
| 85:15:3608:A:H2'   | 85:15:3609:G:H8    | 1.79                     | 0.47              |
| 85:15:3610:A:H2'   | 85:15:3611:A:C8    | 2.48                     | 0.47              |
| 85:15:4606:G:H2'   | 85:15:4607:A:C8    | 2.49                     | 0.47              |
| 85:15:4618:G:C2    | 85:15:4619:U:C5    | 3.02                     | 0.47              |
| 80:CB:44:GLY:HA3   | 80:CB:47:ALA:HB3   | 1.95                     | 0.47              |
| 80:CB:155:LEU:HG   | 80:CB:157:MET:HE1  | 1.96                     | 0.47              |
| 6:SG:70:HIS:HB3    | 6:SG:101:ILE:HB    | 1.96                     | 0.47              |
| 8:SY:26:ASP:N      | 8:SY:26:ASP:OD2    | 2.46                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 85:L5:154:G:H2'    | 85:L5:155:C:C6     | 2.48                     | 0.47              |
| 85:L5:276:C:H2'    | 54:Li:29:ARG:NH1   | 2.30                     | 0.47              |
| 85:L5:352:G:C6     | 24:LC:196:MET:HE2  | 2.49                     | 0.47              |
| 85:L5:1776:A:H2'   | 85:L5:1777:C:O4'   | 2.14                     | 0.47              |
| 85:L5:1866:U:H2'   | 85:L5:1867:A:O4'   | 2.14                     | 0.47              |
| 85:L5:2465:C:H2'   | 85:L5:2466:G:O4'   | 2.14                     | 0.47              |
| 85:L5:3611:A:H2'   | 85:L5:3612:C:C6    | 2.49                     | 0.47              |
| 85:L5:4061:G:O2'   | 85:L5:4062:A:OP1   | 2.31                     | 0.47              |
| 85:L5:4085:A:H5''  | 28:LG:56:LYS:HB2   | 1.96                     | 0.47              |
| 85:L5:4187:G:H4'   | 34:LN:82:GLY:HA2   | 1.95                     | 0.47              |
| 85:L5:4333:C:H2'   | 85:L5:4334:U:C6    | 2.48                     | 0.47              |
| 23:LB:286:LYS:O    | 23:LB:287:ILE:HD13 | 2.15                     | 0.47              |
| 27:LF:66:ARG:HD3   | 27:LF:69:ILE:HD11  | 1.96                     | 0.47              |
| 38:LR:105:LEU:HD11 | 38:LR:109:TYR:CZ   | 2.49                     | 0.47              |
| 48:Lc:38:ILE:HG22  | 48:Lc:43:ALA:HB3   | 1.96                     | 0.47              |
| 54:Li:55:ARG:HA    | 54:Li:58:MET:CG    | 2.40                     | 0.47              |
| 69:SQ:78:VAL:HG22  | 79:S2:1673:U:H5''  | 1.96                     | 0.47              |
| 70:SS:78:LYS:NZ    | 71:ST:32:GLU:HB2   | 2.29                     | 0.47              |
| 72:SU:55:ARG:HE    | 72:SU:87:ARG:NH1   | 2.11                     | 0.47              |
| 77:SZ:86:ALA:O     | 77:SZ:90:GLU:HG3   | 2.14                     | 0.47              |
| 79:S2:949:G:H2'    | 79:S2:950:C:C6     | 2.49                     | 0.47              |
| 79:S2:1082:A:H5''  | 79:S2:1084:A:N7    | 2.28                     | 0.47              |
| 79:S2:1171:G:O2'   | 79:S2:1187:G:O6    | 2.32                     | 0.47              |
| 81:AP:8:U:O2'      | 81:AP:21:A:N1      | 2.46                     | 0.47              |
| 81:AP:38:C:H2'     | 81:AP:39:G:O4'     | 2.14                     | 0.47              |
| 81:AP:53:G:H2'     | 81:AP:54:U:H6      | 1.79                     | 0.47              |
| 1:cH:60:LYS:O      | 1:cH:64:GLU:N      | 2.46                     | 0.47              |
| 1:cH:75:LEU:O      | 1:cH:79:LYS:HG2    | 2.14                     | 0.47              |
| 3:sI:31:ARG:HH21   | 79:s2:380:G:H5''   | 1.79                     | 0.47              |
| 3:sI:201:LYS:HA    | 3:sI:201:LYS:HD3   | 1.75                     | 0.47              |
| 6:sG:15:LEU:HB2    | 79:s2:154:U:O2'    | 2.14                     | 0.47              |
| 8:sY:109:GLU:HG3   | 8:sY:113:ARG:HH21  | 1.79                     | 0.47              |
| 14:sa:37:LYS:HD3   | 14:sa:70:LYS:CE    | 2.45                     | 0.47              |
| 16:sN:3:ARG:NH1    | 16:sN:10:GLY:O     | 2.40                     | 0.47              |
| 18:sW:53:ILE:CG2   | 18:sW:60:LYS:HB2   | 2.44                     | 0.47              |
| 19:sb:19:HIS:CD2   | 19:sb:20:LYS:H     | 2.31                     | 0.47              |
| 21:l8:104:A:P      | 55:lj:42:LYS:HD3   | 2.54                     | 0.47              |
| 23:lB:229:LYS:HA   | 23:lB:229:LYS:HD2  | 1.62                     | 0.47              |
| 25:lD:80:ALA:O     | 25:lD:84:PRO:HD3   | 2.14                     | 0.47              |
| 25:lD:84:PRO:HA    | 25:lD:88:VAL:O     | 2.14                     | 0.47              |
| 26:lE:94:LYS:NZ    | 85:l5:687:U:O3'    | 2.47                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:lf:161:LYS:HG3  | 27:lf:164:LYS:HA   | 1.96                     | 0.47              |
| 29:IH:23:ARG:NH1   | 29:IH:41:ILE:O     | 2.44                     | 0.47              |
| 40:IT:31:MET:SD    | 40:IT:31:MET:N     | 2.79                     | 0.47              |
| 42:IV:65:VAL:CG1   | 42:IV:73:ARG:HA    | 2.44                     | 0.47              |
| 42:IV:85:ARG:N     | 42:IV:101:ASN:OD1  | 2.45                     | 0.47              |
| 61:lp:86:LEU:HA    | 61:lp:89:LEU:HG    | 1.96                     | 0.47              |
| 62:lr:97:ILE:HD11  | 62:lr:104:PRO:HA   | 1.97                     | 0.47              |
| 65:sD:75:LYS:NZ    | 67:sK:20:VAL:O     | 2.45                     | 0.47              |
| 66:sF:55:ARG:NH1   | 79:s2:1647:A:O2'   | 2.46                     | 0.47              |
| 66:sF:55:ARG:HH12  | 79:s2:1648:G:P     | 2.37                     | 0.47              |
| 68:sP:82:ASP:OD2   | 79:s2:1619:A:O2'   | 2.32                     | 0.47              |
| 69:sQ:128:GLU:OE2  | 69:sQ:128:GLU:N    | 2.47                     | 0.47              |
| 73:sc:10:LYS:CE    | 73:sc:34:PHE:HB3   | 2.39                     | 0.47              |
| 75:sg:30:MET:SD    | 75:sg:44:LYS:HG2   | 2.54                     | 0.47              |
| 76:sM:71:GLU:HG3   | 76:sM:72:HIS:CD2   | 2.49                     | 0.47              |
| 79:s2:158:A:H61    | 79:s2:467:G:H1'    | 1.79                     | 0.47              |
| 79:s2:348:A:H2'    | 79:s2:349:A:C8     | 2.49                     | 0.47              |
| 79:s2:907:G:H2'    | 79:s2:908:A:H8     | 1.79                     | 0.47              |
| 79:s2:959:G:H1'    | 79:s2:964:A:N6     | 2.28                     | 0.47              |
| 79:s2:1233:G:N3    | 79:s2:1252:C:O2'   | 2.41                     | 0.47              |
| 79:s2:1379:A:H2'   | 79:s2:1380:C:C6    | 2.50                     | 0.47              |
| 79:s2:1413:G:H2'   | 79:s2:1414:A:C8    | 2.49                     | 0.47              |
| 79:s2:1737:G:H2'   | 79:s2:1738:C:C6    | 2.49                     | 0.47              |
| 80:cB:111:PHE:HE2  | 80:cB:500:SER:N    | 2.12                     | 0.47              |
| 80:cB:286:PRO:HB2  | 80:cB:291:GLN:HG2  | 1.95                     | 0.47              |
| 80:cB:731:ALA:O    | 80:cB:735:THR:HG23 | 2.14                     | 0.47              |
| 85:l5:247:G:H2'    | 85:l5:248:C:H6     | 1.78                     | 0.47              |
| 85:l5:713:C:H2'    | 85:l5:714:G:H8     | 1.78                     | 0.47              |
| 85:l5:937:U:H2'    | 85:l5:938:C:C6     | 2.49                     | 0.47              |
| 85:l5:1309:C:H2'   | 85:l5:1310:C:C6    | 2.48                     | 0.47              |
| 85:l5:1322:A:O2'   | 85:l5:1324:A:OP2   | 2.25                     | 0.47              |
| 85:l5:1942:A:N3    | 85:l5:4432:C:O2'   | 2.41                     | 0.47              |
| 85:l5:2261:G:H2'   | 85:l5:2262:G:C4    | 2.50                     | 0.47              |
| 85:l5:2629:C:H2'   | 85:l5:2630:U:O4'   | 2.14                     | 0.47              |
| 80:CB:260:LEU:HD12 | 80:CB:288:THR:HB   | 1.96                     | 0.47              |
| 5:SX:14:ARG:HG2    | 5:SX:18:ARG:NH1    | 2.28                     | 0.47              |
| 6:SG:136:LYS:HD3   | 79:S2:65:C:C5      | 2.50                     | 0.47              |
| 7:SJ:65:GLU:HG3    | 7:SJ:66:LYS:H      | 1.80                     | 0.47              |
| 10:SA:85:ARG:HE    | 64:SR:81:ARG:NH1   | 2.12                     | 0.47              |
| 10:SA:127:PRO:HA   | 10:SA:134:LEU:HD11 | 1.96                     | 0.47              |
| 11:SB:71:LEU:HD12  | 11:SB:74:LEU:HB3   | 1.97                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 12:SH:43:LEU:HG    | 12:SH:68:GLN:HB2   | 1.96                     | 0.47              |
| 16:SN:62:GLN:NE2   | 79:S2:1016:U:O3'   | 2.46                     | 0.47              |
| 16:SN:109:LYS:HE3  | 79:S2:1032:C:H5''  | 1.96                     | 0.47              |
| 85:L5:104:G:C2     | 85:L5:105:A:C8     | 3.02                     | 0.47              |
| 85:L5:342:G:O2'    | 55:Lj:71:TYR:OH    | 2.32                     | 0.47              |
| 85:L5:736:C:H5'    | 33:LM:74:ARG:HH12  | 1.80                     | 0.47              |
| 85:L5:746:A:H2     | 85:L5:918:G:H22    | 1.62                     | 0.47              |
| 85:L5:1281:G:C5    | 26:LE:128:HIS:HD2  | 2.32                     | 0.47              |
| 85:L5:1541:C:H2'   | 85:L5:1542:U:C6    | 2.49                     | 0.47              |
| 85:L5:1698:C:H3'   | 85:L5:1699:A:O4'   | 2.14                     | 0.47              |
| 85:L5:1718:C:P     | 27:LF:200:ARG:HH22 | 2.37                     | 0.47              |
| 85:L5:1856:C:H2'   | 85:L5:1857:C:H6    | 1.79                     | 0.47              |
| 85:L5:1929:A:C8    | 85:L5:1932:A:H1'   | 2.49                     | 0.47              |
| 85:L5:1951:G:H1'   | 39:LS:117:HIS:CE1  | 2.48                     | 0.47              |
| 85:L5:2079:G:H2'   | 85:L5:2080:U:H6    | 1.79                     | 0.47              |
| 85:L5:2258:C:H41   | 26:LE:88:VAL:HG12  | 1.78                     | 0.47              |
| 85:L5:2532:C:OP1   | 43:LX:125:ASN:ND2  | 2.46                     | 0.47              |
| 85:L5:2722:G:H2'   | 85:L5:2723:U:C6    | 2.49                     | 0.47              |
| 85:L5:2858:A:H2'   | 85:L5:2859:G:C8    | 2.49                     | 0.47              |
| 85:L5:3802:U:O2'   | 85:L5:3803:A:H5'   | 2.14                     | 0.47              |
| 85:L5:3851:U:H2'   | 85:L5:3852:A:O4'   | 2.14                     | 0.47              |
| 85:L5:3868:G:N2    | 85:L5:3900:G:O2'   | 2.43                     | 0.47              |
| 85:L5:4079:C:H2'   | 85:L5:4080:C:C6    | 2.50                     | 0.47              |
| 85:L5:4318:C:O2'   | 60:Lo:18:HIS:ND1   | 2.33                     | 0.47              |
| 85:L5:4953:G:H2'   | 85:L5:4954:G:H8    | 1.79                     | 0.47              |
| 85:L5:5002:U:H3    | 85:L5:5045:G:H1    | 1.62                     | 0.47              |
| 20:L7:73:U:O5'     | 20:L7:74:A:H2'     | 2.14                     | 0.47              |
| 20:L7:88:A:H2'     | 20:L7:89:G:O4'     | 2.15                     | 0.47              |
| 27:LF:60:GLU:O     | 27:LF:64:MET:SD    | 2.72                     | 0.47              |
| 27:LF:142:TRP:CZ2  | 27:LF:235:ASN:HB2  | 2.49                     | 0.47              |
| 30:LI:46:PHE:HB2   | 30:LI:139:ARG:NH1  | 2.29                     | 0.47              |
| 38:LR:10:LEU:O     | 38:LR:14:VAL:HG12  | 2.14                     | 0.47              |
| 40:LT:84:ILE:HD11  | 47:Lb:23:LYS:HA    | 1.96                     | 0.47              |
| 40:LT:151:LEU:H    | 40:LT:151:LEU:CD2  | 2.27                     | 0.47              |
| 49:Ld:115:LYS:HG2  | 49:Ld:116:ASN:ND2  | 2.29                     | 0.47              |
| 66:SF:102:LEU:HD21 | 77:SZ:108:ILE:HG12 | 1.97                     | 0.47              |
| 70:SS:105:ASN:OD1  | 70:SS:106:LYS:HD3  | 2.14                     | 0.47              |
| 71:ST:39:LEU:HD13  | 71:ST:47:PRO:HD3   | 1.97                     | 0.47              |
| 72:SU:51:LYS:HD2   | 72:SU:52:GLY:N     | 2.29                     | 0.47              |
| 73:Sc:13:ARG:N     | 73:Sc:33:GLU:O     | 2.47                     | 0.47              |
| 75:Sg:60:ARG:HD2   | 75:Sg:60:ARG:C     | 2.40                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 75:Sg:107:ASP:OD1  | 75:Sg:125:ARG:NE   | 2.47                     | 0.47              |
| 79:S2:674:C:H2'    | 79:S2:675:U:H6     | 1.80                     | 0.47              |
| 79:S2:1642:U:H2'   | 79:S2:1643:U:H6    | 1.79                     | 0.47              |
| 82:PE:22:G:C2      | 82:PE:23:A:C5      | 3.02                     | 0.47              |
| 87:IW:56:ARG:NH2   | 87:IW:61:LYS:HB3   | 2.29                     | 0.47              |
| 2:sE:90:ILE:HG22   | 2:sE:99:PHE:HD2    | 1.79                     | 0.47              |
| 2:sE:212:ASP:OD1   | 2:sE:216:ASN:N     | 2.47                     | 0.47              |
| 3:sI:8:TRP:CZ3     | 3:sI:20:PRO:HB3    | 2.50                     | 0.47              |
| 4:sL:59:LYS:HD3    | 4:sL:134:LEU:HG    | 1.96                     | 0.47              |
| 4:sL:150:GLY:HA2   | 4:sL:153:LYS:NZ    | 2.30                     | 0.47              |
| 6:sG:92:ARG:O      | 79:s2:453:C:O2'    | 2.28                     | 0.47              |
| 8:sY:19:GLN:NE2    | 8:sY:81:TYR:HD1    | 2.10                     | 0.47              |
| 10:sA:35:GLU:N     | 10:sA:35:GLU:OE1   | 2.47                     | 0.47              |
| 15:sC:224:THR:O    | 79:s2:2:A:O2'      | 2.33                     | 0.47              |
| 16:sN:52:VAL:O     | 16:sN:55:ARG:HG2   | 2.13                     | 0.47              |
| 16:sN:91:LEU:HD21  | 16:sN:121:ARG:HG2  | 1.96                     | 0.47              |
| 21:l8:64:U:C2      | 21:l8:65:A:C8      | 3.03                     | 0.47              |
| 21:l8:79:G:H2'     | 21:l8:80:A:O4'     | 2.13                     | 0.47              |
| 22:lA:117:GLU:OE1  | 22:lA:163:ARG:N    | 2.35                     | 0.47              |
| 23:lB:55:HIS:NE2   | 87:IW:16:GLY:HA3   | 2.29                     | 0.47              |
| 23:lB:291:TYR:HB3  | 23:lB:297:LYS:HE2  | 1.96                     | 0.47              |
| 24:lC:95:MET:HE1   | 85:l5:1520:C:O2'   | 2.15                     | 0.47              |
| 24:lC:349:LEU:HD23 | 24:lC:352:ASP:OD2  | 2.13                     | 0.47              |
| 25:lD:64:ILE:O     | 25:lD:75:VAL:HG22  | 2.14                     | 0.47              |
| 25:lD:271:MET:HB2  | 25:lD:275:GLN:HB2  | 1.97                     | 0.47              |
| 26:lE:110:ARG:O    | 26:lE:110:ARG:HG3  | 2.15                     | 0.47              |
| 31:lJ:32:ARG:HH21  | 31:lJ:35:ARG:CD    | 2.15                     | 0.47              |
| 32:lL:31:ARG:O     | 32:lL:35:ARG:HG3   | 2.14                     | 0.47              |
| 32:lL:192:PHE:CD2  | 54:li:11:LEU:HD11  | 2.50                     | 0.47              |
| 38:lR:170:ARG:HH12 | 38:lR:173:ARG:HG3  | 1.79                     | 0.47              |
| 43:lX:92:ASP:OD1   | 43:lX:92:ASP:C     | 2.56                     | 0.47              |
| 43:lX:139:ARG:HH22 | 85:l5:2533:C:C5'   | 2.22                     | 0.47              |
| 45:lZ:5:MET:HE1    | 45:lZ:82:PRO:HG3   | 1.97                     | 0.47              |
| 45:lZ:78:ASN:ND2   | 85:l5:2656:U:OP1   | 2.41                     | 0.47              |
| 47:lb:109:ARG:HA   | 47:lb:112:ILE:HG12 | 1.97                     | 0.47              |
| 51:lf:46:ARG:HD3   | 51:lf:71:TRP:CZ3   | 2.48                     | 0.47              |
| 64:sR:53:TYR:CG    | 79:s2:1466:G:C8    | 3.01                     | 0.47              |
| 66:sF:43:GLU:HA    | 66:sF:46:ALA:HB2   | 1.95                     | 0.47              |
| 67:sK:73:ASN:HA    | 67:sK:76:ILE:HG12  | 1.97                     | 0.47              |
| 69:sQ:45:ARG:HH22  | 71:sT:10:ASN:HB2   | 1.79                     | 0.47              |
| 79:s2:526:A:H2'    | 79:s2:527:C:H6     | 1.75                     | 0.47              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 79:s2:695:C:H5''  | 79:s2:696:G:C8     | 2.49                     | 0.47              |
| 79:s2:808:A:H2    | 79:s2:855:G:H22    | 1.61                     | 0.47              |
| 79:s2:870:A:C5'   | 79:s2:915:G:H22    | 2.27                     | 0.47              |
| 79:s2:1112:U:H2'  | 79:s2:1113:A:H8    | 1.79                     | 0.47              |
| 79:s2:1500:G:H2'  | 79:s2:1501:C:C6    | 2.50                     | 0.47              |
| 80:cB:401:MET:HE3 | 80:cB:410:PHE:CG   | 2.49                     | 0.47              |
| 80:cB:603:TYR:HB2 | 80:cB:706:ASP:H    | 1.79                     | 0.47              |
| 82:pE:26:A:H2'    | 82:pE:26:A:N3      | 2.28                     | 0.47              |
| 84:lt:57:ARG:HG3  | 84:lt:83:LYS:HD2   | 1.97                     | 0.47              |
| 85:l5:25:A:H2'    | 85:l5:26:C:C6      | 2.49                     | 0.47              |
| 85:l5:169:G:C2    | 85:l5:267:G:C2     | 3.02                     | 0.47              |
| 85:l5:295:A:C2    | 85:l5:317:A:H1'    | 2.50                     | 0.47              |
| 85:l5:956:A:N6    | 85:l5:1283:G:O3'   | 2.47                     | 0.47              |
| 85:l5:1241:C:C5   | 85:l5:1242:G:C8    | 3.03                     | 0.47              |
| 85:l5:1431:C:H2'  | 85:l5:1432:G:O4'   | 2.15                     | 0.47              |
| 85:l5:1953:U:H2'  | 85:l5:1954:U:C6    | 2.49                     | 0.47              |
| 85:l5:1978:C:H2'  | 85:l5:1979:A:O4'   | 2.14                     | 0.47              |
| 85:l5:2784:C:H2'  | 85:l5:2785:C:C6    | 2.49                     | 0.47              |
| 85:l5:4299:U:H2'  | 85:l5:4300:U:H6    | 1.80                     | 0.47              |
| 85:l5:4348:A:C6   | 85:l5:4350:C:C4    | 3.03                     | 0.47              |
| 85:l5:4575:G:C6   | 85:l5:5069:U:C4    | 3.02                     | 0.47              |
| 80:CB:279:SER:OG  | 80:CB:281:GLU:HG2  | 2.15                     | 0.47              |
| 80:CB:404:THR:HA  | 80:CB:411:TYR:CZ   | 2.49                     | 0.47              |
| 80:CB:448:GLN:NE2 | 79:S2:488:U:H5''   | 2.30                     | 0.47              |
| 80:CB:587:SER:O   | 80:CB:605:LYS:NZ   | 2.47                     | 0.47              |
| 2:SE:19:MET:CE    | 79:S2:846:G:C4     | 2.98                     | 0.47              |
| 5:SX:123:VAL:HA   | 5:SX:130:LEU:HD13  | 1.96                     | 0.47              |
| 6:SG:2:LYS:NZ     | 79:S2:156:G:OP1    | 2.46                     | 0.47              |
| 6:SG:57:ASP:HB3   | 6:SG:98:ARG:HG3    | 1.97                     | 0.47              |
| 6:SG:221:LYS:O    | 6:SG:224:ARG:HG3   | 2.15                     | 0.47              |
| 7:SJ:50:LEU:CD1   | 7:SJ:53:ILE:HD11   | 2.44                     | 0.47              |
| 7:SJ:92:MET:SD    | 7:SJ:92:MET:O      | 2.73                     | 0.47              |
| 7:SJ:117:LEU:HD11 | 7:SJ:119:LEU:HB3   | 1.97                     | 0.47              |
| 10:SA:156:TYR:O   | 13:SV:60:ARG:NH2   | 2.46                     | 0.47              |
| 85:L5:227:A:N6    | 85:L5:242:U:O4'    | 2.47                     | 0.47              |
| 85:L5:272:U:H2'   | 85:L5:273:U:H6     | 1.78                     | 0.47              |
| 85:L5:438:G:OP1   | 50:Le:16:ARG:NH2   | 2.43                     | 0.47              |
| 85:L5:693:C:H2'   | 85:L5:694:C:H6     | 1.79                     | 0.47              |
| 85:L5:951:G:H2'   | 85:L5:952:G:C8     | 2.49                     | 0.47              |
| 85:L5:1091:C:H2'  | 85:L5:1092:G:H8    | 1.78                     | 0.47              |
| 85:L5:1346:C:OP1  | 37:LQ:148:VAL:HG12 | 2.14                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 85:L5:1718:C:OP2   | 27:LF:200:ARG:NH2  | 2.45                     | 0.47              |
| 85:L5:1961:G:H1'   | 85:L5:2025:A:N6    | 2.30                     | 0.47              |
| 85:L5:2361:G:O2'   | 85:L5:3859:G:O6    | 2.27                     | 0.47              |
| 85:L5:2480:G:H2'   | 85:L5:2481:G:H8    | 1.78                     | 0.47              |
| 85:L5:2509:C:H2'   | 85:L5:2510:G:C8    | 2.48                     | 0.47              |
| 85:L5:2830:G:H2'   | 85:L5:2831:G:H8    | 1.78                     | 0.47              |
| 85:L5:2868:G:C2    | 85:L5:2883:G:C6    | 3.02                     | 0.47              |
| 85:L5:4096:C:O2    | 85:L5:4110:C:H2'   | 2.14                     | 0.47              |
| 85:L5:4180:G:H2'   | 85:L5:4181:U:H6    | 1.79                     | 0.47              |
| 85:L5:4485:C:C2    | 85:L5:4486:C:C5    | 3.03                     | 0.47              |
| 85:L5:4566:U:H2'   | 85:L5:4567:G:O4'   | 2.15                     | 0.47              |
| 85:L5:4578:G:H2'   | 85:L5:4579:U:H6    | 1.79                     | 0.47              |
| 85:L5:4773:C:N4    | 85:L5:4861:G:O6    | 2.29                     | 0.47              |
| 85:L5:4986:G:H5''  | 23:LB:176:LYS:HB2  | 1.95                     | 0.47              |
| 22:LA:225:ILE:HG12 | 22:LA:234:LYS:HA   | 1.97                     | 0.47              |
| 23:LB:216:MET:HG3  | 23:LB:350:SER:HB2  | 1.96                     | 0.47              |
| 24:LC:86:ARG:HA    | 24:LC:89:GLN:CD    | 2.40                     | 0.47              |
| 25:LD:195:HIS:O    | 25:LD:199:ILE:HG12 | 2.14                     | 0.47              |
| 25:LD:208:MET:HE1  | 25:LD:233:PRO:CG   | 2.44                     | 0.47              |
| 27:LF:226:HIS:CE1  | 27:LF:234:GLY:HA3  | 2.50                     | 0.47              |
| 33:LM:11:ARG:NH1   | 33:LM:58:THR:O     | 2.47                     | 0.47              |
| 34:LN:101:VAL:O    | 34:LN:104:GLU:HG3  | 2.13                     | 0.47              |
| 43:LX:122:ALA:HB3  | 43:LX:139:ARG:HG2  | 1.95                     | 0.47              |
| 44:LY:91:ASN:OD1   | 44:LY:93:THR:HG22  | 2.15                     | 0.47              |
| 45:LZ:11:VAL:N     | 45:LZ:23:ALA:O     | 2.34                     | 0.47              |
| 53:Lh:53:SER:O     | 53:Lh:57:VAL:HG13  | 2.15                     | 0.47              |
| 54:Li:58:MET:HA    | 54:Li:61:LEU:HG    | 1.97                     | 0.47              |
| 60:Lo:59:LYS:N     | 60:Lo:59:LYS:HD3   | 2.30                     | 0.47              |
| 62:Lr:30:ASN:ND2   | 62:Lr:77:TYR:HE2   | 2.12                     | 0.47              |
| 62:Lr:59:GLY:N     | 62:Lr:121:GLN:OE1  | 2.46                     | 0.47              |
| 64:SR:57:LEU:O     | 64:SR:61:ILE:HG22  | 2.14                     | 0.47              |
| 66:SF:88:MET:HA    | 66:SF:91:ARG:CG    | 2.44                     | 0.47              |
| 75:Sg:243:PRO:HG2  | 75:Sg:293:ALA:C    | 2.39                     | 0.47              |
| 75:Sg:245:ARG:HG3  | 75:Sg:247:TRP:HB2  | 1.97                     | 0.47              |
| 79:S2:15:U:O2'     | 79:S2:669:A:N6     | 2.47                     | 0.47              |
| 79:S2:379:C:H2'    | 79:S2:380:G:C8     | 2.49                     | 0.47              |
| 79:S2:692:G:O6     | 79:S2:738:C:O2'    | 2.23                     | 0.47              |
| 79:S2:1133:A:C4    | 79:S2:1134:G:C8    | 3.02                     | 0.47              |
| 81:AP:9:A:H3'      | 81:AP:11:U:H5      | 1.79                     | 0.47              |
| 83:Ls:157:ASP:OD1  | 83:Ls:157:ASP:N    | 2.44                     | 0.47              |
| 84:Lt:114:ARG:CD   | 84:Lt:130:LYS:HD3  | 2.44                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 87:LW:101:ARG:HG3  | 87:LW:105:ARG:HD2  | 1.96                     | 0.47              |
| 2:sE:17:HIS:HE1    | 2:sE:18:TRP:CZ3    | 2.32                     | 0.47              |
| 2:sE:94:LYS:HG2    | 8:sY:17:LEU:CG     | 2.45                     | 0.47              |
| 4:sL:17:PHE:HD2    | 4:sL:20:LYS:HZ2    | 1.63                     | 0.47              |
| 6:sG:138:ALA:HB2   | 6:sG:176:ILE:HD11  | 1.95                     | 0.47              |
| 11:sB:125:VAL:HB   | 11:sB:169:MET:SD   | 2.55                     | 0.47              |
| 12:sH:20:GLU:O     | 12:sH:24:SER:N     | 2.48                     | 0.47              |
| 15:sC:88:ILE:C     | 15:sC:89:LYS:HD2   | 2.39                     | 0.47              |
| 23:lB:365:LEU:HD23 | 23:lB:368:ILE:HD11 | 1.97                     | 0.47              |
| 24:lC:22:VAL:HG11  | 24:lC:257:PHE:HD2  | 1.79                     | 0.47              |
| 26:lE:132:PRO:HG3  | 85:l5:1287:G:C4    | 2.50                     | 0.47              |
| 37:lQ:101:CYS:HB2  | 37:lQ:121:LEU:HB2  | 1.95                     | 0.47              |
| 45:lZ:11:VAL:N     | 45:lZ:23:ALA:O     | 2.26                     | 0.47              |
| 52:lg:115:LYS:NZ   | 85:l5:4097:G:OP2   | 2.44                     | 0.47              |
| 54:li:76:ARG:O     | 85:l5:304:C:O2'    | 2.29                     | 0.47              |
| 56:lk:10:ASP:HA    | 56:lk:13:LEU:HG    | 1.95                     | 0.47              |
| 56:lk:25:ILE:CG1   | 56:lk:68:GLU:HG3   | 2.44                     | 0.47              |
| 59:ln:16:LYS:HE2   | 59:ln:20:MET:HE1   | 1.95                     | 0.47              |
| 64:sR:11:LYS:HA    | 79:s2:1373:C:C1'   | 2.42                     | 0.47              |
| 66:sF:103:LEU:HD13 | 77:sZ:66:LYS:HZ1   | 1.79                     | 0.47              |
| 68:sP:126:VAL:HG12 | 79:s2:1238:U:H1'   | 1.95                     | 0.47              |
| 75:sg:44:LYS:HB2   | 75:sg:54:ILE:HG22  | 1.96                     | 0.47              |
| 75:sg:273:GLU:H    | 75:sg:273:GLU:CD   | 2.18                     | 0.47              |
| 77:sZ:98:LYS:HE3   | 77:sZ:111:ARG:O    | 2.14                     | 0.47              |
| 79:s2:1432:U:H5''  | 79:s2:1433:C:H5''  | 1.96                     | 0.47              |
| 79:s2:1738:C:H2'   | 79:s2:1739:C:H6    | 1.79                     | 0.47              |
| 80:cB:209:LEU:CA   | 80:cB:257:MET:HE1  | 2.38                     | 0.47              |
| 80:cB:398:ILE:O    | 80:cB:482:THR:OG1  | 2.18                     | 0.47              |
| 80:cB:415:ARG:HA   | 80:cB:469:ILE:HA   | 1.97                     | 0.47              |
| 81:aP:30:G:H2'     | 81:aP:31:C:C6      | 2.49                     | 0.47              |
| 81:aP:53:G:H2'     | 81:aP:54:U:C6      | 2.49                     | 0.47              |
| 84:lt:34:PRO:HA    | 84:lt:37:LEU:HG    | 1.96                     | 0.47              |
| 84:lt:77:ALA:HB3   | 84:lt:80:LEU:HB3   | 1.96                     | 0.47              |
| 85:l5:504:G:H2'    | 85:l5:504:G:N3     | 2.29                     | 0.47              |
| 85:l5:1253:G:HO2'  | 85:l5:1257:A:H62   | 1.62                     | 0.47              |
| 85:l5:1372:A:C4    | 85:l5:1373:A:C8    | 3.02                     | 0.47              |
| 85:l5:4260:U:C2    | 85:l5:4261:C:C5    | 3.02                     | 0.47              |
| 85:l5:4548:A:H5'   | 85:l5:4549:G:H5'   | 1.96                     | 0.47              |
| 85:l5:4594:U:H2'   | 85:l5:4595:G:C8    | 2.49                     | 0.47              |
| 80:CB:304:ILE:HG12 | 80:CB:336:LEU:HB2  | 1.95                     | 0.47              |
| 80:CB:485:ILE:HD12 | 80:CB:486:THR:H    | 1.78                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:SI:165:GLN:CD    | 3:SI:171:LEU:HA    | 2.40                     | 0.47              |
| 6:SG:148:SER:N     | 6:SG:151:ASP:OD2   | 2.47                     | 0.47              |
| 7:SJ:91:LYS:HG3    | 7:SJ:96:TYR:CG     | 2.50                     | 0.47              |
| 11:SB:29:ASP:OD1   | 11:SB:51:ARG:NH1   | 2.47                     | 0.47              |
| 11:SB:82:ARG:HB3   | 11:SB:103:MET:CE   | 2.38                     | 0.47              |
| 11:SB:109:LYS:O    | 11:SB:112:SER:N    | 2.47                     | 0.47              |
| 85:L5:112:C:OP2    | 53:Lh:106:LYS:NZ   | 2.48                     | 0.47              |
| 85:L5:440:U:H2'    | 85:L5:441:G:H8     | 1.80                     | 0.47              |
| 85:L5:967:C:N4     | 85:L5:2259:G:O6    | 2.48                     | 0.47              |
| 85:L5:1338:G:H4'   | 85:L5:1339:U:C6    | 2.49                     | 0.47              |
| 85:L5:2077:C:O2'   | 50:Le:15:LYS:NZ    | 2.46                     | 0.47              |
| 85:L5:2654:C:H2'   | 85:L5:2655:C:C6    | 2.49                     | 0.47              |
| 85:L5:2656:U:C4    | 85:L5:2657:G:C6    | 3.02                     | 0.47              |
| 85:L5:2850:A:O3'   | 85:L5:4495:G:H5'   | 2.15                     | 0.47              |
| 85:L5:3708:C:N4    | 85:L5:3742:G:O6    | 2.34                     | 0.47              |
| 85:L5:4102:C:O5'   | 85:L5:4106:G:N3    | 2.47                     | 0.47              |
| 85:L5:4171:C:C2    | 85:L5:4172:A:C8    | 3.02                     | 0.47              |
| 85:L5:4345:C:H2'   | 85:L5:4346:U:H6    | 1.79                     | 0.47              |
| 85:L5:4476:C:O2'   | 85:L5:4478:G:OP2   | 2.27                     | 0.47              |
| 85:L5:4577:U:H3    | 85:L5:4726:G:H1    | 1.62                     | 0.47              |
| 85:L5:4621:C:H2'   | 85:L5:4622:A:C8    | 2.49                     | 0.47              |
| 85:L5:4993:G:C4    | 85:L5:4994:G:C8    | 3.03                     | 0.47              |
| 23:LB:19:ARG:HD3   | 23:LB:19:ARG:HA    | 1.64                     | 0.47              |
| 27:LF:190:LEU:HD12 | 27:LF:191:ILE:HG12 | 1.96                     | 0.47              |
| 28:LG:132:ARG:HA   | 28:LG:133:PRO:HD3  | 1.85                     | 0.47              |
| 30:LI:169:LYS:NZ   | 30:LI:179:ASP:HB3  | 2.28                     | 0.47              |
| 34:LN:6:TYR:CD1    | 54:Li:40:VAL:HG13  | 2.48                     | 0.47              |
| 34:LN:123:GLU:HG3  | 34:LN:124:ASP:H    | 1.79                     | 0.47              |
| 40:LT:64:VAL:HA    | 40:LT:74:ILE:HG22  | 1.95                     | 0.47              |
| 44:LY:47:MET:HE2   | 44:LY:48:PRO:HD2   | 1.95                     | 0.47              |
| 46:La:52:TYR:HD2   | 46:La:53:PHE:CE2   | 2.31                     | 0.47              |
| 50:Le:90:MET:HA    | 50:Le:90:MET:CE    | 2.42                     | 0.47              |
| 64:SR:8:THR:HG21   | 79:S2:1387:G:H21   | 1.79                     | 0.47              |
| 64:SR:116:ASN:CG   | 64:SR:117:LEU:H    | 2.21                     | 0.47              |
| 73:Sc:44:ARG:NH1   | 73:Sc:61:SER:O     | 2.45                     | 0.47              |
| 75:Sg:35:SER:OG    | 75:Sg:36:ARG:N     | 2.47                     | 0.47              |
| 78:Sf:133:ALA:HB3  | 78:Sf:140:TYR:HB3  | 1.96                     | 0.47              |
| 79:S2:323:C:H4'    | 79:S2:324:C:H5     | 1.79                     | 0.47              |
| 79:S2:869:A:C4     | 79:S2:915:G:H1'    | 2.49                     | 0.47              |
| 79:S2:1373:C:H2'   | 79:S2:1374:C:C6    | 2.50                     | 0.47              |
| 84:Lt:53:TRP:NE1   | 84:Lt:56:LEU:HB2   | 2.30                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:sE:137:PRO:HG2   | 2:sE:150:PRO:HD2   | 1.96                     | 0.47              |
| 6:sG:148:SER:N     | 6:sG:151:ASP:OD2   | 2.47                     | 0.47              |
| 7:sJ:15:THR:HG21   | 79:s2:22:A:O3'     | 2.14                     | 0.47              |
| 8:sY:27:VAL:HG12   | 8:sY:69:THR:HB     | 1.95                     | 0.47              |
| 15:sC:88:ILE:HG22  | 15:sC:160:LEU:HD13 | 1.96                     | 0.47              |
| 16:sN:83:ASP:OD1   | 16:sN:83:ASP:C     | 2.56                     | 0.47              |
| 17:sO:66:ARG:HB3   | 79:s2:963:A:P      | 2.55                     | 0.47              |
| 19:sb:51:GLN:HE22  | 79:s2:928:G:C4'    | 2.27                     | 0.47              |
| 21:l8:57:C:H2'     | 21:l8:58:G:C8      | 2.50                     | 0.47              |
| 22:lA:28:ARG:HB2   | 22:lA:123:ARG:CB   | 2.44                     | 0.47              |
| 22:lA:181:LYS:NZ   | 85:l5:1577:G:OP1   | 2.47                     | 0.47              |
| 23:lB:280:ILE:HD11 | 85:l5:4676:G:H4'   | 1.97                     | 0.47              |
| 24:lC:211:TYR:CZ   | 24:lC:218:ILE:HD11 | 2.49                     | 0.47              |
| 25:lD:273:LEU:HD11 | 25:lD:277:LYS:HE3  | 1.96                     | 0.47              |
| 26:lE:181:LEU:HD11 | 26:lE:268:GLN:HA   | 1.97                     | 0.47              |
| 27:lF:80:ASN:OD1   | 40:lT:143:THR:N    | 2.48                     | 0.47              |
| 27:lF:171:ASP:OD2  | 27:lF:171:ASP:C    | 2.58                     | 0.47              |
| 28:lG:140:VAL:HG13 | 85:l5:150:U:OP2    | 2.13                     | 0.47              |
| 28:lG:145:THR:O    | 28:lG:149:ASN:ND2  | 2.47                     | 0.47              |
| 29:lH:15:ASN:OD1   | 29:lH:15:ASN:C     | 2.57                     | 0.47              |
| 30:lI:209:TRP:CD1  | 30:lI:209:TRP:C    | 2.92                     | 0.47              |
| 31:lJ:118:LYS:HG2  | 31:lJ:119:TYR:H    | 1.79                     | 0.47              |
| 32:lL:90:VAL:O     | 32:lL:94:ILE:HG12  | 2.15                     | 0.47              |
| 33:lM:51:PRO:HG2   | 33:lM:54:CYS:SG    | 2.55                     | 0.47              |
| 34:lN:46:ASP:OD1   | 34:lN:46:ASP:C     | 2.57                     | 0.47              |
| 34:lN:123:GLU:O    | 34:lN:124:ASP:HB2  | 2.15                     | 0.47              |
| 42:lV:34:ALA:HB2   | 42:lV:72:LEU:HD21  | 1.96                     | 0.47              |
| 44:lY:20:ASN:N     | 44:lY:20:ASN:OD1   | 2.48                     | 0.47              |
| 44:lY:91:ASN:OD1   | 44:lY:91:ASN:C     | 2.56                     | 0.47              |
| 48:lc:11:LEU:HD23  | 79:s2:1007:C:H5'   | 1.97                     | 0.47              |
| 64:sR:5:ARG:HE     | 79:s2:1367:U:C2'   | 2.27                     | 0.47              |
| 65:sD:90:LYS:HD3   | 65:sD:90:LYS:C     | 2.39                     | 0.47              |
| 66:sF:152:TRP:HD1  | 66:sF:152:TRP:O    | 1.98                     | 0.47              |
| 68:sP:79:HIS:HB2   | 79:s2:1298:G:H1'   | 1.95                     | 0.47              |
| 71:sT:12:GLN:NE2   | 79:s2:1542:C:O4'   | 2.48                     | 0.47              |
| 78:sf:108:VAL:HA   | 78:sf:113:LYS:O    | 2.15                     | 0.47              |
| 79:s2:460:A:H1'    | 79:s2:470:G:N2     | 2.29                     | 0.47              |
| 79:s2:467:G:H2'    | 79:s2:468:A:C8     | 2.49                     | 0.47              |
| 79:s2:693:A:H2'    | 79:s2:694:G:C8     | 2.50                     | 0.47              |
| 79:s2:1240:A:H2'   | 79:s2:1241:A:C8    | 2.50                     | 0.47              |
| 79:s2:1376:A:H3'   | 79:s2:1377:U:H6    | 1.79                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 79:s2:1556:A:O2'   | 79:s2:1557:C:O4'   | 2.32                     | 0.47              |
| 80:cB:61:LYS:C     | 80:cB:62:ASP:OD1   | 2.58                     | 0.47              |
| 80:cB:123:ASP:HA   | 80:cB:368:ARG:HH12 | 1.80                     | 0.47              |
| 80:cB:143:LEU:HD11 | 80:cB:188:ILE:HD12 | 1.96                     | 0.47              |
| 80:cB:559:LYS:HE2  | 80:cB:563:GLU:HG3  | 1.96                     | 0.47              |
| 85:l5:18:C:H2'     | 85:l5:19:G:H8      | 1.79                     | 0.47              |
| 85:l5:353:A:C4     | 85:l5:379:G:C8     | 3.02                     | 0.47              |
| 85:l5:705:G:H2'    | 85:l5:706:C:H6     | 1.76                     | 0.47              |
| 85:l5:1967:A:C6    | 85:l5:2021:G:C6    | 3.02                     | 0.47              |
| 85:l5:2017:A:O2'   | 85:l5:2018:C:H6    | 1.98                     | 0.47              |
| 85:l5:3707:U:H2'   | 85:l5:3708:C:H6    | 1.80                     | 0.47              |
| 85:l5:3802:U:O2'   | 85:l5:3803:A:H5'   | 2.15                     | 0.47              |
| 85:l5:4301:U:OP2   | 85:l5:4303:C:N4    | 2.47                     | 0.47              |
| 85:l5:4597:U:H2'   | 85:l5:4598:C:O4'   | 2.14                     | 0.47              |
| 85:l5:4865:C:H2'   | 85:l5:4866:C:C6    | 2.50                     | 0.47              |
| 2:SE:92:ILE:HG12   | 2:SE:97:GLU:HB2    | 1.95                     | 0.47              |
| 3:SI:75:LYS:HD2    | 79:S2:303:C:H5'    | 1.97                     | 0.47              |
| 3:SI:76:THR:HG22   | 3:SI:108:PRO:HG2   | 1.96                     | 0.47              |
| 4:SL:93:LEU:HD12   | 4:SL:102:PHE:HB3   | 1.95                     | 0.47              |
| 6:SG:94:ARG:NH2    | 79:S2:454:U:O2'    | 2.47                     | 0.47              |
| 7:SJ:39:ASN:HD22   | 79:S2:642:U:H3'    | 1.79                     | 0.47              |
| 7:SJ:94:LEU:H      | 7:SJ:94:LEU:HD12   | 1.79                     | 0.47              |
| 10:SA:4:ALA:HB3    | 13:SV:79:VAL:HG23  | 1.96                     | 0.47              |
| 10:SA:28:THR:OG1   | 10:SA:45:GLY:O     | 2.22                     | 0.47              |
| 12:SH:105:THR:HG23 | 12:SH:107:LYS:H    | 1.80                     | 0.47              |
| 12:SH:121:THR:O    | 12:SH:125:VAL:HG13 | 2.15                     | 0.47              |
| 12:SH:146:VAL:HG11 | 18:SW:50:PHE:CE2   | 2.50                     | 0.47              |
| 12:SH:148:LEU:HA   | 18:SW:42:MET:HE1   | 1.96                     | 0.47              |
| 85:L5:340:C:H42    | 32:LL:20:ARG:NH2   | 2.12                     | 0.47              |
| 85:L5:950:G:H4'    | 51:Lf:109:ARG:HD2  | 1.96                     | 0.47              |
| 85:L5:1176:C:O3'   | 25:LD:279:ARG:NH1  | 2.47                     | 0.47              |
| 85:L5:1578:U:H2'   | 85:L5:1579:C:C6    | 2.50                     | 0.47              |
| 85:L5:1578:U:H2'   | 85:L5:1579:C:H6    | 1.79                     | 0.47              |
| 85:L5:1580:C:H2'   | 85:L5:1581:G:O4'   | 2.15                     | 0.47              |
| 85:L5:1596:U:O2'   | 36:LP:135:ARG:NH2  | 2.46                     | 0.47              |
| 85:L5:1812:C:H2'   | 85:L5:1813:U:H6    | 1.79                     | 0.47              |
| 85:L5:1952:G:H2'   | 85:L5:1953:U:H6    | 1.80                     | 0.47              |
| 85:L5:2306:G:HO2'  | 85:L5:2307:A:P     | 2.36                     | 0.47              |
| 85:L5:2693:G:OP2   | 85:L5:2694:G:O2'   | 2.32                     | 0.47              |
| 85:L5:2884:G:H2'   | 85:L5:2885:A:C8    | 2.49                     | 0.47              |
| 85:L5:3919:C:C5'   | 22:LA:207:VAL:HG12 | 2.45                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 85:L5:3943:A:H5'   | 85:L5:3944:G:OP2   | 2.14                     | 0.47              |
| 85:L5:4096:C:OP1   | 85:L5:4108:G:C5    | 2.67                     | 0.47              |
| 85:L5:4110:C:O3'   | 85:L5:4111:U:H3'   | 2.15                     | 0.47              |
| 85:L5:4457:U:O2    | 23:LB:252:ALA:HB3  | 2.14                     | 0.47              |
| 85:L5:4963:G:C2    | 85:L5:4964:C:C4    | 3.03                     | 0.47              |
| 20:L7:115:A:H2'    | 20:L7:116:G:C8     | 2.48                     | 0.47              |
| 21:L8:37:A:OP1     | 53:Lh:92:ARG:NH2   | 2.45                     | 0.47              |
| 23:LB:385:LYS:O    | 23:LB:389:MET:CB   | 2.61                     | 0.47              |
| 25:LD:262:LYS:HG2  | 25:LD:263:LYS:N    | 2.29                     | 0.47              |
| 29:LH:40:HIS:CE1   | 29:LH:41:ILE:HG12  | 2.49                     | 0.47              |
| 31:LJ:20:LEU:HD13  | 31:LJ:82:ILE:HG23  | 1.96                     | 0.47              |
| 31:LJ:134:LEU:HD11 | 31:LJ:165:TRP:CH2  | 2.49                     | 0.47              |
| 45:LZ:123:LYS:HD2  | 45:LZ:123:LYS:HA   | 1.63                     | 0.47              |
| 48:Lc:15:ASN:OD1   | 48:Lc:16:SER:N     | 2.47                     | 0.47              |
| 53:Lh:17:LEU:HB3   | 53:Lh:61:ILE:HD11  | 1.97                     | 0.47              |
| 56:Lk:6:GLU:N      | 56:Lk:6:GLU:OE1    | 2.48                     | 0.47              |
| 61:Lp:56:HIS:CD2   | 61:Lp:63:THR:HG22  | 2.49                     | 0.47              |
| 62:Lr:28:GLU:OE1   | 62:Lr:28:GLU:N     | 2.46                     | 0.47              |
| 63:Lz:116:LEU:O    | 63:Lz:120:ILE:HG12 | 2.14                     | 0.47              |
| 70:SS:54:LYS:HZ1   | 70:SS:59:LEU:HA    | 1.79                     | 0.47              |
| 71:ST:18:LEU:O     | 71:ST:22:LEU:HG    | 2.14                     | 0.47              |
| 71:ST:128:GLN:HA   | 71:ST:131:LEU:HB2  | 1.97                     | 0.47              |
| 75:Sg:175:LYS:HE3  | 75:Sg:187:ASN:OD1  | 2.15                     | 0.47              |
| 76:SM:24:THR:CG2   | 76:SM:116:LYS:HG2  | 2.44                     | 0.47              |
| 79:S2:186:C:H2'    | 79:S2:187:G:H8     | 1.79                     | 0.47              |
| 79:S2:538:U:O2     | 79:S2:546:G:C2     | 2.68                     | 0.47              |
| 79:S2:609:U:H2'    | 79:S2:610:G:H8     | 1.77                     | 0.47              |
| 79:S2:651:U:H2'    | 79:S2:652:U:C6     | 2.50                     | 0.47              |
| 79:S2:917:U:H2'    | 79:S2:918:U:C6     | 2.49                     | 0.47              |
| 79:S2:1216:C:O2'   | 79:S2:1644:C:OP1   | 2.26                     | 0.47              |
| 79:S2:1866:A:H2'   | 79:S2:1867:U:C6    | 2.49                     | 0.47              |
| 81:AP:9:A:H3'      | 81:AP:11:U:C5      | 2.50                     | 0.47              |
| 84:Lt:151:ILE:HA   | 84:Lt:154:ASP:OD1  | 2.15                     | 0.47              |
| 1:CH:76:GLU:HA     | 1:CH:79:LYS:HD2    | 1.97                     | 0.47              |
| 1:cH:26:ILE:HG12   | 79:s2:547:G:OP2    | 2.15                     | 0.47              |
| 1:cH:34:ALA:O      | 7:sJ:116:LYS:NZ    | 2.47                     | 0.47              |
| 2:sE:58:GLY:O      | 2:sE:61:VAL:HG12   | 2.13                     | 0.47              |
| 4:sL:4:ILE:HG21    | 4:sL:54:THR:O      | 2.14                     | 0.47              |
| 4:sL:97:ARG:NE     | 79:s2:421:G:OP2    | 2.47                     | 0.47              |
| 6:sG:231:ARG:NH2   | 79:s2:786:G:C8     | 2.82                     | 0.47              |
| 7:sJ:122:SER:O     | 7:sJ:124:HIS:N     | 2.46                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:sA:158:ASP:HA   | 13:sV:65:SER:OG    | 2.14                     | 0.47              |
| 12:sH:20:GLU:HB3   | 12:sH:24:SER:OG    | 2.15                     | 0.47              |
| 13:sV:76:ASP:OD1   | 13:sV:76:ASP:N     | 2.40                     | 0.47              |
| 16:sN:64:ARG:HH12  | 79:s2:919:A:P      | 2.38                     | 0.47              |
| 17:sO:40:THR:O     | 17:sO:57:THR:HG23  | 2.15                     | 0.47              |
| 17:sO:75:MET:HB3   | 17:sO:114:SER:OG   | 2.14                     | 0.47              |
| 17:sO:146:ARG:NH2  | 79:s2:1858:G:OP2   | 2.46                     | 0.47              |
| 18:sW:94:LEU:HD12  | 18:sW:100:GLY:HA3  | 1.97                     | 0.47              |
| 21:l8:4:C:H2'      | 21:l8:5:U:C6       | 2.50                     | 0.47              |
| 21:l8:115:G:H2'    | 21:l8:116:C:H6     | 1.79                     | 0.47              |
| 22:lA:178:PRO:HG3  | 61:lp:25:MET:HE1   | 1.96                     | 0.47              |
| 22:lA:181:LYS:HE2  | 85:l5:1577:G:C5    | 2.50                     | 0.47              |
| 22:lA:186:TYR:HB2  | 22:lA:196:TRP:CH2  | 2.50                     | 0.47              |
| 23:lB:14:LEU:HA    | 23:lB:17:LEU:HD22  | 1.96                     | 0.47              |
| 23:lB:145:GLN:NE2  | 23:lB:148:LYS:HE2  | 2.29                     | 0.47              |
| 23:lB:201:LEU:HD23 | 23:lB:201:LEU:HA   | 1.72                     | 0.47              |
| 23:lB:208:ASN:OD1  | 23:lB:208:ASN:N    | 2.44                     | 0.47              |
| 24:lC:121:ARG:O    | 24:lC:124:ILE:HG22 | 2.14                     | 0.47              |
| 24:lC:171:LEU:HD13 | 24:lC:180:ILE:HD11 | 1.95                     | 0.47              |
| 24:lC:211:TYR:HE1  | 24:lC:229:LEU:HB3  | 1.78                     | 0.47              |
| 26:lE:284:HIS:CE1  | 26:lE:285:LYS:HG2  | 2.48                     | 0.47              |
| 27:lF:113:ARG:NH2  | 27:lF:205:ASN:O    | 2.47                     | 0.47              |
| 27:lF:119:ASN:OD1  | 27:lF:212:LYS:NZ   | 2.47                     | 0.47              |
| 30:lI:36:LEU:HD11  | 30:lI:69:ARG:HD2   | 1.97                     | 0.47              |
| 30:lI:47:PRO:HB3   | 30:lI:171:TRP:CZ2  | 2.49                     | 0.47              |
| 30:lI:166:HIS:NE2  | 40:lT:158:PHE:HD2  | 2.11                     | 0.47              |
| 34:lN:10:LEU:HB3   | 54:li:44:ILE:HD12  | 1.96                     | 0.47              |
| 34:lN:96:ARG:HH12  | 34:lN:104:GLU:CD   | 2.22                     | 0.47              |
| 34:lN:145:ASN:OD1  | 34:lN:146:PRO:O    | 2.33                     | 0.47              |
| 34:lN:168:GLY:O    | 34:lN:172:ARG:HG3  | 2.14                     | 0.47              |
| 37:lQ:54:SER:HB2   | 85:l5:1349:G:OP2   | 2.14                     | 0.47              |
| 39:lS:170:LYS:CE   | 85:l5:4875:G:H5''  | 2.44                     | 0.47              |
| 40:lT:110:LYS:NZ   | 85:l5:1808:C:H5'   | 2.30                     | 0.47              |
| 41:lU:22:THR:HB    | 41:lU:69:LYS:HD2   | 1.97                     | 0.47              |
| 42:lV:18:LEU:HD12  | 42:lV:54:ALA:HB3   | 1.96                     | 0.47              |
| 42:lV:92:ASP:OD2   | 42:lV:94:VAL:HG22  | 2.14                     | 0.47              |
| 43:lX:53:ARG:HG2   | 85:l5:12:A:H4'     | 1.97                     | 0.47              |
| 44:lY:32:SER:OG    | 44:lY:101:PRO:O    | 2.28                     | 0.47              |
| 45:lZ:5:MET:SD     | 45:lZ:82:PRO:HB3   | 2.55                     | 0.47              |
| 48:lc:34:THR:HG23  | 48:lc:95:ALA:HB2   | 1.96                     | 0.47              |
| 53:lh:27:GLU:O     | 53:lh:30:GLN:NE2   | 2.48                     | 0.47              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 57:ll:49:LEU:HD13 | 85:l5:2407:G:P     | 2.55                     | 0.47              |
| 60:lo:61:LYS:HE2  | 60:lo:87:ARG:HH12  | 1.80                     | 0.47              |
| 60:lo:99:ARG:HH22 | 60:lo:102:GLN:HG2  | 1.80                     | 0.47              |
| 61:lp:90:LYS:HD3  | 61:lp:91:ASP:N     | 2.30                     | 0.47              |
| 62:lr:20:ARG:HH11 | 62:lr:20:ARG:HB3   | 1.80                     | 0.47              |
| 64:sR:106:LEU:HA  | 64:sR:109:LEU:CD1  | 2.44                     | 0.47              |
| 65:sD:47:GLU:OE2  | 65:sD:87:TYR:CE1   | 2.67                     | 0.47              |
| 66:sF:143:PRO:HD2 | 73:sc:51:ARG:HH22  | 1.79                     | 0.47              |
| 67:sK:35:LEU:HD12 | 67:sK:40:VAL:HG11  | 1.96                     | 0.47              |
| 68:sP:85:ILE:HD13 | 68:sP:116:LEU:HD11 | 1.97                     | 0.47              |
| 69:sQ:117:ARG:O   | 69:sQ:121:VAL:HG12 | 2.15                     | 0.47              |
| 70:sS:84:LEU:H    | 70:sS:84:LEU:HD12  | 1.78                     | 0.47              |
| 70:sS:137:LYS:NZ  | 79:s2:1236:G:H1    | 2.12                     | 0.47              |
| 71:sT:59:SER:OG   | 71:sT:79:TYR:OH    | 2.27                     | 0.47              |
| 71:sT:82:ARG:NH2  | 79:s2:1653:U:O3'   | 2.48                     | 0.47              |
| 72:sU:22:ILE:HG23 | 72:sU:89:ILE:HB    | 1.95                     | 0.47              |
| 72:sU:94:PRO:O    | 72:sU:97:ILE:HG12  | 2.14                     | 0.47              |
| 73:sc:33:GLU:N    | 73:sc:33:GLU:OE1   | 2.48                     | 0.47              |
| 75:sg:44:LYS:HG3  | 75:sg:56:GLN:CD    | 2.39                     | 0.47              |
| 75:sg:121:VAL:HB  | 75:sg:129:ILE:HD11 | 1.97                     | 0.47              |
| 77:sZ:47:LEU:HD23 | 77:sZ:80:ARG:HB2   | 1.96                     | 0.47              |
| 77:sZ:98:LYS:HE3  | 77:sZ:112:ASN:HA   | 1.95                     | 0.47              |
| 79:s2:402:C:C2    | 79:s2:403:G:C8     | 3.02                     | 0.47              |
| 79:s2:608:C:H2'   | 79:s2:609:U:C6     | 2.50                     | 0.47              |
| 79:s2:1259:A:N6   | 79:s2:1518:C:H3'   | 2.26                     | 0.47              |
| 79:s2:1259:A:N6   | 79:s2:1519:U:O5'   | 2.48                     | 0.47              |
| 79:s2:1260:A:C8   | 79:s2:1261:C:H5    | 2.33                     | 0.47              |
| 79:s2:1269:G:H2'  | 79:s2:1270:G:C8    | 2.49                     | 0.47              |
| 79:s2:1276:A:C5   | 79:s2:1322:G:H1'   | 2.50                     | 0.47              |
| 79:s2:1501:C:H2'  | 79:s2:1502:C:H6    | 1.80                     | 0.47              |
| 79:s2:1545:A:H2'  | 79:s2:1546:G:C8    | 2.49                     | 0.47              |
| 79:s2:1855:G:H2'  | 79:s2:1856:C:C6    | 2.50                     | 0.47              |
| 80:cB:28:VAL:HG12 | 80:cB:108:HIS:HA   | 1.95                     | 0.47              |
| 80:cB:196:GLU:HG3 | 80:cB:197:SER:H    | 1.79                     | 0.47              |
| 80:cB:259:LYS:HE2 | 80:cB:273:PHE:HD2  | 1.78                     | 0.47              |
| 80:cB:329:ASP:OD2 | 80:cB:330:LYS:N    | 2.47                     | 0.47              |
| 80:cB:554:LEU:HA  | 80:cB:557:CYS:SG   | 2.54                     | 0.47              |
| 80:cB:627:GLU:OE2 | 80:cB:628:LEU:N    | 2.46                     | 0.47              |
| 81:aP:4:U:H2'     | 81:aP:5:C:H6       | 1.78                     | 0.47              |
| 84:lt:65:GLN:HG2  | 84:lt:70:GLN:CD    | 2.39                     | 0.47              |
| 84:lt:146:ARG:HG3 | 84:lt:151:ILE:HD11 | 1.96                     | 0.47              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 85:l5:163:A:H2'    | 85:l5:164:G:C8    | 2.49                     | 0.47              |
| 85:l5:260:C:H2'    | 85:l5:261:G:H8    | 1.79                     | 0.47              |
| 85:l5:920:C:H2'    | 85:l5:921:C:H6    | 1.80                     | 0.47              |
| 85:l5:1305:C:H2'   | 85:l5:1306:C:H6   | 1.80                     | 0.47              |
| 85:l5:1334:A:H2'   | 85:l5:1335:G:H8   | 1.80                     | 0.47              |
| 85:l5:1356:U:H2'   | 85:l5:1357:C:C6   | 2.49                     | 0.47              |
| 85:l5:1764:G:H8    | 85:l5:1766:A:OP2  | 1.98                     | 0.47              |
| 85:l5:1806:G:H2'   | 85:l5:1807:C:C6   | 2.50                     | 0.47              |
| 85:l5:2012:A:C2    | 85:l5:2013:A:H1'  | 2.50                     | 0.47              |
| 85:l5:2491:C:H2'   | 85:l5:2492:C:C6   | 2.50                     | 0.47              |
| 85:l5:2748:C:H2'   | 85:l5:2749:C:C6   | 2.50                     | 0.47              |
| 85:l5:2826:U:H4'   | 85:l5:2827:G:O4'  | 2.15                     | 0.47              |
| 85:l5:2870:A:H2'   | 85:l5:2871:A:H8   | 1.79                     | 0.47              |
| 85:l5:2884:G:H2'   | 85:l5:2885:A:H8   | 1.79                     | 0.47              |
| 85:l5:2897:G:H2'   | 85:l5:2898:G:C8   | 2.48                     | 0.47              |
| 85:l5:3911:C:H2'   | 85:l5:3912:U:C6   | 2.49                     | 0.47              |
| 85:l5:3936:A:N6    | 85:l5:4175:G:O6   | 2.48                     | 0.47              |
| 85:l5:4236:G:H2'   | 85:l5:4237:C:H6   | 1.79                     | 0.47              |
| 85:l5:4508:C:N3    | 85:l5:4512:U:H5   | 2.13                     | 0.47              |
| 85:l5:4565:C:H2'   | 85:l5:4566:U:H6   | 1.80                     | 0.47              |
| 85:l5:4600:G:H1'   | 85:l5:4601:U:H5   | 1.80                     | 0.47              |
| 85:l5:4629:U:C2    | 85:l5:4630:G:C8   | 3.03                     | 0.47              |
| 80:CB:27:HIS:CE1   | 80:CB:28:VAL:HG22 | 2.50                     | 0.47              |
| 80:CB:90:LYS:HD3   | 80:CB:90:LYS:HA   | 1.61                     | 0.47              |
| 80:CB:568:ILE:HD12 | 80:CB:569:PRO:HD2 | 1.97                     | 0.47              |
| 2:SE:229:GLY:HA3   | 2:SE:234:PRO:HA   | 1.95                     | 0.47              |
| 11:SB:167:LYS:HD2  | 11:SB:170:GLU:OE1 | 2.15                     | 0.47              |
| 12:SH:98:ARG:HG3   | 12:SH:125:VAL:HB  | 1.97                     | 0.47              |
| 15:SC:183:LYS:HA   | 15:SC:195:LEU:O   | 2.14                     | 0.47              |
| 15:SC:206:SER:HG   | 15:SC:210:PRO:HG2 | 1.79                     | 0.47              |
| 15:SC:207:ALA:HB2  | 79:S2:4:C:H4'     | 1.96                     | 0.47              |
| 15:SC:254:ASP:O    | 15:SC:257:LYS:NZ  | 2.48                     | 0.47              |
| 18:SW:22:LYS:HA    | 19:Sb:3:LEU:CD1   | 2.45                     | 0.47              |
| 85:L5:62:A:N3      | 85:L5:77:U:O2'    | 2.45                     | 0.47              |
| 85:L5:89:C:H4'     | 85:L5:293:G:H5'   | 1.97                     | 0.47              |
| 85:L5:271:C:C2     | 85:L5:272:U:C5    | 3.03                     | 0.47              |
| 85:L5:342:G:H2'    | 85:L5:343:C:C6    | 2.50                     | 0.47              |
| 85:L5:469:C:H2'    | 85:L5:470:A:O4'   | 2.15                     | 0.47              |
| 85:L5:699:C:O2'    | 85:L5:968:C:O2    | 2.31                     | 0.47              |
| 85:L5:705:G:H2'    | 85:L5:706:C:C6    | 2.49                     | 0.47              |
| 85:L5:1238:A:H2'   | 27:LF:51:TYR:HE2  | 1.80                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 85:L5:1253:G:H4'   | 85:L5:1254:A:N7    | 2.29                     | 0.47              |
| 85:L5:1302:U:H3'   | 85:L5:1303:A:H8    | 1.79                     | 0.47              |
| 85:L5:1373:A:H2'   | 85:L5:1374:G:H8    | 1.80                     | 0.47              |
| 85:L5:1387:A:O2'   | 85:L5:1396:G:N2    | 2.48                     | 0.47              |
| 85:L5:1418:C:H2'   | 85:L5:1419:G:C8    | 2.50                     | 0.47              |
| 85:L5:1431:C:H2'   | 85:L5:1432:G:O4'   | 2.15                     | 0.47              |
| 85:L5:1502:G:OP2   | 37:LQ:62:SER:OG    | 2.29                     | 0.47              |
| 85:L5:1554:A:OP2   | 61:Lp:4:ARG:NE     | 2.42                     | 0.47              |
| 85:L5:1569:U:H2'   | 85:L5:1570:G:C8    | 2.50                     | 0.47              |
| 85:L5:1999:A:H2'   | 85:L5:2000:G:C4    | 2.49                     | 0.47              |
| 85:L5:2020:U:O3'   | 83:Ls:57:LYS:HA    | 2.15                     | 0.47              |
| 85:L5:2669:C:H2'   | 85:L5:2670:C:O4'   | 2.14                     | 0.47              |
| 85:L5:2732:G:H2'   | 85:L5:2733:C:C6    | 2.50                     | 0.47              |
| 85:L5:2904:U:H3'   | 85:L5:2904:U:OP2   | 2.14                     | 0.47              |
| 85:L5:3613:U:H2'   | 85:L5:3614:G:C8    | 2.49                     | 0.47              |
| 85:L5:3696:C:O2'   | 85:L5:3816:A:N1    | 2.46                     | 0.47              |
| 85:L5:4100:C:O3'   | 85:L5:4107:G:OP2   | 2.33                     | 0.47              |
| 85:L5:4160:C:H2'   | 85:L5:4161:G:C8    | 2.49                     | 0.47              |
| 85:L5:4357:G:H2'   | 85:L5:4358:U:H6    | 1.80                     | 0.47              |
| 85:L5:4505:C:H2'   | 85:L5:4506:C:H6    | 1.79                     | 0.47              |
| 85:L5:4602:A:H5''  | 29:LH:98:HIS:CE1   | 2.49                     | 0.47              |
| 85:L5:4713:G:C5    | 85:L5:4714:C:C5    | 3.02                     | 0.47              |
| 85:L5:4901:G:H2'   | 85:L5:4902:C:O4'   | 2.14                     | 0.47              |
| 85:L5:4928:C:H2'   | 33:LM:118:MET:HE2  | 1.96                     | 0.47              |
| 85:L5:4929:C:H2'   | 85:L5:4930:C:H6    | 1.78                     | 0.47              |
| 85:L5:4947:U:H2'   | 85:L5:4948:C:C6    | 2.50                     | 0.47              |
| 85:L5:4998:G:H2'   | 85:L5:4999:G:H8    | 1.80                     | 0.47              |
| 85:L5:5002:U:H2'   | 85:L5:5003:U:H6    | 1.79                     | 0.47              |
| 85:L5:5010:U:H2'   | 85:L5:5011:A:H8    | 1.79                     | 0.47              |
| 21:L8:13:G:C4      | 21:L8:14:U:C5      | 3.02                     | 0.47              |
| 21:L8:20:A:H2'     | 21:L8:21:C:C6      | 2.49                     | 0.47              |
| 23:LB:289:GLN:HB3  | 23:LB:301:ASN:HD22 | 1.79                     | 0.47              |
| 24:LC:35:ASP:OD1   | 24:LC:35:ASP:N     | 2.47                     | 0.47              |
| 25:LD:91:GLY:O     | 25:LD:94:ASN:ND2   | 2.45                     | 0.47              |
| 26:LE:264:ILE:HD11 | 26:LE:267:LEU:HD22 | 1.96                     | 0.47              |
| 27:LF:182:TYR:HB3  | 27:LF:200:ARG:HG3  | 1.97                     | 0.47              |
| 28:LG:108:GLN:O    | 28:LG:112:GLN:HG2  | 2.15                     | 0.47              |
| 28:LG:174:CYS:HB2  | 28:LG:181:TYR:HD1  | 1.80                     | 0.47              |
| 28:LG:182:CYS:HA   | 28:LG:226:TYR:CE2  | 2.49                     | 0.47              |
| 30:LI:9:TYR:CE2    | 30:LI:97:ILE:HD13  | 2.50                     | 0.47              |
| 31:LJ:158:SER:OG   | 31:LJ:159:LYS:N    | 2.47                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 32:LL:79:GLU:O     | 32:LL:82:ARG:HG2   | 2.14                     | 0.47              |
| 33:LM:41:PRO:HG3   | 33:LM:74:ARG:HG2   | 1.96                     | 0.47              |
| 34:LN:68:ARG:HD3   | 34:LN:125:SER:O    | 2.14                     | 0.47              |
| 34:LN:150:TRP:CD1  | 34:LN:150:TRP:N    | 2.82                     | 0.47              |
| 37:LQ:122:THR:O    | 37:LQ:125:GLN:HG2  | 2.14                     | 0.47              |
| 38:LR:140:GLU:HB3  | 38:LR:144:LYS:NZ   | 2.29                     | 0.47              |
| 38:LR:168:GLU:O    | 38:LR:172:ARG:HG3  | 2.14                     | 0.47              |
| 40:LT:50:LYS:HE3   | 40:LT:50:LYS:HB3   | 1.66                     | 0.47              |
| 44:LY:39:ARG:NH1   | 44:LY:45:ARG:HG3   | 2.29                     | 0.47              |
| 45:LZ:97:ASN:OD1   | 45:LZ:100:VAL:HG23 | 2.14                     | 0.47              |
| 53:Lh:117:ARG:HA   | 53:Lh:117:ARG:HD2  | 1.68                     | 0.47              |
| 63:Lz:1:MET:N      | 63:Lz:1:MET:SD     | 2.87                     | 0.47              |
| 63:Lz:39:LYS:HD3   | 63:Lz:41:TYR:CE2   | 2.50                     | 0.47              |
| 63:Lz:193:LEU:O    | 63:Lz:194:LEU:HG   | 2.14                     | 0.47              |
| 68:SP:43:ARG:NH2   | 79:S2:1617:G:N7    | 2.62                     | 0.47              |
| 69:SQ:22:VAL:CG2   | 69:SQ:71:ARG:HE    | 2.28                     | 0.47              |
| 69:SQ:47:LEU:HB3   | 69:SQ:50:LYS:HG3   | 1.96                     | 0.47              |
| 72:SU:61:LEU:HD23  | 72:SU:82:MET:HB3   | 1.97                     | 0.47              |
| 75:Sg:225:LYS:HZ2  | 75:Sg:226:HIS:H    | 1.61                     | 0.47              |
| 76:SM:84:LYS:HG3   | 76:SM:88:TRP:NE1   | 2.29                     | 0.47              |
| 77:SZ:46:ASN:O     | 77:SZ:78:LYS:HG2   | 2.15                     | 0.47              |
| 79:S2:17:C:H2'     | 79:S2:18:C:H6      | 1.78                     | 0.47              |
| 79:S2:149:A:N7     | 79:S2:169:U:O2     | 2.48                     | 0.47              |
| 79:S2:360:A:C2     | 79:S2:363:A:H5'    | 2.50                     | 0.47              |
| 79:S2:535:G:N2     | 79:S2:536:A:H62    | 2.13                     | 0.47              |
| 79:S2:1075:C:H2'   | 79:S2:1076:G:C8    | 2.50                     | 0.47              |
| 79:S2:1265:A:O2'   | 79:S2:1327:G:OP2   | 2.22                     | 0.47              |
| 79:S2:1387:G:H2'   | 79:S2:1388:A:O4'   | 2.15                     | 0.47              |
| 79:S2:1568:C:H2'   | 79:S2:1569:A:N9    | 2.29                     | 0.47              |
| 79:S2:1758:G:O3'   | 79:S2:1774:C:N4    | 2.47                     | 0.47              |
| 83:Ls:123:VAL:HG12 | 83:Ls:180:ILE:CD1  | 2.40                     | 0.47              |
| 1:cH:100:ASN:HD21  | 79:s2:635:G:H22    | 1.63                     | 0.47              |
| 3:sI:42:ARG:CZ     | 3:sI:59:ARG:HH22   | 2.27                     | 0.47              |
| 4:sL:29:GLY:HA3    | 4:sL:30:LYS:HA     | 1.49                     | 0.47              |
| 6:sG:6:SER:HA      | 6:sG:13:GLN:HB3    | 1.95                     | 0.47              |
| 6:sG:136:LYS:HB2   | 79:s2:170:A:O5'    | 2.15                     | 0.47              |
| 7:sJ:22:LYS:HE2    | 79:s2:604:A:H5''   | 1.97                     | 0.47              |
| 10:sA:125:THR:HA   | 10:sA:147:LEU:HB3  | 1.96                     | 0.47              |
| 15:sC:65:LYS:O     | 15:sC:69:LEU:HG    | 2.15                     | 0.47              |
| 22:lA:80:GLU:OE2   | 61:lp:73:THR:HG23  | 2.15                     | 0.47              |
| 23:lB:21:ARG:HB3   | 23:lB:274:TYR:HD2  | 1.80                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:1C:9:SER:HA     | 24:1C:21:ASN:HA    | 1.96                     | 0.47              |
| 24:1C:134:PRO:O    | 24:1C:138:MET:HG2  | 2.14                     | 0.47              |
| 24:1C:163:LYS:NZ   | 85:15:224:U:OP1    | 2.38                     | 0.47              |
| 24:1C:268:ARG:HH22 | 85:15:654:C:H5'    | 1.80                     | 0.47              |
| 27:1F:40:LYS:HE3   | 27:1F:40:LYS:HB2   | 1.71                     | 0.47              |
| 27:1F:154:ILE:HG21 | 27:1F:191:ILE:CD1  | 2.44                     | 0.47              |
| 34:1N:135:ILE:HD12 | 34:1N:135:ILE:HA   | 1.56                     | 0.47              |
| 35:1O:82:ARG:NH1   | 85:15:3887:C:OP2   | 2.44                     | 0.47              |
| 36:1P:50:ASP:OD1   | 36:1P:56:GLN:NE2   | 2.48                     | 0.47              |
| 37:1Q:4:ASP:O      | 37:1Q:4:ASP:OD1    | 2.32                     | 0.47              |
| 41:1U:103:VAL:HG11 | 85:15:2702:C:H4'   | 1.97                     | 0.47              |
| 49:1d:75:LYS:HB2   | 49:1d:79:ASN:O     | 2.14                     | 0.47              |
| 65:sD:122:VAL:O    | 65:sD:126:ILE:HG23 | 2.14                     | 0.47              |
| 65:sD:157:MET:HE3  | 65:sD:187:LYS:HE2  | 1.97                     | 0.47              |
| 75:sg:43:TRP:HA    | 75:sg:54:ILE:O     | 2.15                     | 0.47              |
| 79:s2:613:G:O2'    | 79:s2:626:G:H4'    | 2.14                     | 0.47              |
| 79:s2:799:U:C4     | 79:s2:800:U:C4     | 3.03                     | 0.47              |
| 79:s2:857:U:H2'    | 79:s2:858:A:C8     | 2.50                     | 0.47              |
| 79:s2:1210:G:H3'   | 79:s2:1211:G:P     | 2.55                     | 0.47              |
| 79:s2:1287:A:H2'   | 79:s2:1315:U:O2    | 2.14                     | 0.47              |
| 79:s2:1593:C:H2'   | 79:s2:1594:A:H8    | 1.79                     | 0.47              |
| 79:s2:1601:A:O4'   | 79:s2:1636:G:N2    | 2.43                     | 0.47              |
| 80:cB:206:ASP:HB3  | 80:cB:209:LEU:CD2  | 2.45                     | 0.47              |
| 80:cB:401:MET:HE1  | 80:cB:529:LYS:HB3  | 1.97                     | 0.47              |
| 80:cB:428:ARG:HB3  | 80:cB:428:ARG:CZ   | 2.44                     | 0.47              |
| 80:cB:753:GLU:O    | 80:cB:756:VAL:HG23 | 2.15                     | 0.47              |
| 82:pE:41:U:H2'     | 82:pE:42:G:H8      | 1.79                     | 0.47              |
| 85:15:734:G:C2     | 85:15:735:G:C8     | 3.03                     | 0.47              |
| 85:15:1180:C:O2    | 85:15:1183:C:N4    | 2.48                     | 0.47              |
| 85:15:1274:A:O2'   | 85:15:1275:G:H8    | 1.98                     | 0.47              |
| 85:15:1406:G:C6    | 85:15:1412:G:C6    | 3.02                     | 0.47              |
| 85:15:1430:C:C2    | 85:15:1455:G:C2    | 3.02                     | 0.47              |
| 85:15:1475:G:H2'   | 85:15:1476:C:C6    | 2.50                     | 0.47              |
| 85:15:1669:A:H4'   | 85:15:1685:G:H22   | 1.78                     | 0.47              |
| 85:15:2843:U:O2'   | 85:15:4632:U:OP1   | 2.30                     | 0.47              |
| 85:15:2870:A:H2'   | 85:15:2871:A:C8    | 2.50                     | 0.47              |
| 85:15:3695:U:H2'   | 85:15:3696:C:H6    | 1.80                     | 0.47              |
| 85:15:3923:A:H2'   | 85:15:3924:C:C6    | 2.50                     | 0.47              |
| 85:15:4729:A:H5''  | 85:15:4965:U:H1'   | 1.97                     | 0.47              |
| 85:15:4769:G:H5'   | 85:15:4873:G:H1    | 1.80                     | 0.47              |
| 85:15:4770:U:H2'   | 85:15:4771:C:C5    | 2.49                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 80:CB:45:ILE:CD1   | 80:CB:77:LEU:C     | 2.88                     | 0.47              |
| 80:CB:144:ARG:HH22 | 80:CB:809:PHE:HE2  | 1.63                     | 0.47              |
| 80:CB:592:LEU:HG   | 80:CB:602:LEU:O    | 2.15                     | 0.47              |
| 2:SE:11:ARG:HD2    | 2:SE:25:GLY:O      | 2.15                     | 0.47              |
| 3:SI:2:GLY:N       | 79:S2:441:C:OP1    | 2.47                     | 0.47              |
| 3:SI:104:ILE:O     | 3:SI:171:LEU:N     | 2.48                     | 0.47              |
| 4:SL:113:LEU:HD11  | 4:SL:117:PHE:HB2   | 1.97                     | 0.47              |
| 5:SX:67:ARG:HH22   | 79:S2:618:C:H41    | 1.62                     | 0.47              |
| 10:SA:19:LEU:HD12  | 64:SR:96:ILE:HD13  | 1.97                     | 0.47              |
| 14:Sa:17:HIS:HB3   | 79:S2:999:G:C8     | 2.50                     | 0.47              |
| 14:Sa:57:SER:OG    | 14:Sa:59:PHE:O     | 2.24                     | 0.47              |
| 17:SO:78:ALA:HB3   | 17:SO:118:ALA:HB3  | 1.97                     | 0.47              |
| 19:Sb:19:HIS:HB3   | 19:Sb:22:LYS:HG2   | 1.97                     | 0.47              |
| 85:L5:15:A:H2'     | 85:L5:16:G:O4'     | 2.14                     | 0.47              |
| 85:L5:129:C:H2'    | 85:L5:130:C:C6     | 2.49                     | 0.47              |
| 85:L5:440:U:H2'    | 85:L5:441:G:C8     | 2.50                     | 0.47              |
| 85:L5:1310:C:H2'   | 85:L5:1311:G:O4'   | 2.15                     | 0.47              |
| 85:L5:1372:A:C4    | 85:L5:1373:A:C8    | 3.03                     | 0.47              |
| 85:L5:1450:C:H2'   | 85:L5:1451:G:O4'   | 2.15                     | 0.47              |
| 85:L5:1981:G:H2'   | 85:L5:1982:G:C8    | 2.49                     | 0.47              |
| 85:L5:2458:C:H1'   | 85:L5:3671:G:H21   | 1.79                     | 0.47              |
| 85:L5:2691:U:H2'   | 85:L5:2692:U:C6    | 2.50                     | 0.47              |
| 85:L5:2864:A:H2'   | 85:L5:2865:U:C6    | 2.50                     | 0.47              |
| 85:L5:3710:G:N2    | 85:L5:3711:A:H62   | 2.13                     | 0.47              |
| 85:L5:4383:U:H2'   | 85:L5:4384:U:C6    | 2.49                     | 0.47              |
| 20:L7:62:U:O2'     | 20:L7:64:G:O4'     | 2.32                     | 0.47              |
| 21:L8:83:C:N3      | 44:LY:50:ARG:NH2   | 2.63                     | 0.47              |
| 21:L8:142:U:C2     | 21:L8:143:G:C8     | 3.03                     | 0.47              |
| 23:LB:90:VAL:HB    | 23:LB:163:ILE:HD11 | 1.97                     | 0.47              |
| 26:LE:223:ARG:HA   | 26:LE:224:LYS:HA   | 1.71                     | 0.47              |
| 28:LG:60:TYR:O     | 28:LG:64:GLN:HG2   | 2.15                     | 0.47              |
| 34:LN:25:VAL:O     | 34:LN:29:GLN:HG3   | 2.14                     | 0.47              |
| 36:LP:47:TYR:O     | 36:LP:51:VAL:HG23  | 2.14                     | 0.47              |
| 40:LT:17:ARG:HB2   | 40:LT:22:HIS:CD2   | 2.50                     | 0.47              |
| 43:LX:145:ASP:OD2  | 43:LX:148:ASP:N    | 2.32                     | 0.47              |
| 44:LY:2:LYS:NZ     | 44:LY:7:VAL:HG13   | 2.30                     | 0.47              |
| 54:Li:58:MET:HB2   | 54:Li:62:LYS:HZ1   | 1.78                     | 0.47              |
| 58:Lm:94:MET:HG2   | 58:Lm:104:HIS:O    | 2.13                     | 0.47              |
| 63:Lz:60:ARG:HB3   | 63:Lz:61:PRO:HD3   | 1.97                     | 0.47              |
| 64:SR:51:ALA:O     | 64:SR:55:THR:HG23  | 2.14                     | 0.47              |
| 66:SF:30:ILE:HD11  | 66:SF:35:LEU:HD21  | 1.96                     | 0.47              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 71:ST:133:ARG:O    | 71:ST:137:GLN:OE1 | 2.32                     | 0.47              |
| 74:Sd:22:ARG:NH1   | 79:S2:1553:C:H41  | 2.13                     | 0.47              |
| 79:S2:37:C:H3'     | 79:S2:38:A:H8     | 1.80                     | 0.47              |
| 79:S2:336:A:H2'    | 79:S2:337:C:O4'   | 2.14                     | 0.47              |
| 79:S2:614:C:H2'    | 79:S2:626:G:C8    | 2.50                     | 0.47              |
| 79:S2:642:U:H4'    | 79:S2:644:G:H4'   | 1.97                     | 0.47              |
| 79:S2:804:U:C2     | 79:S2:860:G:N2    | 2.83                     | 0.47              |
| 79:S2:1238:U:O2    | 79:S2:1242:U:H5   | 1.98                     | 0.47              |
| 79:S2:1369:A:H2'   | 79:S2:1370:A:C8   | 2.50                     | 0.47              |
| 79:S2:1500:G:H2'   | 79:S2:1501:C:C6   | 2.50                     | 0.47              |
| 79:S2:1772:C:O2    | 79:S2:1772:C:H2'  | 2.15                     | 0.47              |
| 84:Lt:61:LYS:NZ    | 84:Lt:63:THR:OG1  | 2.38                     | 0.47              |
| 1:cH:93:LYS:O      | 1:cH:97:THR:HG23  | 2.15                     | 0.47              |
| 3:sI:27:TYR:CE1    | 79:s2:349:A:H4'   | 2.49                     | 0.47              |
| 5:sX:90:CYS:O      | 5:sX:94:ILE:HG22  | 2.14                     | 0.47              |
| 6:sG:85:ARG:HH22   | 8:sY:118:ARG:HG2  | 1.79                     | 0.47              |
| 6:sG:147:LEU:HB3   | 6:sG:151:ASP:CB   | 2.44                     | 0.47              |
| 9:se:12:VAL:O      | 9:se:16:THR:HG23  | 2.15                     | 0.47              |
| 11:sB:158:HIS:N    | 79:s2:932:G:OP1   | 2.42                     | 0.47              |
| 12:sH:160:LYS:HA   | 12:sH:189:PHE:CD2 | 2.49                     | 0.47              |
| 13:sV:24:ILE:HD13  | 13:sV:31:SER:HB2  | 1.96                     | 0.47              |
| 13:sV:67:ASP:O     | 13:sV:71:ARG:HG3  | 2.15                     | 0.47              |
| 15:sC:194:ARG:HH21 | 79:s2:1155:U:P    | 2.38                     | 0.47              |
| 16:sN:39:LYS:HA    | 16:sN:42:LYS:CE   | 2.45                     | 0.47              |
| 22:lA:32:VAL:HG12  | 22:lA:37:ARG:HH21 | 1.80                     | 0.47              |
| 23:lB:83:PRO:HB2   | 23:lB:204:GLN:HG2 | 1.97                     | 0.47              |
| 28:lG:150:LYS:NZ   | 28:lG:177:MET:HB2 | 2.29                     | 0.47              |
| 29:lH:150:ASP:OD1  | 29:lH:151:ILE:N   | 2.48                     | 0.47              |
| 32:lL:100:PRO:O    | 54:li:25:ARG:NH2  | 2.48                     | 0.47              |
| 35:lO:93:LYS:CD    | 85:l5:1308:C:H5'' | 2.45                     | 0.47              |
| 36:lP:115:GLU:OE2  | 36:lP:151:THR:CG2 | 2.62                     | 0.47              |
| 37:lQ:72:LEU:HD12  | 37:lQ:75:ARG:NH1  | 2.30                     | 0.47              |
| 39:lS:11:LYS:NZ    | 39:lS:67:VAL:HG22 | 2.30                     | 0.47              |
| 46:la:126:ALA:HB3  | 46:la:129:PHE:CZ  | 2.49                     | 0.47              |
| 47:lb:57:MET:HE3   | 85:l5:1811:G:H21  | 1.80                     | 0.47              |
| 55:lj:46:LYS:HB3   | 55:lj:46:LYS:HE2  | 1.68                     | 0.47              |
| 63:lz:95:LYS:HD2   | 63:lz:104:ALA:HB1 | 1.97                     | 0.47              |
| 64:sR:5:ARG:HG2    | 64:sR:9:VAL:HG23  | 1.96                     | 0.47              |
| 67:sK:34:GLU:N     | 67:sK:34:GLU:CD   | 2.73                     | 0.47              |
| 69:sQ:8:GLN:HE22   | 69:sQ:27:ARG:CZ   | 2.28                     | 0.47              |
| 69:sQ:130:LYS:NZ   | 79:s2:1669:G:OP2  | 2.32                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 70:sS:104:ASP:OD1  | 70:sS:104:ASP:N    | 2.48                     | 0.47              |
| 75:sg:89:LEU:HD12  | 75:sg:98:THR:HB    | 1.96                     | 0.47              |
| 75:sg:139:LYS:HG3  | 75:sg:140:TYR:H    | 1.80                     | 0.47              |
| 76:sM:47:ALA:HB1   | 76:sM:110:VAL:HG21 | 1.97                     | 0.47              |
| 79:s2:1121:G:C4    | 79:s2:1122:A:C8    | 3.03                     | 0.47              |
| 79:s2:1214:A:C2    | 79:s2:1217:A:C8    | 3.03                     | 0.47              |
| 79:s2:1352:G:H2'   | 79:s2:1353:A:C8    | 2.50                     | 0.47              |
| 80:cB:762:VAL:HG21 | 80:cB:800:LEU:HD13 | 1.97                     | 0.47              |
| 85:l5:750:U:H1'    | 85:l5:917:A:C8     | 2.49                     | 0.47              |
| 85:l5:3608:A:H2'   | 85:l5:3609:G:C8    | 2.50                     | 0.47              |
| 85:l5:3730:U:H2'   | 85:l5:3731:C:H6    | 1.80                     | 0.47              |
| 85:l5:3805:U:H2'   | 85:l5:3806:G:C8    | 2.48                     | 0.47              |
| 85:l5:3911:C:C2    | 85:l5:3912:U:C5    | 3.03                     | 0.47              |
| 85:l5:4499:G:N2    | 85:l5:4529:G:H1'   | 2.30                     | 0.47              |
| 85:l5:4640:C:H2'   | 85:l5:4641:U:C6    | 2.49                     | 0.47              |
| 85:l5:4642:U:H2'   | 85:l5:4643:G:C8    | 2.50                     | 0.47              |
| 85:l5:4959:U:H2'   | 85:l5:4960:G:C8    | 2.49                     | 0.47              |
| 4:SL:32:LYS:HD3    | 4:SL:33:LEU:N      | 2.29                     | 0.47              |
| 10:SA:42:LYS:HZ2   | 10:SA:44:ASP:HB3   | 1.79                     | 0.47              |
| 11:SB:187:LYS:NZ   | 11:SB:192:SER:OG   | 2.47                     | 0.47              |
| 15:SC:104:ASP:OD1  | 15:SC:105:GLU:N    | 2.48                     | 0.47              |
| 15:SC:108:LYS:NZ   | 15:SC:233:LEU:HB3  | 2.30                     | 0.47              |
| 17:SO:95:ILE:HB    | 17:SO:129:ILE:HD13 | 1.95                     | 0.47              |
| 85:L5:25:A:H2'     | 85:L5:26:C:C6      | 2.49                     | 0.47              |
| 85:L5:80:C:H2'     | 85:L5:81:C:H6      | 1.80                     | 0.47              |
| 85:L5:173:C:OP1    | 32:LL:129:ARG:NH1  | 2.47                     | 0.47              |
| 85:L5:181:C:H3'    | 85:L5:182:G:C8     | 2.43                     | 0.47              |
| 85:L5:481:G:H2'    | 85:L5:482:G:C8     | 2.50                     | 0.47              |
| 85:L5:667:A:H5'    | 62:Lr:46:ARG:HH22  | 1.80                     | 0.47              |
| 85:L5:958:G:C2     | 26:LE:124:LYS:HD2  | 2.50                     | 0.47              |
| 85:L5:1185:G:H2'   | 85:L5:1186:U:C6    | 2.49                     | 0.47              |
| 85:L5:1688:G:H2'   | 85:L5:1689:G:C8    | 2.50                     | 0.47              |
| 85:L5:1778:C:H2'   | 85:L5:1779:U:C6    | 2.49                     | 0.47              |
| 85:L5:1922:G:OP1   | 39:LS:160:ARG:NH1  | 2.48                     | 0.47              |
| 85:L5:2349:A:H61   | 24:LC:95:MET:CE    | 2.28                     | 0.47              |
| 85:L5:2402:G:C2    | 85:L5:2403:A:C8    | 3.03                     | 0.47              |
| 85:L5:2478:C:O2    | 85:L5:2591:A:O2'   | 2.32                     | 0.47              |
| 85:L5:2521:G:H2'   | 85:L5:2522:G:C8    | 2.49                     | 0.47              |
| 85:L5:2675:G:O6    | 48:Lc:30:GLY:HA3   | 2.15                     | 0.47              |
| 85:L5:3615:G:H1'   | 87:LW:44:ARG:HD2   | 1.97                     | 0.47              |
| 85:L5:4059:C:O2'   | 85:L5:4060:U:H5'   | 2.14                     | 0.47              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 85:L5:4597:U:H2'  | 85:L5:4598:C:O4'   | 2.15                     | 0.47              |
| 85:L5:4600:G:O2'  | 85:L5:4601:U:P     | 2.73                     | 0.47              |
| 85:L5:4765:G:H2'  | 85:L5:4766:C:O4'   | 2.15                     | 0.47              |
| 23:LB:162:VAL:N   | 23:LB:183:ILE:O    | 2.39                     | 0.47              |
| 25:LD:116:ASP:OD1 | 25:LD:117:LYS:N    | 2.48                     | 0.47              |
| 31:LJ:121:PRO:CD  | 70:SS:101:ASN:CG   | 2.88                     | 0.47              |
| 31:LJ:136:ARG:HD2 | 31:LJ:155:HIS:CD2  | 2.50                     | 0.47              |
| 36:LP:61:ARG:HA   | 36:LP:78:TRP:CZ2   | 2.50                     | 0.47              |
| 37:LQ:43:PHE:CD1  | 37:LQ:133:GLY:HA3  | 2.50                     | 0.47              |
| 37:LQ:80:ALA:HB3  | 37:LQ:100:VAL:HG23 | 1.96                     | 0.47              |
| 38:LR:49:LEU:H    | 38:LR:49:LEU:HD12  | 1.80                     | 0.47              |
| 45:LZ:42:LEU:HA   | 45:LZ:74:VAL:HA    | 1.96                     | 0.47              |
| 48:Lc:9:LYS:N     | 79:S2:1006:C:OP1   | 2.48                     | 0.47              |
| 53:Lh:20:GLN:HA   | 53:Lh:20:GLN:OE1   | 2.15                     | 0.47              |
| 53:Lh:20:GLN:O    | 53:Lh:24:LEU:HB2   | 2.14                     | 0.47              |
| 60:Lo:21:HIS:NE2  | 60:Lo:72:CYS:HB3   | 2.30                     | 0.47              |
| 61:Lp:80:LYS:O    | 61:Lp:83:ILE:HD12  | 2.15                     | 0.47              |
| 62:Lr:97:ILE:HD13 | 62:Lr:107:ARG:HB2  | 1.97                     | 0.47              |
| 65:SD:90:LYS:HA   | 65:SD:90:LYS:HD2   | 1.81                     | 0.47              |
| 66:SF:145:ARG:NH1 | 73:Sc:47:LYS:HE2   | 2.29                     | 0.47              |
| 67:SK:7:ASN:O     | 67:SK:11:ILE:HG12  | 2.15                     | 0.47              |
| 70:SS:111:LEU:O   | 70:SS:115:LYS:HG2  | 2.15                     | 0.47              |
| 71:ST:144:LYS:HD3 | 71:ST:144:LYS:HA   | 1.70                     | 0.47              |
| 74:Sd:19:ARG:CD   | 74:Sd:32:ARG:HH11  | 2.28                     | 0.47              |
| 75:Sg:42:MET:O    | 75:Sg:55:PRO:HA    | 2.15                     | 0.47              |
| 77:SZ:69:THR:HB   | 77:SZ:108:ILE:HD12 | 1.96                     | 0.47              |
| 79:S2:429:C:H2'   | 79:S2:430:C:C6     | 2.49                     | 0.47              |
| 79:S2:479:C:H2'   | 79:S2:480:G:H8     | 1.80                     | 0.47              |
| 79:S2:1041:G:H2'  | 79:S2:1042:A:H8    | 1.80                     | 0.47              |
| 79:S2:1278:A:H2'  | 79:S2:1279:C:C6    | 2.49                     | 0.47              |
| 79:S2:1384:C:C2   | 79:S2:1385:G:C8    | 3.03                     | 0.47              |
| 79:S2:1804:U:H2'  | 79:S2:1805:G:H8    | 1.79                     | 0.47              |
| 1:CH:85:ARG:HG2   | 1:CH:95:LEU:HD12   | 1.97                     | 0.47              |
| 1:CH:104:GLN:NE2  | 79:S2:1501:C:OP1   | 2.48                     | 0.47              |
| 1:cH:85:ARG:CZ    | 1:cH:90:LEU:O      | 2.63                     | 0.47              |
| 2:sE:94:LYS:CG    | 8:sY:17:LEU:HD21   | 2.45                     | 0.47              |
| 6:sG:87:ARG:N     | 6:sG:91:GLU:OE1    | 2.48                     | 0.47              |
| 10:sA:90:PHE:CE1  | 10:sA:94:THR:HG21  | 2.50                     | 0.47              |
| 14:sa:15:ARG:HB3  | 79:s2:993:G:O6     | 2.15                     | 0.47              |
| 18:sW:55:ASP:OD2  | 18:sW:57:ARG:N     | 2.37                     | 0.47              |
| 19:sb:81:ARG:NH1  | 19:sb:82:LYS:HG3   | 2.29                     | 0.47              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 20:l7:75:G:O2'    | 20:l7:99:G:O6      | 2.27                     | 0.47              |
| 21:l8:32:C:H3'    | 21:l8:33:G:H8      | 1.80                     | 0.47              |
| 23:lB:93:VAL:HG13 | 23:lB:102:PHE:HB2  | 1.97                     | 0.47              |
| 24:lC:304:ALA:HB1 | 85:l5:1701:A:H5'   | 1.97                     | 0.47              |
| 25:lD:152:ARG:HD2 | 25:lD:152:ARG:HA   | 1.69                     | 0.47              |
| 25:lD:254:GLU:N   | 25:lD:254:GLU:OE1  | 2.48                     | 0.47              |
| 26:lE:58:SER:OG   | 85:l5:1238:A:OP2   | 2.32                     | 0.47              |
| 26:lE:66:LYS:HE2  | 85:l5:979:C:OP1    | 2.15                     | 0.47              |
| 26:lE:93:THR:HA   | 26:lE:106:VAL:HA   | 1.95                     | 0.47              |
| 26:lE:201:ILE:O   | 26:lE:201:ILE:HG13 | 2.15                     | 0.47              |
| 26:lE:268:GLN:O   | 26:lE:272:ARG:HG3  | 2.14                     | 0.47              |
| 27:lF:68:GLU:HA   | 27:lF:71:MET:HE1   | 1.95                     | 0.47              |
| 30:lI:143:GLN:OE1 | 30:lI:143:GLN:N    | 2.33                     | 0.47              |
| 30:lI:183:ASP:OD1 | 30:lI:187:LYS:NZ   | 2.42                     | 0.47              |
| 30:lI:209:TRP:O   | 30:lI:213:HIS:ND1  | 2.46                     | 0.47              |
| 32:lL:36:ARG:NH2  | 85:l5:1363:C:H3'   | 2.29                     | 0.47              |
| 32:lL:65:ARG:HG2  | 32:lL:66:TYR:CD2   | 2.49                     | 0.47              |
| 33:lM:53:LYS:N    | 33:lM:53:LYS:HD2   | 2.30                     | 0.47              |
| 35:lO:3:GLU:OE1   | 35:lO:31:ARG:CZ    | 2.63                     | 0.47              |
| 37:lQ:63:LEU:HD12 | 37:lQ:66:MET:CE    | 2.45                     | 0.47              |
| 38:lR:73:GLY:HA2  | 38:lR:76:MET:HE1   | 1.97                     | 0.47              |
| 44:lY:47:MET:HE3  | 44:lY:47:MET:HA    | 1.97                     | 0.47              |
| 53:lh:52:LYS:HA   | 53:lh:52:LYS:HD3   | 1.73                     | 0.47              |
| 61:lp:60:CYS:O    | 61:lp:62:LYS:HG2   | 2.15                     | 0.47              |
| 62:lr:98:ARG:NH1  | 85:l5:2262:G:OP2   | 2.44                     | 0.47              |
| 64:sR:3:ARG:CZ    | 79:s2:1467:C:H1'   | 2.45                     | 0.47              |
| 65:sD:190:LEU:HB2 | 65:sD:200:PRO:HD3  | 1.96                     | 0.47              |
| 70:sS:8:LYS:HD2   | 70:sS:8:LYS:C      | 2.40                     | 0.47              |
| 74:sd:17:GLY:HA2  | 74:sd:27:ARG:NH2   | 2.30                     | 0.47              |
| 75:sg:176:VAL:O   | 75:sg:184:LEU:HD22 | 2.14                     | 0.47              |
| 77:sZ:98:LYS:NZ   | 77:sZ:111:ARG:O    | 2.46                     | 0.47              |
| 79:s2:604:A:H1'   | 79:s2:639:C:O2'    | 2.15                     | 0.47              |
| 79:s2:948:C:C2'   | 79:s2:949:G:H5'    | 2.44                     | 0.47              |
| 79:s2:962:A:N1    | 79:s2:1055:A:O2'   | 2.48                     | 0.47              |
| 79:s2:1265:A:H5'  | 79:s2:1266:C:OP2   | 2.15                     | 0.47              |
| 79:s2:1633:A:H2'  | 79:s2:1634:A:C8    | 2.50                     | 0.47              |
| 79:s2:1777:G:H8   | 79:s2:1777:G:OP2   | 1.98                     | 0.47              |
| 79:s2:1827:U:H2'  | 79:s2:1828:C:C6    | 2.50                     | 0.47              |
| 80:cB:338:ALA:HA  | 80:cB:341:ARG:NH2  | 2.30                     | 0.47              |
| 80:cB:613:LEU:O   | 80:cB:617:ILE:HG13 | 2.15                     | 0.47              |
| 83:ls:28:PHE:HZ   | 83:ls:189:ILE:HB   | 1.80                     | 0.47              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 83:ls:63:LYS:HA    | 83:ls:66:ARG:HG2  | 1.95                     | 0.47              |
| 84:lt:59:THR:HA    | 84:lt:80:LEU:HD13 | 1.97                     | 0.47              |
| 85:l5:122:U:H2'    | 85:l5:123:C:H6    | 1.80                     | 0.47              |
| 85:l5:269:G:H2'    | 85:l5:270:U:C6    | 2.49                     | 0.47              |
| 85:l5:386:A:H3'    | 85:l5:387:G:H5''  | 1.97                     | 0.47              |
| 85:l5:713:C:H2'    | 85:l5:714:G:C8    | 2.49                     | 0.47              |
| 85:l5:1426:G:N1    | 85:l5:1458:C:OP2  | 2.41                     | 0.47              |
| 85:l5:1807:C:H2'   | 85:l5:1808:C:H6   | 1.80                     | 0.47              |
| 85:l5:2081:C:H2'   | 85:l5:2082:G:H8   | 1.80                     | 0.47              |
| 85:l5:2094:G:H2'   | 85:l5:2095:A:C4   | 2.50                     | 0.47              |
| 85:l5:2497:C:H2'   | 85:l5:2498:C:C6   | 2.49                     | 0.47              |
| 85:l5:2772:C:N3    | 85:l5:2773:G:C8   | 2.82                     | 0.47              |
| 85:l5:3972:A:H1'   | 85:l5:4050:A:N6   | 2.29                     | 0.47              |
| 85:l5:4180:G:H2'   | 85:l5:4181:U:C6   | 2.50                     | 0.47              |
| 85:l5:4760:G:N1    | 85:l5:4767:C:OP1  | 2.48                     | 0.47              |
| 80:CB:772:GLU:HG2  | 80:CB:785:LYS:HD2 | 1.96                     | 0.47              |
| 80:CB:820:LEU:HD12 | 80:CB:821:PRO:HD2 | 1.97                     | 0.47              |
| 8:SY:88:LYS:HB3    | 8:SY:97:TYR:CE2   | 2.49                     | 0.47              |
| 11:SB:129:THR:OG1  | 11:SB:131:ASP:OD1 | 2.28                     | 0.47              |
| 12:SH:176:VAL:O    | 12:SH:180:LEU:HG  | 2.14                     | 0.47              |
| 12:SH:181:THR:HG22 | 12:SH:183:LYS:HG3 | 1.96                     | 0.47              |
| 16:SN:20:ARG:HD3   | 18:SW:56:HIS:CD2  | 2.50                     | 0.47              |
| 85:L5:40:G:C4      | 85:L5:4378:A:C6   | 3.02                     | 0.47              |
| 85:L5:229:G:H2'    | 85:L5:230:G:C8    | 2.47                     | 0.47              |
| 85:L5:307:A:H2'    | 85:L5:308:G:N3    | 2.30                     | 0.47              |
| 85:L5:1339:U:H2'   | 85:L5:1340:C:H6   | 1.78                     | 0.47              |
| 85:L5:1505:C:H2'   | 85:L5:1506:G:C8   | 2.49                     | 0.47              |
| 85:L5:1995:G:O2'   | 84:Lt:122:ALA:O   | 2.26                     | 0.47              |
| 85:L5:1998:A:H1'   | 85:L5:2019:C:O2'  | 2.15                     | 0.47              |
| 85:L5:2406:G:P     | 55:Lj:14:LYS:HZ1  | 2.38                     | 0.47              |
| 85:L5:2638:G:H2'   | 85:L5:2639:U:C6   | 2.50                     | 0.47              |
| 85:L5:3689:G:OP1   | 22:LA:201:GLY:N   | 2.48                     | 0.47              |
| 85:L5:3783:A:C8    | 85:L5:3792:G:C8   | 3.03                     | 0.47              |
| 85:L5:4266:G:H4'   | 85:L5:4267:G:C4   | 2.50                     | 0.47              |
| 85:L5:4431:U:H2'   | 85:L5:4432:C:C6   | 2.49                     | 0.47              |
| 85:L5:4518:A:OP2   | 85:L5:4518:A:H8   | 1.98                     | 0.47              |
| 85:L5:4710:C:H2'   | 85:L5:4711:C:H6   | 1.79                     | 0.47              |
| 85:L5:4728:U:OP1   | 23:LB:132:LYS:NZ  | 2.44                     | 0.47              |
| 85:L5:4768:G:H4'   | 85:L5:4873:G:C2   | 2.50                     | 0.47              |
| 85:L5:4771:C:H2'   | 85:L5:4772:C:C6   | 2.50                     | 0.47              |
| 85:L5:4906:C:H2'   | 85:L5:4907:G:C8   | 2.49                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 85:L5:4919:G:H2'   | 85:L5:4920:C:H6    | 1.80                     | 0.47              |
| 20:L7:28:C:O3'     | 31:LJ:138:GLY:HA2  | 2.15                     | 0.47              |
| 20:L7:33:U:H2'     | 20:L7:34:C:C6      | 2.50                     | 0.47              |
| 22:LA:51:ASP:CG    | 22:LA:58:LEU:HD21  | 2.40                     | 0.47              |
| 22:LA:65:ASP:OD2   | 22:LA:68:ARG:HG2   | 2.15                     | 0.47              |
| 23:LB:189:THR:O    | 23:LB:193:LYS:HG2  | 2.14                     | 0.47              |
| 23:LB:242:ARG:HA   | 23:LB:248:LEU:HD13 | 1.96                     | 0.47              |
| 24:LC:67:TRP:HE1   | 24:LC:71:ARG:HD2   | 1.80                     | 0.47              |
| 24:LC:218:ILE:HG13 | 24:LC:219:LYS:N    | 2.29                     | 0.47              |
| 24:LC:297:GLU:OE1  | 24:LC:297:GLU:N    | 2.40                     | 0.47              |
| 31:LJ:78:LYS:O     | 31:LJ:82:ILE:HG22  | 2.15                     | 0.47              |
| 34:LN:160:GLU:HG2  | 34:LN:161:MET:HE1  | 1.97                     | 0.47              |
| 38:LR:38:ARG:C     | 38:LR:40:GLN:H     | 2.23                     | 0.47              |
| 39:LS:79:GLY:HA2   | 39:LS:96:GLU:HA    | 1.97                     | 0.47              |
| 41:LU:29:VAL:HG12  | 41:LU:34:MET:O     | 2.15                     | 0.47              |
| 42:LV:90:ARG:C     | 42:LV:92:ASP:H     | 2.23                     | 0.47              |
| 43:LX:75:ALA:O     | 43:LX:78:LYS:NZ    | 2.47                     | 0.47              |
| 44:LY:73:VAL:HG12  | 44:LY:80:ILE:HG23  | 1.96                     | 0.47              |
| 49:Ld:28:ASN:ND2   | 49:Ld:31:LYS:HB3   | 2.29                     | 0.47              |
| 62:Lr:3:ALA:HB1    | 62:Lr:44:ILE:HD12  | 1.96                     | 0.47              |
| 64:SR:3:ARG:HH11   | 64:SR:3:ARG:HG3    | 1.80                     | 0.47              |
| 67:SK:16:PHE:HD2   | 67:SK:83:LEU:HD21  | 1.80                     | 0.47              |
| 70:SS:26:ILE:O     | 70:SS:30:ILE:HD12  | 2.15                     | 0.47              |
| 71:ST:11:GLN:HG2   | 71:ST:62:ARG:CZ    | 2.45                     | 0.47              |
| 75:Sg:84:ASP:HB2   | 75:Sg:86:THR:HG23  | 1.97                     | 0.47              |
| 75:Sg:143:GLN:NE2  | 75:Sg:144:ASP:OD2  | 2.48                     | 0.47              |
| 76:SM:23:LYS:O     | 76:SM:27:ILE:HG12  | 2.15                     | 0.47              |
| 76:SM:88:TRP:CD1   | 76:SM:88:TRP:N     | 2.80                     | 0.47              |
| 76:SM:95:ASP:O     | 76:SM:97:GLU:N     | 2.48                     | 0.47              |
| 78:Sf:87:THR:HA    | 79:S2:1507:G:H1    | 1.80                     | 0.47              |
| 79:S2:480:G:H2'    | 79:S2:481:C:C6     | 2.50                     | 0.47              |
| 79:S2:496:C:H2'    | 79:S2:497:C:C6     | 2.47                     | 0.47              |
| 79:S2:499:G:N1     | 79:S2:501:C:O2     | 2.47                     | 0.47              |
| 79:S2:872:A:C8     | 79:S2:874:G:C8     | 3.03                     | 0.47              |
| 79:S2:925:G:C2     | 79:S2:1018:U:C2    | 3.03                     | 0.47              |
| 79:S2:1141:G:H2'   | 79:S2:1142:G:C8    | 2.50                     | 0.47              |
| 79:S2:1164:G:O2'   | 79:S2:1165:G:H5'   | 2.15                     | 0.47              |
| 79:S2:1236:G:H2'   | 79:S2:1237:C:C6    | 2.50                     | 0.47              |
| 79:S2:1410:C:O2'   | 79:S2:1411:G:H5'   | 2.15                     | 0.47              |
| 81:AP:66:C:H3'     | 81:AP:67:G:H8      | 1.80                     | 0.47              |
| 83:Ls:41:GLN:O     | 83:Ls:45:MET:SD    | 2.73                     | 0.47              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:CH:40:THR:HG22  | 86:Se:44:ASN:HB3   | 1.97                     | 0.46              |
| 1:CH:53:SER:N     | 1:CH:119:GLN:OE1   | 2.48                     | 0.46              |
| 4:sL:39:ASN:O     | 79:s2:292:A:O2'    | 2.22                     | 0.46              |
| 4:sL:59:LYS:NZ    | 4:sL:134:LEU:HB3   | 2.30                     | 0.46              |
| 4:sL:133:PRO:HD2  | 79:s2:383:G:H1'    | 1.97                     | 0.46              |
| 4:sL:133:PRO:O    | 79:s2:383:G:O2'    | 2.33                     | 0.46              |
| 6:sG:5:ILE:HD12   | 6:sG:14:LYS:H      | 1.79                     | 0.46              |
| 6:sG:131:ARG:HH22 | 79:s2:167:G:H2'    | 1.79                     | 0.46              |
| 7:sJ:88:ASP:OD1   | 7:sJ:89:GLU:N      | 2.48                     | 0.46              |
| 7:sJ:122:SER:O    | 7:sJ:122:SER:OG    | 2.28                     | 0.46              |
| 8:sY:74:MET:HA    | 8:sY:74:MET:HE3    | 1.96                     | 0.46              |
| 8:sY:105:LYS:HE2  | 79:s2:491:C:OP2    | 2.15                     | 0.46              |
| 10:sA:39:TYR:N    | 10:sA:48:ILE:O     | 2.46                     | 0.46              |
| 15:sC:208:PRO:O   | 15:sC:212:LYS:HG2  | 2.15                     | 0.46              |
| 17:sO:13:GLN:HA   | 17:sO:13:GLN:OE1   | 2.15                     | 0.46              |
| 21:l8:45:C:H2'    | 21:l8:46:G:C8      | 2.50                     | 0.46              |
| 21:l8:112:G:HO2'  | 85:l5:2444:U:HO2'  | 1.63                     | 0.46              |
| 22:lA:40:TYR:HE2  | 22:lA:89:TYR:CD1   | 2.32                     | 0.46              |
| 26:lE:220:LYS:HD2 | 26:lE:221:LYS:H    | 1.78                     | 0.46              |
| 28:lG:50:ASP:OD2  | 28:lG:52:THR:N     | 2.29                     | 0.46              |
| 30:lI:48:LEU:O    | 30:lI:139:ARG:HA   | 2.14                     | 0.46              |
| 35:lO:130:LYS:NZ  | 85:l5:2055:G:O5'   | 2.47                     | 0.46              |
| 36:lP:35:ALA:HB2  | 36:lP:58:VAL:HG23  | 1.97                     | 0.46              |
| 39:lS:32:ILE:HD12 | 39:lS:32:ILE:N     | 2.31                     | 0.46              |
| 47:lb:3:LYS:NZ    | 85:l5:4195:G:OP2   | 2.36                     | 0.46              |
| 52:lg:98:GLU:O    | 52:lg:102:ILE:HG12 | 2.15                     | 0.46              |
| 62:lr:97:ILE:HD13 | 62:lr:107:ARG:HA   | 1.96                     | 0.46              |
| 64:sR:56:HIS:CE1  | 79:s2:1461:G:H1    | 2.33                     | 0.46              |
| 65:sD:24:PHE:O    | 67:sK:61:GLN:NE2   | 2.43                     | 0.46              |
| 66:sF:83:ASN:OD1  | 79:s2:1651:A:O2'   | 2.19                     | 0.46              |
| 76:sM:106:CYS:SG  | 79:s2:1284:A:O2'   | 2.72                     | 0.46              |
| 76:sM:120:ALA:HA  | 76:sM:123:VAL:HG22 | 1.97                     | 0.46              |
| 77:sZ:94:LYS:O    | 77:sZ:94:LYS:HD2   | 2.15                     | 0.46              |
| 79:s2:36:U:H2'    | 79:s2:37:C:O4'     | 2.16                     | 0.46              |
| 79:s2:496:C:H2'   | 79:s2:497:C:H6     | 1.80                     | 0.46              |
| 79:s2:529:A:H2'   | 79:s2:530:U:H6     | 1.79                     | 0.46              |
| 79:s2:563:G:N7    | 79:s2:586:G:N2     | 2.63                     | 0.46              |
| 79:s2:594:A:H4'   | 79:s2:595:U:H5'    | 1.96                     | 0.46              |
| 79:s2:690:G:OP2   | 79:s2:690:G:N2     | 2.37                     | 0.46              |
| 79:s2:1049:A:OP2  | 79:s2:1068:G:N1    | 2.43                     | 0.46              |
| 79:s2:1421:A:H5'' | 79:s2:1422:G:C4    | 2.50                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 79:s2:1428:G:O2'   | 79:s2:1585:U:O4    | 2.31                     | 0.46              |
| 79:s2:1552:G:H1'   | 79:s2:1557:C:N4    | 2.30                     | 0.46              |
| 79:s2:1648:G:H22   | 79:s2:1675:A:P     | 2.37                     | 0.46              |
| 79:s2:1736:G:H2'   | 79:s2:1737:G:C8    | 2.50                     | 0.46              |
| 79:s2:1754:G:C6    | 79:s2:1755:C:C2    | 3.03                     | 0.46              |
| 79:s2:1796:G:H2'   | 79:s2:1797:U:C6    | 2.50                     | 0.46              |
| 80:cB:208:VAL:HG13 | 80:cB:258:LYS:HA   | 1.96                     | 0.46              |
| 84:lt:66:ASN:N     | 84:lt:69:ALA:O     | 2.45                     | 0.46              |
| 85:l5:353:A:C4     | 85:l5:379:G:N7     | 2.83                     | 0.46              |
| 85:l5:369:G:N1     | 85:l5:373:G:C6     | 2.83                     | 0.46              |
| 85:l5:1202:C:H3'   | 85:l5:1203:G:H4'   | 1.97                     | 0.46              |
| 85:l5:1604:G:H2'   | 85:l5:1605:G:H8    | 1.79                     | 0.46              |
| 85:l5:1964:A:H2'   | 85:l5:1965:G:C8    | 2.50                     | 0.46              |
| 85:l5:2353:U:H2'   | 85:l5:2354:G:C8    | 2.48                     | 0.46              |
| 85:l5:2902:G:N2    | 85:l5:3597:G:O6    | 2.48                     | 0.46              |
| 85:l5:4072:C:C2    | 85:l5:4073:A:C8    | 3.03                     | 0.46              |
| 85:l5:4180:G:H2'   | 85:l5:4181:U:H6    | 1.79                     | 0.46              |
| 80:CB:398:ILE:HG22 | 80:CB:483:GLY:C    | 2.39                     | 0.46              |
| 80:CB:416:VAL:HG12 | 80:CB:466:CYS:HA   | 1.96                     | 0.46              |
| 80:CB:453:MET:HE3  | 80:CB:453:MET:H    | 1.80                     | 0.46              |
| 2:SE:148:ARG:NH1   | 2:SE:149:TYR:CZ    | 2.83                     | 0.46              |
| 2:SE:181:CYS:SG    | 2:SE:195:ILE:HG13  | 2.55                     | 0.46              |
| 4:SL:46:THR:HA     | 4:SL:62:PHE:CE1    | 2.50                     | 0.46              |
| 5:SX:45:SER:OG     | 79:S2:649:U:H1'    | 2.14                     | 0.46              |
| 5:SX:125:VAL:O     | 5:SX:126:ALA:C     | 2.58                     | 0.46              |
| 6:SG:174:PRO:HB3   | 79:S2:65:C:C6      | 2.50                     | 0.46              |
| 7:SJ:35:TYR:HE1    | 7:SJ:112:THR:HG21  | 1.79                     | 0.46              |
| 8:SY:3:ASP:OD1     | 8:SY:4:THR:N       | 2.47                     | 0.46              |
| 8:SY:21:LYS:HB2    | 8:SY:75:ILE:HD11   | 1.97                     | 0.46              |
| 10:SA:118:GLU:OE1  | 15:SC:65:LYS:HG2   | 2.15                     | 0.46              |
| 11:SB:205:TYR:CE1  | 79:S2:1122:A:H4'   | 2.50                     | 0.46              |
| 14:Sa:22:ARG:HH12  | 17:SO:142:ARG:H    | 1.62                     | 0.46              |
| 15:SC:62:PRO:HG3   | 15:SC:71:LYS:HB2   | 1.97                     | 0.46              |
| 15:SC:108:LYS:HE2  | 15:SC:233:LEU:HD23 | 1.97                     | 0.46              |
| 15:SC:277:HIS:O    | 15:SC:279:ARG:HA   | 2.15                     | 0.46              |
| 17:SO:12:GLU:HA    | 17:SO:13:GLN:HA    | 1.68                     | 0.46              |
| 19:Sb:82:LYS:O     | 19:Sb:83:GLN:HG3   | 2.15                     | 0.46              |
| 85:L5:480:C:H2'    | 85:L5:481:G:C8     | 2.51                     | 0.46              |
| 85:L5:1195:G:H2'   | 85:L5:1196:G:C8    | 2.51                     | 0.46              |
| 85:L5:1204:C:N4    | 85:L5:1205:G:O6    | 2.48                     | 0.46              |
| 85:L5:1348:U:H2'   | 85:L5:1349:G:H8    | 1.80                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 85:L5:1517:G:N1    | 24:LC:104:PRO:HD2  | 2.23                     | 0.46              |
| 85:L5:1536:U:H2'   | 85:L5:1537:A:H8    | 1.80                     | 0.46              |
| 85:L5:1956:A:H2'   | 85:L5:1957:U:H6    | 1.81                     | 0.46              |
| 85:L5:2060:G:H2'   | 85:L5:2061:U:C6    | 2.51                     | 0.46              |
| 85:L5:2523:G:H2'   | 85:L5:2524:U:C6    | 2.49                     | 0.46              |
| 85:L5:4173:G:H2'   | 85:L5:4174:U:C6    | 2.50                     | 0.46              |
| 85:L5:4200:G:C6    | 85:L5:4201:G:C5    | 3.03                     | 0.46              |
| 28:LG:116:ALA:O    | 28:LG:120:LYS:HE3  | 2.15                     | 0.46              |
| 28:LG:123:ALA:HA   | 28:LG:124:GLY:HA2  | 1.72                     | 0.46              |
| 28:LG:175:ARG:NH2  | 28:LG:234:ARG:HH12 | 2.13                     | 0.46              |
| 31:LJ:58:ARG:O     | 31:LJ:58:ARG:HG2   | 2.14                     | 0.46              |
| 35:LO:42:ASN:OD1   | 35:LO:135:PHE:HB2  | 2.14                     | 0.46              |
| 39:LS:127:MET:HE1  | 40:LT:154:ILE:C    | 2.40                     | 0.46              |
| 40:LT:110:LYS:HA   | 40:LT:113:ASP:OD1  | 2.15                     | 0.46              |
| 48:Lc:12:GLU:HA    | 48:Lc:15:ASN:ND2   | 2.30                     | 0.46              |
| 56:Lk:19:ASP:OD1   | 56:Lk:19:ASP:N     | 2.45                     | 0.46              |
| 56:Lk:64:LEU:HD12  | 56:Lk:65:ALA:H     | 1.81                     | 0.46              |
| 63:Lz:59:PRO:HB3   | 63:Lz:171:HIS:H    | 1.79                     | 0.46              |
| 63:Lz:73:HIS:HE1   | 63:Lz:111:LEU:HD21 | 1.79                     | 0.46              |
| 66:SF:145:ARG:HA   | 66:SF:148:ASN:HB2  | 1.96                     | 0.46              |
| 70:SS:137:LYS:HG3  | 79:S2:1521:C:C4    | 2.49                     | 0.46              |
| 73:Sc:31:ARG:N     | 73:Sc:43:ILE:HD12  | 2.28                     | 0.46              |
| 74:Sd:38:MET:SD    | 74:Sd:42:CYS:HB2   | 2.55                     | 0.46              |
| 79:S2:20:G:H5'     | 79:S2:620:G:C8     | 2.50                     | 0.46              |
| 79:S2:374:G:H2'    | 79:S2:375:U:C6     | 2.50                     | 0.46              |
| 79:S2:1461:G:C2    | 79:S2:1466:G:C6    | 3.03                     | 0.46              |
| 83:Ls:13:TYR:CD2   | 83:Ls:60:MET:HE2   | 2.50                     | 0.46              |
| 83:Ls:146:LYS:HE3  | 83:Ls:155:LEU:HD22 | 1.96                     | 0.46              |
| 87:LW:117:LYS:HD3  | 87:LW:117:LYS:HA   | 1.75                     | 0.46              |
| 2:sE:164:LEU:HG    | 2:sE:165:GLU:HG3   | 1.96                     | 0.46              |
| 16:sN:38:TYR:OH    | 16:sN:78:LYS:HB2   | 2.16                     | 0.46              |
| 16:sN:87:ASP:CG    | 79:s2:924:G:H21    | 2.24                     | 0.46              |
| 16:sN:96:VAL:HG11  | 16:sN:150:VAL:HG11 | 1.96                     | 0.46              |
| 18:sW:25:VAL:O     | 18:sW:62:VAL:HA    | 2.15                     | 0.46              |
| 21:l8:88:A:H2'     | 21:l8:89:U:O4'     | 2.15                     | 0.46              |
| 21:l8:115:G:H2'    | 21:l8:116:C:C6     | 2.50                     | 0.46              |
| 21:l8:120:G:C6     | 21:l8:131:G:C6     | 3.03                     | 0.46              |
| 22:lA:147:ARG:CZ   | 79:s2:949:G:H5''   | 2.45                     | 0.46              |
| 24:lC:120:LYS:HD2  | 85:l5:1374:G:OP1   | 2.15                     | 0.46              |
| 24:lC:158:VAL:HA   | 24:lC:161:TYR:CD1  | 2.50                     | 0.46              |
| 26:lE:150:LEU:HD13 | 26:lE:194:VAL:HG21 | 1.95                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:lf:182:TYR:CE2  | 27:lf:203:GLU:HG2  | 2.50                     | 0.46              |
| 31:lj:129:ASP:OD1  | 31:lj:129:ASP:N    | 2.46                     | 0.46              |
| 32:il:101:ARG:NH1  | 85:l5:76:A:H5'     | 2.30                     | 0.46              |
| 35:lo:18:ARG:HE    | 35:lo:128:ARG:NH2  | 2.14                     | 0.46              |
| 38:lr:20:LYS:HD2   | 85:l5:2823:G:N7    | 2.31                     | 0.46              |
| 42:lv:62:MET:HE1   | 85:l5:4507:A:O3'   | 2.15                     | 0.46              |
| 42:lv:64:THR:HG22  | 42:lv:75:LYS:O     | 2.15                     | 0.46              |
| 43:lx:60:TYR:CD1   | 53:lh:78:TYR:CD2   | 3.00                     | 0.46              |
| 43:lx:74:TYR:CB    | 53:lh:25:LYS:HD3   | 2.45                     | 0.46              |
| 43:lx:83:THR:HG23  | 43:lx:86:ALA:H     | 1.80                     | 0.46              |
| 49:ld:54:MET:HE1   | 49:ld:59:THR:C     | 2.40                     | 0.46              |
| 50:le:48:ARG:HH22  | 85:l5:2279:A:HO2'  | 1.63                     | 0.46              |
| 51:lf:100:ARG:HE   | 85:l5:4753:U:P     | 2.38                     | 0.46              |
| 53:lh:78:TYR:CZ    | 85:l5:16:G:H4'     | 2.49                     | 0.46              |
| 55:lj:75:ARG:NH1   | 85:l5:343:C:O2'    | 2.35                     | 0.46              |
| 61:lp:47:MET:CE    | 61:lp:57:CYS:HB2   | 2.46                     | 0.46              |
| 63:lz:198:TRP:HE1  | 63:lz:199:GLN:HE21 | 1.63                     | 0.46              |
| 64:sR:5:ARG:NH1    | 79:s2:1368:U:H4'   | 2.30                     | 0.46              |
| 70:sS:67:VAL:C     | 70:sS:71:MET:HE3   | 2.40                     | 0.46              |
| 70:sS:75:ARG:HH11  | 70:sS:95:TYR:HB2   | 1.79                     | 0.46              |
| 74:sd:14:PHE:CD2   | 79:s2:1661:A:C8    | 3.04                     | 0.46              |
| 75:sg:181:ASN:HD21 | 75:sg:183:LYS:HD2  | 1.79                     | 0.46              |
| 79:s2:186:C:H2'    | 79:s2:187:G:C8     | 2.51                     | 0.46              |
| 79:s2:876:C:H2'    | 79:s2:877:C:C6     | 2.51                     | 0.46              |
| 79:s2:1133:A:H2'   | 79:s2:1134:G:C8    | 2.47                     | 0.46              |
| 79:s2:1203:G:C6    | 79:s2:1204:A:C6    | 3.03                     | 0.46              |
| 80:cB:154:VAL:HG23 | 80:cB:211:THR:OG1  | 2.15                     | 0.46              |
| 83:ls:57:LYS:HA    | 85:l5:2021:G:P     | 2.55                     | 0.46              |
| 84:lt:65:GLN:HG2   | 84:lt:70:GLN:NE2   | 2.30                     | 0.46              |
| 85:l5:513:U:C2     | 85:l5:516:C:H5     | 2.33                     | 0.46              |
| 85:l5:743:G:N1     | 85:l5:922:C:N3     | 2.64                     | 0.46              |
| 85:l5:1368:A:H2'   | 85:l5:1369:C:O4'   | 2.15                     | 0.46              |
| 85:l5:1577:G:H5'   | 85:l5:1578:U:H5''  | 1.98                     | 0.46              |
| 85:l5:2497:C:H2'   | 85:l5:2498:C:H6    | 1.80                     | 0.46              |
| 85:l5:2655:C:C2    | 85:l5:2656:U:C5    | 3.03                     | 0.46              |
| 85:l5:2689:C:H2'   | 85:l5:2690:C:H6    | 1.81                     | 0.46              |
| 85:l5:2706:G:N2    | 85:l5:2709:C:H5''  | 2.31                     | 0.46              |
| 85:l5:2817:C:H2'   | 85:l5:2818:C:H6    | 1.79                     | 0.46              |
| 85:l5:3633:C:H2'   | 85:l5:3634:G:H8    | 1.79                     | 0.46              |
| 85:l5:3730:U:H2'   | 85:l5:3731:C:C6    | 2.50                     | 0.46              |
| 85:l5:3968:U:O4    | 85:l5:4053:A:O2'   | 2.26                     | 0.46              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 85:L5:4215:C:C2   | 85:L5:4216:G:C8    | 3.03                     | 0.46              |
| 85:L5:4729:A:OP2  | 85:L5:5068:G:N1    | 2.37                     | 0.46              |
| 85:L5:4954:G:C2   | 85:L5:4955:A:C5    | 3.03                     | 0.46              |
| 80:CB:13:MET:HE2  | 80:CB:13:MET:C     | 2.41                     | 0.46              |
| 80:CB:45:ILE:HG23 | 80:CB:45:ILE:HD12  | 1.65                     | 0.46              |
| 80:CB:631:ARG:HG3 | 80:CB:635:LEU:HD23 | 1.97                     | 0.46              |
| 2:SE:157:ASN:O    | 2:SE:157:ASN:ND2   | 2.48                     | 0.46              |
| 3:SI:134:GLU:O    | 3:SI:138:ASN:ND2   | 2.48                     | 0.46              |
| 5:SX:124:LYS:HD3  | 79:S2:29:G:H5''    | 1.96                     | 0.46              |
| 6:SG:23:LYS:HD2   | 6:SG:41:LEU:HA     | 1.97                     | 0.46              |
| 6:SG:183:ARG:HH22 | 79:S2:316:G:H3'    | 1.78                     | 0.46              |
| 7:SJ:93:LYS:HZ2   | 7:SJ:95:ASP:HB3    | 1.80                     | 0.46              |
| 16:SN:49:GLN:O    | 16:SN:52:VAL:HG22  | 2.15                     | 0.46              |
| 16:SN:110:ASP:OD1 | 79:S2:934:G:N2     | 2.37                     | 0.46              |
| 85:L5:53:C:C2     | 85:L5:54:G:C8      | 3.03                     | 0.46              |
| 85:L5:106:A:H2'   | 85:L5:107:G:O4'    | 2.15                     | 0.46              |
| 85:L5:466:A:H2'   | 85:L5:467:U:C6     | 2.50                     | 0.46              |
| 85:L5:481:G:H2'   | 85:L5:482:G:H8     | 1.79                     | 0.46              |
| 85:L5:966:A:C2    | 85:L5:2093:A:H2    | 2.33                     | 0.46              |
| 85:L5:1176:C:H2'  | 85:L5:1177:U:H6    | 1.80                     | 0.46              |
| 85:L5:1617:G:H1'  | 85:L5:2513:A:N6    | 2.31                     | 0.46              |
| 85:L5:1875:C:H2'  | 85:L5:1876:U:H6    | 1.81                     | 0.46              |
| 85:L5:1933:G:H8   | 85:L5:1933:G:O5'   | 1.98                     | 0.46              |
| 85:L5:2010:A:H2'  | 85:L5:2011:C:O4'   | 2.16                     | 0.46              |
| 85:L5:2018:C:H2'  | 85:L5:2019:C:H6    | 1.79                     | 0.46              |
| 85:L5:2434:G:H2'  | 85:L5:2435:G:C8    | 2.49                     | 0.46              |
| 85:L5:2455:G:H1'  | 85:L5:2471:G:C5    | 2.50                     | 0.46              |
| 85:L5:2508:U:H2'  | 85:L5:2509:C:H6    | 1.79                     | 0.46              |
| 85:L5:2662:G:H2'  | 85:L5:2663:G:H8    | 1.78                     | 0.46              |
| 85:L5:2732:G:H2'  | 85:L5:2733:C:H6    | 1.81                     | 0.46              |
| 85:L5:3870:C:H2'  | 85:L5:3871:A:C8    | 2.50                     | 0.46              |
| 85:L5:3949:A:H61  | 85:L5:4064:C:H42   | 1.63                     | 0.46              |
| 85:L5:3951:G:C2   | 85:L5:4062:A:N1    | 2.84                     | 0.46              |
| 85:L5:4110:C:O2'  | 85:L5:4112:C:O2    | 2.32                     | 0.46              |
| 85:L5:4348:A:H61  | 85:L5:4364:G:H1    | 1.62                     | 0.46              |
| 85:L5:4444:C:H2'  | 85:L5:4445:U:H6    | 1.80                     | 0.46              |
| 85:L5:4740:G:C6   | 85:L5:4959:U:O2    | 2.68                     | 0.46              |
| 20:L7:35:U:O2     | 20:L7:45:U:O2'     | 2.32                     | 0.46              |
| 21:L8:4:C:H2'     | 21:L8:5:U:H6       | 1.79                     | 0.46              |
| 21:L8:44:A:H2'    | 21:L8:45:C:C6      | 2.50                     | 0.46              |
| 22:LA:60:LYS:O    | 22:LA:60:LYS:HD3   | 2.14                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:LA:140:ASN:HD21 | 22:LA:143:THR:HG22 | 1.80                     | 0.46              |
| 22:LA:235:VAL:HG22 | 22:LA:236:GLY:H    | 1.80                     | 0.46              |
| 30:LI:51:HIS:O     | 30:LI:52:MET:HE2   | 2.15                     | 0.46              |
| 35:LO:120:VAL:HG22 | 39:LS:167:PHE:HD2  | 1.78                     | 0.46              |
| 35:LO:147:TRP:HE1  | 35:LO:149:TYR:HB2  | 1.80                     | 0.46              |
| 49:Ld:18:ASN:OD1   | 49:Ld:19:GLU:N     | 2.48                     | 0.46              |
| 51:Lf:40:GLU:O     | 51:Lf:109:ARG:NH2  | 2.49                     | 0.46              |
| 54:Li:52:PRO:O     | 54:Li:55:ARG:HG2   | 2.16                     | 0.46              |
| 62:Lr:56:ASP:OD1   | 62:Lr:56:ASP:C     | 2.57                     | 0.46              |
| 65:SD:11:PHE:O     | 65:SD:14:ASP:OD2   | 2.32                     | 0.46              |
| 66:SF:45:TYR:HD1   | 66:SF:45:TYR:C     | 2.23                     | 0.46              |
| 66:SF:68:ILE:HD11  | 66:SF:116:ILE:HG13 | 1.96                     | 0.46              |
| 68:SP:47:ARG:NH1   | 79:S2:1619:A:OP1   | 2.48                     | 0.46              |
| 69:SQ:106:LYS:HA   | 69:SQ:109:LYS:HZ2  | 1.79                     | 0.46              |
| 70:SS:132:ARG:HD3  | 79:S2:1623:A:C6    | 2.50                     | 0.46              |
| 71:ST:102:ARG:HD3  | 71:ST:102:ARG:HA   | 1.63                     | 0.46              |
| 76:SM:17:ALA:HB1   | 76:SM:123:VAL:HG23 | 1.97                     | 0.46              |
| 79:S2:573:U:H1'    | 79:S2:576:A:C8     | 2.51                     | 0.46              |
| 79:S2:647:U:H2'    | 79:S2:648:A:C8     | 2.50                     | 0.46              |
| 79:S2:1203:G:H2'   | 79:S2:1204:A:H8    | 1.76                     | 0.46              |
| 79:S2:1854:U:H2'   | 79:S2:1855:G:C8    | 2.43                     | 0.46              |
| 81:AP:5:C:H2'      | 81:AP:6:C:H6       | 1.80                     | 0.46              |
| 84:Lt:81:ILE:HD12  | 84:Lt:82:ILE:HD13  | 1.97                     | 0.46              |
| 3:sI:147:LYS:NZ    | 79:s2:203:G:OP2    | 2.41                     | 0.46              |
| 6:sG:64:LYS:HE2    | 6:sG:77:LEU:HD11   | 1.96                     | 0.46              |
| 7:sJ:27:GLN:HA     | 7:sJ:27:GLN:OE1    | 2.15                     | 0.46              |
| 10:sA:84:GLN:O     | 10:sA:88:LEU:HG    | 2.16                     | 0.46              |
| 18:sW:11:LEU:HD22  | 18:sW:74:VAL:HB    | 1.96                     | 0.46              |
| 19:sb:69:GLY:HA3   | 79:s2:1105:G:O3'   | 2.15                     | 0.46              |
| 21:l8:25:G:H2'     | 21:l8:26:C:C6      | 2.50                     | 0.46              |
| 21:l8:123:U:H3'    | 21:l8:124:U:O4'    | 2.14                     | 0.46              |
| 25:lD:163:LEU:O    | 25:lD:167:VAL:HG13 | 2.15                     | 0.46              |
| 25:lD:164:LYS:HE2  | 25:lD:195:HIS:NE2  | 2.30                     | 0.46              |
| 26:lE:73:TYR:HE1   | 85:l5:981:C:C2     | 2.33                     | 0.46              |
| 29:lH:110:SER:C    | 29:lH:128:MET:HE1  | 2.41                     | 0.46              |
| 31:lJ:114:ASP:N    | 31:lJ:114:ASP:OD1  | 2.49                     | 0.46              |
| 32:lL:77:SER:N     | 32:lL:80:GLU:OE1   | 2.42                     | 0.46              |
| 36:lP:93:HIS:NE2   | 85:l5:397:G:O6     | 2.47                     | 0.46              |
| 37:lQ:181:ARG:NH2  | 85:l5:1391:A:OP1   | 2.38                     | 0.46              |
| 42:lV:26:ILE:HB    | 42:lV:101:ASN:O    | 2.15                     | 0.46              |
| 42:lV:61:VAL:O     | 42:lV:79:ALA:N     | 2.41                     | 0.46              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 43:IX:130:PRO:HG3 | 85:l5:2436:U:O4    | 2.15                     | 0.46              |
| 44:IY:34:LEU:HG   | 44:IY:106:ILE:HD11 | 1.96                     | 0.46              |
| 46:la:71:PRO:HD2  | 46:la:109:TYR:CD2  | 2.50                     | 0.46              |
| 46:la:85:GLN:HA   | 46:la:88:VAL:HG22  | 1.96                     | 0.46              |
| 51:lf:60:PRO:HG3  | 85:l5:4943:A:C4    | 2.51                     | 0.46              |
| 52:lg:104:VAL:HA  | 52:lg:107:LEU:CD2  | 2.43                     | 0.46              |
| 53:lh:13:LYS:HE2  | 53:lh:15:GLU:CB    | 2.45                     | 0.46              |
| 54:li:12:ASN:OD1  | 54:li:16:LYS:NZ    | 2.49                     | 0.46              |
| 55:lj:11:ARG:HB2  | 85:l5:1534:A:N3    | 2.30                     | 0.46              |
| 64:sR:57:LEU:HD23 | 64:sR:57:LEU:HA    | 1.72                     | 0.46              |
| 64:sR:77:GLU:O    | 64:sR:81:ARG:HG2   | 2.15                     | 0.46              |
| 65:sD:77:PHE:HB2  | 65:sD:79:PHE:CE2   | 2.51                     | 0.46              |
| 65:sD:167:TYR:CE1 | 65:sD:200:PRO:HG2  | 2.50                     | 0.46              |
| 66:sF:127:ARG:HG3 | 66:sF:128:ILE:H    | 1.81                     | 0.46              |
| 69:sQ:23:ALA:HA   | 69:sQ:70:VAL:HA    | 1.96                     | 0.46              |
| 70:sS:39:ARG:O    | 70:sS:43:VAL:HG13  | 2.16                     | 0.46              |
| 74:sd:10:HIS:O    | 74:sd:12:ARG:NH1   | 2.49                     | 0.46              |
| 79:s2:351:G:C2    | 79:s2:352:U:C6     | 3.03                     | 0.46              |
| 79:s2:382:C:H2'   | 79:s2:383:G:C8     | 2.50                     | 0.46              |
| 79:s2:409:C:N4    | 79:s2:427:U:OP1    | 2.45                     | 0.46              |
| 79:s2:496:C:H2'   | 79:s2:497:C:C6     | 2.50                     | 0.46              |
| 79:s2:1276:A:N7   | 79:s2:1322:G:H1'   | 2.30                     | 0.46              |
| 79:s2:1421:A:H3'  | 79:s2:1422:G:C8    | 2.51                     | 0.46              |
| 79:s2:1422:G:H4'  | 79:s2:1423:C:H3'   | 1.97                     | 0.46              |
| 79:s2:1464:C:H2'  | 79:s2:1465:A:C5    | 2.51                     | 0.46              |
| 80:cB:333:LYS:O   | 80:cB:336:LEU:HB3  | 2.15                     | 0.46              |
| 80:cB:428:ARG:HD2 | 80:cB:489:GLU:CD   | 2.41                     | 0.46              |
| 82:pE:55:U:H2'    | 82:pE:57:A:N7      | 2.30                     | 0.46              |
| 83:ls:26:LYS:HD2  | 83:ls:95:LEU:HG    | 1.97                     | 0.46              |
| 85:l5:732:A:H2'   | 85:l5:733:A:O4'    | 2.14                     | 0.46              |
| 85:l5:2037:C:H2'  | 85:l5:2038:U:H6    | 1.79                     | 0.46              |
| 85:l5:2624:G:H2'  | 85:l5:2625:U:C6    | 2.51                     | 0.46              |
| 85:l5:3833:C:H2'  | 85:l5:3834:C:H6    | 1.80                     | 0.46              |
| 85:l5:4139:G:H1'  | 85:l5:4146:G:N1    | 2.30                     | 0.46              |
| 85:l5:4642:U:H2'  | 85:l5:4643:G:H8    | 1.79                     | 0.46              |
| 80:CB:227:GLN:O   | 80:CB:231:MET:SD   | 2.73                     | 0.46              |
| 6:SG:126:ASP:OD1  | 6:SG:126:ASP:C     | 2.58                     | 0.46              |
| 7:SJ:124:HIS:CG   | 86:Se:35:ARG:HD2   | 2.51                     | 0.46              |
| 10:SA:39:TYR:CZ   | 64:SR:105:MET:HB2  | 2.50                     | 0.46              |
| 12:SH:91:HIS:CD2  | 12:SH:169:LYS:HG2  | 2.50                     | 0.46              |
| 13:SV:32:ILE:HD12 | 13:SV:32:ILE:HA    | 1.79                     | 0.46              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 13:SV:51:LYS:HD2  | 13:SV:52:THR:N     | 2.29                     | 0.46              |
| 16:SN:20:ARG:HH21 | 16:SN:64:ARG:HH21  | 1.63                     | 0.46              |
| 18:SW:6:VAL:HG23  | 18:SW:34:ILE:HD11  | 1.96                     | 0.46              |
| 18:SW:41:MET:HE1  | 18:SW:129:PHE:HB3  | 1.96                     | 0.46              |
| 85:L5:80:C:C2     | 85:L5:81:C:C5      | 3.03                     | 0.46              |
| 85:L5:196:C:O2'   | 44:LY:126:ARG:HA   | 2.15                     | 0.46              |
| 85:L5:334:A:H2'   | 85:L5:335:A:C8     | 2.50                     | 0.46              |
| 85:L5:406:C:O2'   | 85:L5:407:A:OP1    | 2.31                     | 0.46              |
| 85:L5:454:U:C4    | 85:L5:703:G:C8     | 3.04                     | 0.46              |
| 85:L5:458:C:H2'   | 85:L5:459:C:C6     | 2.50                     | 0.46              |
| 85:L5:652:G:H2'   | 85:L5:653:U:O4'    | 2.14                     | 0.46              |
| 85:L5:749:G:N1    | 85:L5:912:G:O2'    | 2.37                     | 0.46              |
| 85:L5:1786:A:H2'  | 85:L5:1789:C:H5    | 1.76                     | 0.46              |
| 85:L5:1806:G:H2'  | 85:L5:1807:C:C6    | 2.50                     | 0.46              |
| 85:L5:1863:U:H2'  | 85:L5:1864:G:H8    | 1.79                     | 0.46              |
| 85:L5:1895:G:H2'  | 85:L5:1896:A:O4'   | 2.16                     | 0.46              |
| 85:L5:1978:C:OP1  | 84:Lt:83:LYS:NZ    | 2.46                     | 0.46              |
| 85:L5:2323:C:H2'  | 85:L5:2324:C:C6    | 2.50                     | 0.46              |
| 85:L5:2372:U:H2'  | 85:L5:2373:C:C6    | 2.50                     | 0.46              |
| 85:L5:2752:G:H3'  | 85:L5:2753:G:H8    | 1.79                     | 0.46              |
| 85:L5:3667:C:H2'  | 85:L5:3668:C:H6    | 1.80                     | 0.46              |
| 85:L5:3760:A:H5'  | 85:L5:3760:A:N3    | 2.30                     | 0.46              |
| 85:L5:4117:U:N3   | 22:LA:40:TYR:O     | 2.41                     | 0.46              |
| 85:L5:4192:A:H2'  | 85:L5:4193:C:C6    | 2.50                     | 0.46              |
| 85:L5:4258:C:H2'  | 85:L5:4259:C:H6    | 1.80                     | 0.46              |
| 85:L5:4538:G:H2'  | 85:L5:4539:U:H6    | 1.80                     | 0.46              |
| 85:L5:4572:U:H2'  | 85:L5:4573:G:C8    | 2.50                     | 0.46              |
| 21:L8:108:A:H2'   | 21:L8:109:C:C6     | 2.50                     | 0.46              |
| 22:LA:129:ALA:HB3 | 22:LA:132:ASN:ND2  | 2.30                     | 0.46              |
| 23:LB:103:LYS:HB2 | 23:LB:153:MET:HE1  | 1.98                     | 0.46              |
| 24:LC:208:CYS:HA  | 24:LC:228:THR:CG2  | 2.45                     | 0.46              |
| 25:LD:208:MET:SD  | 25:LD:209:ARG:N    | 2.88                     | 0.46              |
| 25:LD:222:GLN:HG3 | 25:LD:223:PHE:CD1  | 2.49                     | 0.46              |
| 28:LG:104:PRO:HG2 | 28:LG:194:VAL:HG23 | 1.97                     | 0.46              |
| 30:LI:207:ASP:OD1 | 30:LI:207:ASP:N    | 2.46                     | 0.46              |
| 34:LN:123:GLU:O   | 34:LN:124:ASP:HB2  | 2.14                     | 0.46              |
| 36:LP:9:GLU:OE1   | 36:LP:9:GLU:N      | 2.41                     | 0.46              |
| 40:LT:29:THR:HG23 | 40:LT:30:TYR:CD1   | 2.50                     | 0.46              |
| 44:LY:91:ASN:OD1  | 44:LY:92:GLY:N     | 2.49                     | 0.46              |
| 48:Lc:32:LYS:HG2  | 48:Lc:33:GLN:OE1   | 2.16                     | 0.46              |
| 48:Lc:33:GLN:OE1  | 48:Lc:33:GLN:N     | 2.46                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 51:Lf:79:GLY:O     | 51:Lf:81:SER:N     | 2.47                     | 0.46              |
| 59:Ln:2:ARG:HD2    | 79:S2:1841:C:OP1   | 2.16                     | 0.46              |
| 60:Lo:71:GLU:OE1   | 60:Lo:80:LYS:HG2   | 2.15                     | 0.46              |
| 62:Lr:11:ARG:HE    | 62:Lr:12:ASN:HB2   | 1.81                     | 0.46              |
| 63:Lz:17:VAL:HB    | 63:Lz:180:VAL:HG12 | 1.97                     | 0.46              |
| 63:Lz:148:VAL:HG23 | 63:Lz:149:ASP:H    | 1.80                     | 0.46              |
| 65:SD:55:THR:O     | 65:SD:59:LEU:N     | 2.43                     | 0.46              |
| 68:SP:75:VAL:HG22  | 68:SP:93:MET:SD    | 2.55                     | 0.46              |
| 70:SS:75:ARG:NH1   | 70:SS:95:TYR:HB2   | 2.29                     | 0.46              |
| 70:SS:139:THR:OG1  | 79:S2:1230:C:OP2   | 2.29                     | 0.46              |
| 73:Sc:33:GLU:OE1   | 73:Sc:35:MET:N     | 2.49                     | 0.46              |
| 74:Sd:32:ARG:NH2   | 79:S2:1661:A:OP2   | 2.48                     | 0.46              |
| 79:S2:386:C:H2'    | 79:S2:387:C:C6     | 2.50                     | 0.46              |
| 79:S2:676:C:H2'    | 79:S2:677:G:O4'    | 2.16                     | 0.46              |
| 79:S2:907:G:H2'    | 79:S2:908:A:H8     | 1.79                     | 0.46              |
| 79:S2:1035:A:H2'   | 79:S2:1036:A:H8    | 1.81                     | 0.46              |
| 79:S2:1201:U:H2'   | 79:S2:1202:U:H6    | 1.80                     | 0.46              |
| 79:S2:1452:A:H5'   | 79:S2:1453:C:C6    | 2.51                     | 0.46              |
| 79:S2:1581:C:H5'   | 79:S2:1582:C:C5    | 2.42                     | 0.46              |
| 83:Ls:37:SER:O     | 83:Ls:40:MET:SD    | 2.74                     | 0.46              |
| 83:Ls:52:VAL:HG23  | 83:Ls:90:PHE:HB2   | 1.97                     | 0.46              |
| 87:LW:93:LYS:HA    | 87:LW:93:LYS:HD2   | 1.65                     | 0.46              |
| 2:sE:54:TYR:OH     | 8:sY:18:LEU:N      | 2.48                     | 0.46              |
| 2:sE:121:TYR:HA    | 2:sE:163:ASP:HA    | 1.96                     | 0.46              |
| 4:sL:147:LYS:HG2   | 4:sL:151:THR:HG23  | 1.96                     | 0.46              |
| 5:sX:48:LYS:HZ2    | 79:s2:483:C:H5''   | 1.80                     | 0.46              |
| 6:sG:20:ASP:OD1    | 6:sG:22:ARG:NE     | 2.47                     | 0.46              |
| 7:sJ:5:ARG:HG2     | 79:s2:38:A:OP1     | 2.16                     | 0.46              |
| 10:sA:220:LYS:HA   | 10:sA:220:LYS:HD3  | 1.71                     | 0.46              |
| 11:sB:40:ASN:OD1   | 11:sB:40:ASN:N     | 2.48                     | 0.46              |
| 14:sa:10:ARG:NH1   | 79:s2:1860:A:OP2   | 2.46                     | 0.46              |
| 15:sC:135:GLY:HA2  | 15:sC:217:ALA:O    | 2.15                     | 0.46              |
| 16:sN:121:ARG:HD3  | 79:s2:924:G:O3'    | 2.16                     | 0.46              |
| 18:sW:3:ARG:NH2    | 18:sW:9:ASP:OD2    | 2.48                     | 0.46              |
| 18:sW:24:GLN:HA    | 18:sW:63:VAL:O     | 2.15                     | 0.46              |
| 21:l8:14:U:H5''    | 36:lP:123:PRO:HG3  | 1.98                     | 0.46              |
| 21:l8:137:A:H2'    | 21:l8:138:C:H6     | 1.79                     | 0.46              |
| 21:l8:144:U:H2'    | 21:l8:145:C:C6     | 2.50                     | 0.46              |
| 22:lA:147:ARG:HA   | 22:lA:157:VAL:HA   | 1.97                     | 0.46              |
| 22:lA:206:PRO:HD3  | 22:lA:213:GLY:CA   | 2.45                     | 0.46              |
| 23:lB:89:ILE:HD11  | 23:lB:197:ALA:HB1  | 1.98                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:1B:120:LYS:NZ   | 85:15:4579:U:OP1   | 2.48                     | 0.46              |
| 24:1C:209:ILE:HB   | 24:1C:229:LEU:HD13 | 1.97                     | 0.46              |
| 26:1E:130:LYS:HG2  | 85:15:1284:G:N3    | 2.30                     | 0.46              |
| 27:1F:96:ARG:HG3   | 27:1F:139:TYR:HA   | 1.97                     | 0.46              |
| 27:1F:122:PHE:HD2  | 27:1F:194:ILE:HD13 | 1.81                     | 0.46              |
| 27:1F:156:LYS:HG3  | 27:1F:157:ARG:HG3  | 1.97                     | 0.46              |
| 29:1H:167:VAL:HG22 | 29:1H:170:LYS:HB2  | 1.97                     | 0.46              |
| 32:1L:8:MET:HE1    | 37:1Q:168:ARG:N    | 2.31                     | 0.46              |
| 33:1M:126:GLU:OE1  | 33:1M:127:VAL:N    | 2.48                     | 0.46              |
| 34:1N:96:ARG:NH1   | 34:1N:104:GLU:OE1  | 2.47                     | 0.46              |
| 38:1R:163:ARG:O    | 38:1R:167:LYS:HG2  | 2.15                     | 0.46              |
| 42:1V:96:LEU:HD23  | 42:1V:96:LEU:H     | 1.79                     | 0.46              |
| 46:1a:79:TRP:HB3   | 46:1a:87:ARG:HH22  | 1.79                     | 0.46              |
| 51:1f:8:LYS:HB2    | 51:1f:100:ARG:CZ   | 2.45                     | 0.46              |
| 51:1f:36:ARG:HH11  | 51:1f:79:GLY:H     | 1.63                     | 0.46              |
| 52:1g:25:THR:HG22  | 52:1g:29:ARG:HG2   | 1.97                     | 0.46              |
| 63:1z:23:ARG:NH1   | 63:1z:212:LYS:O    | 2.49                     | 0.46              |
| 64:sR:14:ARG:CZ    | 79:s2:1373:C:H1'   | 2.46                     | 0.46              |
| 65:sD:42:THR:OG1   | 65:sD:45:ARG:O     | 2.23                     | 0.46              |
| 65:sD:126:ILE:HG13 | 65:sD:127:MET:H    | 1.79                     | 0.46              |
| 69:sQ:15:ARG:HG2   | 69:sQ:20:THR:HG22  | 1.97                     | 0.46              |
| 70:sS:132:ARG:HD3  | 79:s2:1623:A:N6    | 2.31                     | 0.46              |
| 71:sT:139:ALA:HA   | 71:sT:142:ASN:ND2  | 2.30                     | 0.46              |
| 75:sg:237:ASN:OD1  | 75:sg:237:ASN:N    | 2.46                     | 0.46              |
| 76:sM:117:GLU:HA   | 76:sM:120:ALA:HB3  | 1.97                     | 0.46              |
| 79:s2:530:U:H5''   | 79:s2:531:A:O4'    | 2.15                     | 0.46              |
| 79:s2:595:U:H2'    | 79:s2:596:U:C6     | 2.51                     | 0.46              |
| 79:s2:899:U:H3'    | 79:s2:900:C:C5'    | 2.46                     | 0.46              |
| 79:s2:1352:G:C4    | 79:s2:1353:A:C8    | 3.04                     | 0.46              |
| 80:cB:61:LYS:C     | 80:cB:63:GLU:H     | 2.22                     | 0.46              |
| 80:cB:116:THR:O    | 80:cB:497:MET:HE1  | 2.15                     | 0.46              |
| 80:cB:196:GLU:CG   | 80:cB:197:SER:H    | 2.29                     | 0.46              |
| 80:cB:649:ILE:HG23 | 80:cB:661:ILE:HD11 | 1.97                     | 0.46              |
| 85:15:432:U:H4'    | 85:15:433:A:H5''   | 1.96                     | 0.46              |
| 85:15:980:U:H2'    | 85:15:981:C:C6     | 2.50                     | 0.46              |
| 85:15:1309:C:H2'   | 85:15:1310:C:H6    | 1.81                     | 0.46              |
| 85:15:1384:C:C2    | 85:15:1385:G:C8    | 3.04                     | 0.46              |
| 85:15:1634:A:C6    | 85:15:1635:C:C4    | 3.03                     | 0.46              |
| 85:15:1647:U:H2'   | 85:15:1648:C:C6    | 2.51                     | 0.46              |
| 85:15:1709:C:N3    | 85:15:1716:G:C2    | 2.83                     | 0.46              |
| 85:15:2633:U:H2'   | 85:15:2634:C:C6    | 2.47                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 85:L5:3832:U:H2'   | 85:L5:3833:C:C6    | 2.50                     | 0.46              |
| 85:L5:4219:A:H2'   | 85:L5:4220:A:C8    | 2.50                     | 0.46              |
| 85:L5:4355:G:C2    | 85:L5:4356:G:C8    | 3.04                     | 0.46              |
| 85:L5:4918:C:H2'   | 85:L5:4919:G:C8    | 2.49                     | 0.46              |
| 85:L5:4957:C:H2'   | 85:L5:4958:C:H6    | 1.81                     | 0.46              |
| 80:CB:402:VAL:HG22 | 80:CB:411:TYR:HB2  | 1.97                     | 0.46              |
| 80:CB:659:PRO:HG2  | 80:CB:698:ARG:HA   | 1.97                     | 0.46              |
| 11:SB:123:ALA:HB2  | 11:SB:165:ARG:HG3  | 1.98                     | 0.46              |
| 14:Sa:31:PRO:HB2   | 14:Sa:33:ASP:OD1   | 2.15                     | 0.46              |
| 14:Sa:88:SER:OG    | 79:S2:1691:U:H4'   | 2.16                     | 0.46              |
| 18:SW:81:VAL:N     | 18:SW:123:GLY:O    | 2.48                     | 0.46              |
| 85:L5:337:U:OP1    | 32:LL:35:ARG:NH1   | 2.41                     | 0.46              |
| 85:L5:473:C:H2'    | 85:L5:474:C:C6     | 2.50                     | 0.46              |
| 85:L5:484:U:O4     | 85:L5:665:C:H2'    | 2.15                     | 0.46              |
| 85:L5:683:C:H2'    | 85:L5:684:G:O4'    | 2.15                     | 0.46              |
| 85:L5:739:G:C2     | 85:L5:740:G:C2     | 3.04                     | 0.46              |
| 85:L5:1086:C:H2'   | 85:L5:1087:A:H8    | 1.81                     | 0.46              |
| 85:L5:1305:C:H2'   | 85:L5:1306:C:H6    | 1.80                     | 0.46              |
| 85:L5:1507:C:H2'   | 85:L5:1508:A:C8    | 2.49                     | 0.46              |
| 85:L5:2029:A:H2'   | 85:L5:2030:A:H8    | 1.79                     | 0.46              |
| 85:L5:2072:C:C2    | 85:L5:2073:C:C5    | 3.03                     | 0.46              |
| 85:L5:2079:G:OP1   | 50:Le:64:LYS:HE3   | 2.16                     | 0.46              |
| 85:L5:3874:G:H2'   | 85:L5:3875:G:C8    | 2.51                     | 0.46              |
| 85:L5:4087:G:O5'   | 22:LA:37:ARG:NH2   | 2.48                     | 0.46              |
| 85:L5:4467:A:H61   | 85:L5:4490:C:H42   | 1.62                     | 0.46              |
| 85:L5:4910:G:O2'   | 85:L5:4911:A:H8    | 1.99                     | 0.46              |
| 20:L7:61:G:C5'     | 25:LD:271:MET:HE1  | 2.45                     | 0.46              |
| 21:L8:73:U:H2'     | 21:L8:74:U:O4'     | 2.15                     | 0.46              |
| 21:L8:96:C:H2'     | 21:L8:97:A:C8      | 2.51                     | 0.46              |
| 23:LB:213:GLN:HG3  | 23:LB:214:ASP:OD2  | 2.15                     | 0.46              |
| 24:LC:152:LEU:HD23 | 24:LC:251:ILE:HD12 | 1.97                     | 0.46              |
| 25:LD:111:ASN:HA   | 25:LD:116:ASP:HB3  | 1.96                     | 0.46              |
| 27:LF:227:PHE:HA   | 27:LF:231:GLY:O    | 2.15                     | 0.46              |
| 31:LJ:63:ARG:HB3   | 31:LJ:66:GLU:OE2   | 2.14                     | 0.46              |
| 45:LZ:11:VAL:CG2   | 45:LZ:80:LEU:HB2   | 2.44                     | 0.46              |
| 45:LZ:87:VAL:HG12  | 45:LZ:127:ASN:ND2  | 2.29                     | 0.46              |
| 46:La:119:LYS:HB3  | 46:La:119:LYS:HE2  | 1.74                     | 0.46              |
| 48:Lc:59:GLU:OE1   | 48:Lc:60:ILE:HD13  | 2.16                     | 0.46              |
| 50:Le:89:LEU:HD12  | 50:Le:90:MET:SD    | 2.55                     | 0.46              |
| 51:Lf:31:GLU:OE1   | 51:Lf:31:GLU:N     | 2.46                     | 0.46              |
| 54:Li:55:ARG:O     | 54:Li:59:GLU:HG3   | 2.15                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 55:Lj:56:ARG:O     | 55:Lj:56:ARG:HD3   | 2.15                     | 0.46              |
| 62:Lr:93:ILE:HA    | 62:Lr:96:MET:HG2   | 1.95                     | 0.46              |
| 65:SD:158:ILE:HG23 | 65:SD:164:VAL:HG12 | 1.97                     | 0.46              |
| 66:SF:138:ALA:HB3  | 66:SF:204:ARG:HA   | 1.97                     | 0.46              |
| 70:SS:30:ILE:O     | 70:SS:36:VAL:HG11  | 2.16                     | 0.46              |
| 75:Sg:83:TRP:HA    | 75:Sg:107:ASP:HB2  | 1.97                     | 0.46              |
| 75:Sg:240:CYS:N    | 75:Sg:249:CYS:O    | 2.31                     | 0.46              |
| 79:S2:93:U:H2'     | 79:S2:94:G:O4'     | 2.16                     | 0.46              |
| 79:S2:364:A:H2'    | 79:S2:365:C:H6     | 1.80                     | 0.46              |
| 79:S2:375:U:H2'    | 79:S2:376:A:H8     | 1.78                     | 0.46              |
| 79:S2:806:U:H2'    | 79:S2:807:G:H8     | 1.80                     | 0.46              |
| 79:S2:1266:C:H2'   | 79:S2:1267:C:H6    | 1.80                     | 0.46              |
| 79:S2:1405:A:H5'   | 79:S2:1580:A:C8    | 2.51                     | 0.46              |
| 79:S2:1642:U:H2'   | 79:S2:1643:U:C6    | 2.51                     | 0.46              |
| 82:PE:21:A:H2'     | 82:PE:22:G:C8      | 2.50                     | 0.46              |
| 87:IW:58:LYS:HG2   | 87:IW:59:HIS:HD2   | 1.80                     | 0.46              |
| 1:CH:37:ASP:CG     | 86:Se:47:PRO:HD2   | 2.38                     | 0.46              |
| 1:CH:100:ASN:O     | 79:S2:608:C:O2'    | 2.29                     | 0.46              |
| 4:sL:86:ILE:O      | 4:sL:111:VAL:N     | 2.33                     | 0.46              |
| 5:sX:53:GLU:O      | 5:sX:70:VAL:HG23   | 2.15                     | 0.46              |
| 6:sG:118:GLU:CD    | 6:sG:119:LYS:HG3   | 2.40                     | 0.46              |
| 6:sG:213:LEU:O     | 6:sG:217:MET:SD    | 2.74                     | 0.46              |
| 7:sJ:30:LYS:HA     | 9:se:38:TYR:CE2    | 2.47                     | 0.46              |
| 7:sJ:114:VAL:HG23  | 7:sJ:126:ALA:HB1   | 1.98                     | 0.46              |
| 7:sJ:136:ARG:N     | 7:sJ:158:ASP:O     | 2.45                     | 0.46              |
| 8:sY:82:ALA:O      | 8:sY:86:GLU:HB2    | 2.14                     | 0.46              |
| 11:sB:150:ILE:HD12 | 64:sR:131:PRO:CD   | 2.43                     | 0.46              |
| 19:sb:72:ARG:NH1   | 79:s2:1119:A:O2'   | 2.48                     | 0.46              |
| 24:IC:142:HIS:ND1  | 24:IC:249:PHE:HB3  | 2.29                     | 0.46              |
| 25:ID:40:ASP:OD2   | 40:IT:69:GLN:HA    | 2.15                     | 0.46              |
| 25:ID:236:MET:HA   | 25:ID:239:MET:SD   | 2.56                     | 0.46              |
| 26:IE:126:LEU:HD21 | 85:l5:970:G:C2     | 2.51                     | 0.46              |
| 27:IF:227:PHE:HA   | 27:IF:231:GLY:O    | 2.15                     | 0.46              |
| 32:IL:36:ARG:NH2   | 85:l5:1364:U:OP2   | 2.48                     | 0.46              |
| 34:IN:124:ASP:HB3  | 34:IN:127:TYR:N    | 2.31                     | 0.46              |
| 34:IN:195:ARG:HD3  | 85:l5:98:A:OP1     | 2.16                     | 0.46              |
| 38:IR:18:GLY:HA3   | 85:l5:2822:G:H5''  | 1.98                     | 0.46              |
| 38:IR:57:VAL:HG13  | 85:l5:4646:U:H5''  | 1.96                     | 0.46              |
| 40:IT:158:PHE:HE1  | 40:IT:160:ALA:C    | 2.23                     | 0.46              |
| 49:ld:70:LYS:NZ    | 85:l5:2388:A:O3'   | 2.48                     | 0.46              |
| 50:le:122:VAL:HG23 | 50:le:125:PRO:HD3  | 1.97                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 51:lf:66:LYS:HB2   | 51:lf:66:LYS:HE2   | 1.73                     | 0.46              |
| 59:ln:1:MET:CE     | 59:ln:2:ARG:HB3    | 2.46                     | 0.46              |
| 64:sR:35:CYS:HA    | 64:sR:38:ILE:HD11  | 1.96                     | 0.46              |
| 64:sR:46:LEU:HG    | 79:s2:1369:A:N7    | 2.30                     | 0.46              |
| 67:sK:1:MET:N      | 67:sK:1:MET:HE2    | 2.31                     | 0.46              |
| 69:sQ:13:PHE:N     | 79:s2:1397:U:O4    | 2.36                     | 0.46              |
| 70:sS:63:GLU:OE1   | 70:sS:63:GLU:N     | 2.38                     | 0.46              |
| 71:sT:56:ARG:NH1   | 79:s2:1541:G:OP1   | 2.48                     | 0.46              |
| 71:sT:124:THR:HG23 | 71:sT:127:GLY:H    | 1.81                     | 0.46              |
| 74:sd:40:ARG:HH21  | 79:s2:1256:G:P     | 2.38                     | 0.46              |
| 75:sg:42:MET:HE2   | 75:sg:56:GLN:NE2   | 2.30                     | 0.46              |
| 75:sg:199:THR:OG1  | 75:sg:239:LEU:HB2  | 2.16                     | 0.46              |
| 76:sM:31:LEU:HB3   | 76:sM:109:VAL:HG23 | 1.97                     | 0.46              |
| 76:sM:95:ASP:OD1   | 76:sM:95:ASP:N     | 2.46                     | 0.46              |
| 79:s2:344:U:H2'    | 79:s2:345:U:C6     | 2.51                     | 0.46              |
| 79:s2:512:A:C2     | 79:s2:513:G:C8     | 3.04                     | 0.46              |
| 81:aP:26:G:N1      | 81:aP:44:A:C2      | 2.81                     | 0.46              |
| 85:l5:178:C:N4     | 85:l5:179:G:O6     | 2.47                     | 0.46              |
| 85:l5:1172:C:H1'   | 85:l5:1189:G:H22   | 1.80                     | 0.46              |
| 85:l5:1243:C:H2'   | 85:l5:1244:G:O4'   | 2.16                     | 0.46              |
| 85:l5:1727:U:H2'   | 85:l5:1728:U:C6    | 2.51                     | 0.46              |
| 85:l5:1811:G:H2'   | 85:l5:1812:C:H6    | 1.79                     | 0.46              |
| 85:l5:2372:U:H2'   | 85:l5:2373:C:C6    | 2.50                     | 0.46              |
| 85:l5:2878:G:OP2   | 85:l5:2879:A:O2'   | 2.24                     | 0.46              |
| 85:l5:3932:U:H2'   | 85:l5:3933:G:H8    | 1.80                     | 0.46              |
| 85:l5:4683:U:C4    | 85:l5:4707:A:C5    | 3.03                     | 0.46              |
| 85:l5:4684:A:H2'   | 85:l5:4685:U:O4'   | 2.14                     | 0.46              |
| 85:l5:5037:U:H2'   | 85:l5:5038:A:H8    | 1.79                     | 0.46              |
| 80:CB:308:LYS:HB2  | 80:CB:311:GLU:HB3  | 1.97                     | 0.46              |
| 80:CB:403:PRO:HA   | 80:CB:410:PHE:CD2  | 2.50                     | 0.46              |
| 80:CB:613:LEU:HG   | 80:CB:639:TYR:CD2  | 2.50                     | 0.46              |
| 2:SE:49:ARG:NH1    | 79:S2:495:U:OP1    | 2.48                     | 0.46              |
| 6:SG:126:ASP:OD1   | 6:SG:127:THR:HG23  | 2.15                     | 0.46              |
| 6:SG:177:GLN:HE22  | 79:S2:63:U:H5''    | 1.79                     | 0.46              |
| 7:SJ:113:GLN:NE2   | 7:SJ:149:VAL:HG22  | 2.31                     | 0.46              |
| 10:SA:141:ASN:HD21 | 15:SC:86:LEU:HA    | 1.80                     | 0.46              |
| 11:SB:34:LYS:HG2   | 11:SB:95:ASN:OD1   | 2.15                     | 0.46              |
| 14:Sa:73:TYR:CD1   | 14:Sa:83:VAL:HG21  | 2.50                     | 0.46              |
| 15:SC:187:ARG:HH22 | 15:SC:190:SER:HA   | 1.80                     | 0.46              |
| 15:SC:199:PRO:HG2  | 15:SC:202:THR:HG21 | 1.97                     | 0.46              |
| 17:SO:96:LYS:HD3   | 17:SO:96:LYS:HA    | 1.79                     | 0.46              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 18:SW:23:ARG:C     | 18:SW:23:ARG:HD2  | 2.40                     | 0.46              |
| 85:L5:186:G:H4'    | 85:L5:187:U:H5'   | 1.97                     | 0.46              |
| 85:L5:416:U:H2'    | 85:L5:417:G:O4'   | 2.14                     | 0.46              |
| 85:L5:1244:G:H2'   | 85:L5:1245:C:H6   | 1.80                     | 0.46              |
| 85:L5:1292:C:H2'   | 85:L5:1293:G:N3   | 2.30                     | 0.46              |
| 85:L5:1655:C:O2    | 85:L5:4390:A:O2'  | 2.33                     | 0.46              |
| 85:L5:1727:U:O2'   | 27:LF:127:LYS:HE3 | 2.15                     | 0.46              |
| 85:L5:1762:C:H5''  | 85:L5:1764:G:H22  | 1.81                     | 0.46              |
| 85:L5:2570:U:H2'   | 85:L5:2571:C:C6   | 2.50                     | 0.46              |
| 85:L5:2821:U:C2    | 85:L5:2822:G:C8   | 3.04                     | 0.46              |
| 85:L5:3680:U:OP1   | 22:LA:54:ARG:NH1  | 2.45                     | 0.46              |
| 85:L5:4102:C:C5    | 85:L5:4105:A:O4'  | 2.68                     | 0.46              |
| 85:L5:4154:G:H2'   | 85:L5:4155:C:C6   | 2.50                     | 0.46              |
| 85:L5:4561:C:H2'   | 85:L5:4562:C:H6   | 1.80                     | 0.46              |
| 85:L5:4988:U:H4'   | 85:L5:4989:U:C5   | 2.50                     | 0.46              |
| 21:L8:64:U:C2      | 21:L8:65:A:C8     | 3.03                     | 0.46              |
| 22:LA:45:VAL:HG23  | 22:LA:84:THR:HA   | 1.97                     | 0.46              |
| 25:LD:108:ARG:NH2  | 25:LD:253:TYR:HB2 | 2.30                     | 0.46              |
| 25:LD:212:MET:HE1  | 25:LD:219:TYR:CZ  | 2.51                     | 0.46              |
| 28:LG:154:LEU:HD23 | 28:LG:204:PHE:CD2 | 2.50                     | 0.46              |
| 29:LH:113:GLU:CD   | 29:LH:115:ARG:HE  | 2.23                     | 0.46              |
| 31:LJ:97:ASN:OD1   | 31:LJ:97:ASN:N    | 2.49                     | 0.46              |
| 33:LM:20:HIS:HB3   | 33:LM:23:LYS:HG3  | 1.97                     | 0.46              |
| 33:LM:127:VAL:O    | 33:LM:131:GLN:HG2 | 2.15                     | 0.46              |
| 34:LN:113:LEU:HD22 | 34:LN:136:ASP:HA  | 1.97                     | 0.46              |
| 35:LO:124:LEU:HD23 | 35:LO:124:LEU:HA  | 1.70                     | 0.46              |
| 38:LR:168:GLU:O    | 38:LR:171:LYS:HG3 | 2.15                     | 0.46              |
| 44:LY:43:ASN:O     | 44:LY:126:ARG:HD3 | 2.15                     | 0.46              |
| 65:SD:51:LEU:HD12  | 65:SD:91:VAL:HG23 | 1.97                     | 0.46              |
| 66:SF:100:ILE:HD13 | 66:SF:174:ALA:HB1 | 1.98                     | 0.46              |
| 69:SQ:128:GLU:OE1  | 69:SQ:128:GLU:N   | 2.47                     | 0.46              |
| 70:SS:101:ASN:OD1  | 70:SS:101:ASN:N   | 2.46                     | 0.46              |
| 71:ST:56:ARG:HD2   | 71:ST:79:TYR:CZ   | 2.50                     | 0.46              |
| 75:Sg:216:ALA:N    | 75:Sg:230:LEU:O   | 2.48                     | 0.46              |
| 79:S2:463:C:O2'    | 79:S2:466:G:O6    | 2.26                     | 0.46              |
| 79:S2:958:G:H2'    | 79:S2:959:G:C8    | 2.51                     | 0.46              |
| 79:S2:1461:G:H2'   | 79:S2:1463:U:O2   | 2.15                     | 0.46              |
| 79:S2:1630:A:N3    | 79:S2:1630:A:H2'  | 2.31                     | 0.46              |
| 1:CH:109:TYR:HA    | 1:CH:114:ALA:HB2  | 1.96                     | 0.46              |
| 3:sI:119:LEU:O     | 3:sI:121:LEU:HD22 | 2.16                     | 0.46              |
| 6:sG:190:ARG:NH1   | 79:s2:333:G:O5'   | 2.48                     | 0.46              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 10:sA:38:ILE:CD1   | 10:sA:47:TYR:HB3  | 2.45                     | 0.46              |
| 10:sA:84:GLN:O     | 10:sA:87:VAL:HG22 | 2.16                     | 0.46              |
| 11:sB:30:TRP:CG    | 17:sO:19:PRO:HG3  | 2.51                     | 0.46              |
| 11:sB:104:ASP:OD2  | 11:sB:105:LEU:N   | 2.40                     | 0.46              |
| 13:sV:9:VAL:O      | 13:sV:9:VAL:HG13  | 2.15                     | 0.46              |
| 15:sC:190:SER:HB3  | 79:s2:14:C:H5'    | 1.98                     | 0.46              |
| 16:sN:124:ARG:HG2  | 16:sN:127:ARG:NH2 | 2.31                     | 0.46              |
| 17:sO:138:ASP:HB2  | 79:s2:986:G:O4'   | 2.16                     | 0.46              |
| 20:l7:98:G:H2'     | 20:l7:99:G:O4'    | 2.15                     | 0.46              |
| 24:lC:361:LEU:HD23 | 24:lC:364:LYS:NZ  | 2.30                     | 0.46              |
| 26:lE:108:LYS:HB2  | 26:lE:108:LYS:HE3 | 1.78                     | 0.46              |
| 27:lF:91:PHE:HB2   | 27:lF:145:PRO:HG3 | 1.97                     | 0.46              |
| 31:lJ:95:ARG:HG2   | 31:lJ:96:LYS:H    | 1.81                     | 0.46              |
| 34:lN:123:GLU:HB2  | 34:lN:128:LYS:HA  | 1.98                     | 0.46              |
| 34:lN:193:ARG:NH1  | 85:l5:27:C:OP1    | 2.40                     | 0.46              |
| 37:lQ:172:ARG:CZ   | 37:lQ:173:LYS:HG2 | 2.46                     | 0.46              |
| 42:lV:117:ILE:HD11 | 42:lV:135:ASN:HB3 | 1.98                     | 0.46              |
| 51:lf:104:MET:SD   | 51:lf:104:MET:N   | 2.89                     | 0.46              |
| 57:ll:36:ARG:HG3   | 57:ll:37:TYR:CE1  | 2.51                     | 0.46              |
| 60:lo:6:LYS:O      | 60:lo:23:VAL:HG22 | 2.16                     | 0.46              |
| 60:lo:105:GLN:N    | 60:lo:105:GLN:OE1 | 2.48                     | 0.46              |
| 64:sR:128:PHE:CG   | 64:sR:129:LYS:N   | 2.84                     | 0.46              |
| 65:sD:90:LYS:HZ2   | 65:sD:92:ALA:HA   | 1.80                     | 0.46              |
| 66:sF:167:LYS:NZ   | 66:sF:171:GLU:HG3 | 2.30                     | 0.46              |
| 69:sQ:11:GLN:OE1   | 79:s2:1442:U:H1'  | 2.15                     | 0.46              |
| 72:sU:18:HIS:ND1   | 72:sU:94:PRO:HA   | 2.30                     | 0.46              |
| 72:sU:20:ILE:CG2   | 72:sU:91:LEU:HB2  | 2.45                     | 0.46              |
| 73:sc:13:ARG:HG2   | 73:sc:35:MET:HE3  | 1.97                     | 0.46              |
| 76:sM:61:TYR:HE1   | 76:sM:107:SER:CB  | 2.29                     | 0.46              |
| 79:s2:19:A:H2'     | 79:s2:20:G:O4'    | 2.15                     | 0.46              |
| 79:s2:634:A:C2     | 79:s2:635:G:C5    | 3.04                     | 0.46              |
| 79:s2:833:C:C4     | 79:s2:834:C:N4    | 2.84                     | 0.46              |
| 79:s2:1122:A:C6    | 79:s2:1123:C:C5   | 3.03                     | 0.46              |
| 79:s2:1220:A:H2'   | 79:s2:1221:G:O4'  | 2.15                     | 0.46              |
| 79:s2:1511:U:H2'   | 79:s2:1512:C:H6   | 1.80                     | 0.46              |
| 79:s2:1686:G:H2'   | 79:s2:1687:C:H6   | 1.80                     | 0.46              |
| 79:s2:1773:C:H2'   | 79:s2:1774:C:H5'' | 1.96                     | 0.46              |
| 79:s2:1839:U:H2'   | 79:s2:1840:U:C6   | 2.50                     | 0.46              |
| 79:s2:1839:U:H2'   | 79:s2:1840:U:H6   | 1.81                     | 0.46              |
| 80:cB:509:VAL:HG13 | 80:cB:544:HIS:HB2 | 1.98                     | 0.46              |
| 84:lt:32:ILE:O     | 84:lt:32:ILE:HG13 | 2.16                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 85:L5:18:C:H2'     | 85:L5:19:G:C8      | 2.51                     | 0.46              |
| 85:L5:452:A:H4'    | 85:L5:453:G:H5'    | 1.98                     | 0.46              |
| 85:L5:665:C:H1'    | 85:L5:666:G:N7     | 2.29                     | 0.46              |
| 85:L5:1211:G:H2'   | 85:L5:1212:G:C8    | 2.50                     | 0.46              |
| 85:L5:1418:C:H2'   | 85:L5:1419:G:O4'   | 2.16                     | 0.46              |
| 85:L5:1662:C:H2'   | 85:L5:1663:C:C6    | 2.51                     | 0.46              |
| 85:L5:1762:C:N4    | 85:L5:1770:A:H2    | 2.06                     | 0.46              |
| 85:L5:1779:U:H2'   | 85:L5:1780:A:H8    | 1.81                     | 0.46              |
| 85:L5:2059:C:H2'   | 85:L5:2060:G:H8    | 1.81                     | 0.46              |
| 85:L5:2286:G:H2'   | 85:L5:2287:G:C8    | 2.51                     | 0.46              |
| 85:L5:2699:C:H2'   | 85:L5:2700:G:C8    | 2.50                     | 0.46              |
| 85:L5:2885:A:H2'   | 85:L5:2886:U:H6    | 1.80                     | 0.46              |
| 85:L5:3759:A:OP2   | 85:L5:3765:G:N1    | 2.33                     | 0.46              |
| 85:L5:4485:C:H2'   | 85:L5:4486:C:C6    | 2.51                     | 0.46              |
| 85:L5:4713:G:C5    | 85:L5:4714:C:C5    | 3.04                     | 0.46              |
| 85:L5:5003:U:H2'   | 85:L5:5004:C:C6    | 2.51                     | 0.46              |
| 80:CB:167:LEU:HD22 | 29:LH:100:PRO:HD2  | 1.97                     | 0.46              |
| 80:CB:830:ARG:H    | 80:CB:830:ARG:HG2  | 1.55                     | 0.46              |
| 2:SE:21:ASP:OD1    | 2:SE:24:THR:OG1    | 2.20                     | 0.46              |
| 2:SE:43:PRO:HB2    | 2:SE:45:ILE:HG22   | 1.97                     | 0.46              |
| 3:SI:83:TYR:HA     | 3:SI:91:VAL:HG21   | 1.97                     | 0.46              |
| 7:SJ:22:LYS:HA     | 7:SJ:25:LEU:HD12   | 1.98                     | 0.46              |
| 10:SA:81:ASN:HA    | 10:SA:84:GLN:OE1   | 2.16                     | 0.46              |
| 12:SH:147:LYS:O    | 12:SH:149:ASP:N    | 2.49                     | 0.46              |
| 17:SO:57:THR:O     | 17:SO:60:MET:HG2   | 2.16                     | 0.46              |
| 19:Sb:54:VAL:C     | 19:Sb:55:LEU:HD23  | 2.41                     | 0.46              |
| 85:L5:369:G:N1     | 85:L5:373:G:C6     | 2.83                     | 0.46              |
| 85:L5:663:G:C6     | 85:L5:664:G:C6     | 3.04                     | 0.46              |
| 85:L5:911:U:H2'    | 85:L5:912:G:C4     | 2.51                     | 0.46              |
| 85:L5:1298:C:H2'   | 85:L5:1299:G:C8    | 2.51                     | 0.46              |
| 85:L5:1350:C:H2'   | 85:L5:1351:G:C8    | 2.51                     | 0.46              |
| 85:L5:1515:A:H2'   | 85:L5:1516:G:O4'   | 2.16                     | 0.46              |
| 85:L5:1918:U:O2    | 85:L5:2064:G:O6    | 2.33                     | 0.46              |
| 85:L5:2028:C:H2'   | 85:L5:2029:A:H8    | 1.81                     | 0.46              |
| 85:L5:2249:C:H2'   | 85:L5:2250:C:H5    | 1.81                     | 0.46              |
| 85:L5:2459:G:N2    | 85:L5:2462:C:OP2   | 2.43                     | 0.46              |
| 85:L5:2654:C:C2    | 85:L5:2655:C:C5    | 3.03                     | 0.46              |
| 85:L5:2838:G:H2'   | 85:L5:2839:U:C6    | 2.51                     | 0.46              |
| 85:L5:3919:C:H5''  | 22:LA:207:VAL:HG12 | 1.96                     | 0.46              |
| 85:L5:4110:C:H4'   | 85:L5:4112:C:O5'   | 2.15                     | 0.46              |
| 85:L5:4233:A:P     | 60:Lo:97:LYS:HD2   | 2.56                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 85:L5:4237:C:H2'   | 85:L5:4238:G:C8    | 2.50                     | 0.46              |
| 20:L7:1:G:H4'      | 25:LD:265:ARG:NE   | 2.31                     | 0.46              |
| 23:LB:279:GLU:OE2  | 23:LB:338:VAL:HB   | 2.16                     | 0.46              |
| 24:LC:253:THR:HG23 | 24:LC:256:ALA:H    | 1.80                     | 0.46              |
| 26:LE:72:LYS:HA    | 47:Lb:117:ARG:HH12 | 1.81                     | 0.46              |
| 29:LH:90:TYR:HB2   | 29:LH:146:LEU:HD21 | 1.97                     | 0.46              |
| 32:LL:65:ARG:HG3   | 46:La:69:PHE:CD1   | 2.51                     | 0.46              |
| 33:LM:113:MET:SD   | 33:LM:114:LYS:N    | 2.89                     | 0.46              |
| 34:LN:65:ARG:HB2   | 34:LN:129:PHE:CE1  | 2.51                     | 0.46              |
| 35:LO:111:PRO:C    | 35:LO:112:TYR:HD2  | 2.23                     | 0.46              |
| 36:LP:48:LEU:O     | 36:LP:52:THR:HG23  | 2.16                     | 0.46              |
| 39:LS:45:TRP:HH2   | 39:LS:59:GLY:HA3   | 1.81                     | 0.46              |
| 45:LZ:33:THR:C     | 45:LZ:35:ASP:H     | 2.24                     | 0.46              |
| 47:Lb:103:LYS:HE2  | 47:Lb:104:LEU:HG   | 1.98                     | 0.46              |
| 48:Lc:44:LYS:N     | 48:Lc:44:LYS:HD2   | 2.30                     | 0.46              |
| 53:Lh:52:LYS:HD3   | 53:Lh:52:LYS:HA    | 1.70                     | 0.46              |
| 54:Li:60:LEU:HD21  | 54:Li:65:LYS:O     | 2.15                     | 0.46              |
| 72:SU:35:VAL:CG1   | 72:SU:107:GLU:HG2  | 2.45                     | 0.46              |
| 79:S2:85:A:H2'     | 79:S2:86:C:H6      | 1.80                     | 0.46              |
| 79:S2:114:G:O2'    | 79:S2:115:U:O5'    | 2.34                     | 0.46              |
| 79:S2:394:G:H2'    | 79:S2:394:G:N3     | 2.31                     | 0.46              |
| 79:S2:568:C:H2'    | 79:S2:569:A:O4'    | 2.16                     | 0.46              |
| 79:S2:604:A:N3     | 79:S2:639:C:O2'    | 2.40                     | 0.46              |
| 79:S2:1006:C:H2'   | 79:S2:1007:C:H6    | 1.80                     | 0.46              |
| 79:S2:1414:A:H5'   | 79:S2:1415:C:OP2   | 2.16                     | 0.46              |
| 79:S2:1495:G:H2'   | 79:S2:1496:U:C6    | 2.50                     | 0.46              |
| 79:S2:1515:G:H2'   | 79:S2:1516:G:C8    | 2.51                     | 0.46              |
| 2:sE:173:ILE:HD11  | 2:sE:235:TRP:CZ2   | 2.50                     | 0.46              |
| 5:sX:104:GLY:O     | 79:s2:648:A:H4'    | 2.15                     | 0.46              |
| 8:sY:37:LYS:HE2    | 79:s2:571:U:OP1    | 2.15                     | 0.46              |
| 9:se:44:ASN:OD1    | 9:se:44:ASN:N      | 2.48                     | 0.46              |
| 11:sB:71:LEU:HD21  | 11:sB:84:PHE:CD1   | 2.50                     | 0.46              |
| 11:sB:82:ARG:NH2   | 11:sB:191:ASP:OD1  | 2.48                     | 0.46              |
| 11:sB:107:ARG:NH2  | 17:sO:132:VAL:C    | 2.73                     | 0.46              |
| 14:sa:4:LYS:HE3    | 14:sa:5:ARG:NH1    | 2.31                     | 0.46              |
| 17:sO:55:ARG:HH11  | 79:s2:974:C:H1'    | 1.80                     | 0.46              |
| 22:lA:2:GLY:HA2    | 85:l5:4185:G:OP1   | 2.15                     | 0.46              |
| 26:lE:203:ILE:HD12 | 26:lE:260:LYS:HE3  | 1.98                     | 0.46              |
| 27:lF:220:MET:HB2  | 27:lF:232:ASP:OD1  | 2.15                     | 0.46              |
| 29:lH:71:ARG:HH11  | 85:l5:4691:A:H4'   | 1.80                     | 0.46              |
| 30:lI:16:PRO:HG3   | 30:lI:128:ARG:CZ   | 2.45                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 32:1L:185:ALA:HB1  | 54:1i:10:GLY:HA3   | 1.97                     | 0.46              |
| 33:1M:24:LEU:O     | 33:1M:43:THR:HG21  | 2.16                     | 0.46              |
| 34:1N:47:LYS:NZ    | 85:15:280:G:OP1    | 2.27                     | 0.46              |
| 34:1N:85:VAL:HG23  | 34:1N:86:HIS:CD2   | 2.51                     | 0.46              |
| 36:1P:41:ILE:HG22  | 36:1P:112:LEU:O    | 2.15                     | 0.46              |
| 38:1R:124:TYR:O    | 38:1R:127:VAL:HG12 | 2.16                     | 0.46              |
| 38:1R:176:ARG:NH2  | 38:1R:180:LYS:HE3  | 2.26                     | 0.46              |
| 43:1X:94:ASN:ND2   | 43:1X:94:ASN:O     | 2.49                     | 0.46              |
| 44:1Y:2:LYS:HE3    | 44:1Y:2:LYS:HB3    | 1.72                     | 0.46              |
| 47:1b:118:LEU:HD11 | 85:15:1241:C:C6    | 2.51                     | 0.46              |
| 50:1e:64:LYS:HG2   | 85:15:2078:C:OP1   | 2.15                     | 0.46              |
| 50:1e:80:HIS:N     | 50:1e:84:GLU:OE2   | 2.49                     | 0.46              |
| 55:1j:39:TYR:O     | 55:1j:39:TYR:CG    | 2.65                     | 0.46              |
| 55:1j:67:LEU:O     | 55:1j:71:TYR:CD2   | 2.69                     | 0.46              |
| 58:1m:79:GLU:OE2   | 58:1m:81:SER:HB3   | 2.15                     | 0.46              |
| 61:1p:16:THR:HG22  | 85:15:2876:G:C8    | 2.51                     | 0.46              |
| 63:1z:106:LYS:HE2  | 63:1z:106:LYS:HA   | 1.98                     | 0.46              |
| 75:sg:168:CYS:HB2  | 75:sg:198:VAL:HB   | 1.97                     | 0.46              |
| 79:s2:452:G:H2'    | 79:s2:453:C:C6     | 2.49                     | 0.46              |
| 79:s2:566:U:H3'    | 79:s2:567:C:C6     | 2.50                     | 0.46              |
| 79:s2:639:C:H2'    | 79:s2:640:A:C8     | 2.41                     | 0.46              |
| 79:s2:747:U:H2'    | 79:s2:748:C:O4'    | 2.16                     | 0.46              |
| 79:s2:900:C:H5'    | 79:s2:901:G:N7     | 2.31                     | 0.46              |
| 79:s2:1048:G:N1    | 79:s2:1069:U:OP2   | 2.44                     | 0.46              |
| 79:s2:1444:U:H2'   | 79:s2:1445:U:O4'   | 2.15                     | 0.46              |
| 79:s2:1856:C:H2'   | 79:s2:1857:G:H8    | 1.81                     | 0.46              |
| 80:cB:79:TYR:CD1   | 80:cB:351:LEU:HD13 | 2.51                     | 0.46              |
| 83:1s:54:LEU:HD12  | 83:1s:54:LEU:HA    | 1.72                     | 0.46              |
| 84:1t:143:VAL:O    | 84:1t:146:ARG:HG2  | 2.16                     | 0.46              |
| 85:15:1407:C:O2'   | 85:15:1408:G:H5'   | 2.15                     | 0.46              |
| 85:15:2414:G:C6    | 85:15:2431:A:C6    | 3.03                     | 0.46              |
| 85:15:2656:U:H2'   | 85:15:2657:G:C8    | 2.51                     | 0.46              |
| 85:15:2765:A:H2'   | 85:15:2766:A:C8    | 2.51                     | 0.46              |
| 85:15:2857:A:H2'   | 85:15:2858:A:O4'   | 2.16                     | 0.46              |
| 85:15:2898:G:H2'   | 85:15:2899:C:C6    | 2.50                     | 0.46              |
| 85:15:4113:U:H4'   | 85:15:4115:G:C8    | 2.51                     | 0.46              |
| 85:15:4152:G:H2'   | 85:15:4153:C:H6    | 1.80                     | 0.46              |
| 85:15:4503:A:H2'   | 85:15:4504:C:H6    | 1.79                     | 0.46              |
| 85:15:4633:G:N2    | 85:15:4664:A:OP2   | 2.37                     | 0.46              |
| 85:15:5051:C:H2'   | 85:15:5052:C:C6    | 2.50                     | 0.46              |
| 80:CB:45:ILE:HD11  | 80:CB:77:LEU:O     | 2.15                     | 0.46              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 80:CB:111:PHE:CD2 | 80:CB:111:PHE:O    | 2.69                     | 0.46              |
| 80:CB:481:LYS:N   | 80:CB:529:LYS:HZ3  | 2.12                     | 0.46              |
| 80:CB:639:TYR:O   | 80:CB:640:GLU:HG3  | 2.16                     | 0.46              |
| 4:SL:71:ARG:HH21  | 79:S2:855:G:HO2'   | 1.62                     | 0.46              |
| 4:SL:133:PRO:HG2  | 79:S2:383:G:H21    | 1.81                     | 0.46              |
| 7:SJ:107:GLU:CD   | 7:SJ:108:ARG:HD2   | 2.41                     | 0.46              |
| 16:SN:69:ASN:ND2  | 16:SN:74:ILE:HG13  | 2.30                     | 0.46              |
| 85:L5:302:C:H2'   | 85:L5:303:C:H6     | 1.80                     | 0.46              |
| 85:L5:461:G:H2'   | 85:L5:462:G:C8     | 2.50                     | 0.46              |
| 85:L5:505:G:C6    | 85:L5:654:C:C2     | 3.04                     | 0.46              |
| 85:L5:671:G:H2'   | 85:L5:672:C:H6     | 1.80                     | 0.46              |
| 85:L5:726:G:H2'   | 85:L5:727:C:H6     | 1.81                     | 0.46              |
| 85:L5:750:U:C2    | 85:L5:751:G:C8     | 3.04                     | 0.46              |
| 85:L5:918:G:H5'   | 33:LM:72:TYR:CE1   | 2.50                     | 0.46              |
| 85:L5:1336:G:H21  | 85:L5:2349:A:H62   | 1.64                     | 0.46              |
| 85:L5:1656:U:C2   | 85:L5:1657:G:C8    | 3.04                     | 0.46              |
| 85:L5:1672:U:H2'  | 85:L5:1673:U:H6    | 1.80                     | 0.46              |
| 85:L5:2004:U:H2'  | 85:L5:2005:G:C8    | 2.51                     | 0.46              |
| 85:L5:2078:C:OP1  | 50:Le:64:LYS:HG2   | 2.16                     | 0.46              |
| 85:L5:3794:C:H2'  | 85:L5:3795:A:H8    | 1.80                     | 0.46              |
| 85:L5:3835:C:H2'  | 85:L5:3836:A:C8    | 2.51                     | 0.46              |
| 85:L5:3951:G:H8   | 85:L5:3951:G:OP2   | 1.99                     | 0.46              |
| 85:L5:3963:A:H3'  | 85:L5:3965:A:H5'   | 1.98                     | 0.46              |
| 85:L5:4182:G:O2'  | 85:L5:4184:G:N7    | 2.44                     | 0.46              |
| 85:L5:4303:C:H3'  | 85:L5:4305:G:N2    | 2.31                     | 0.46              |
| 85:L5:4343:U:H2'  | 85:L5:4344:U:H6    | 1.81                     | 0.46              |
| 85:L5:4378:A:O2'  | 85:L5:4379:A:H2'   | 2.16                     | 0.46              |
| 85:L5:4941:G:H5'  | 26:LE:187:ARG:HG3  | 1.98                     | 0.46              |
| 21:L8:60:G:O6     | 21:L8:96:C:O2'     | 2.30                     | 0.46              |
| 23:LB:286:LYS:HG2 | 23:LB:332:MET:CE   | 2.45                     | 0.46              |
| 26:LE:209:PRO:HB2 | 26:LE:212:LEU:HD21 | 1.98                     | 0.46              |
| 27:LF:226:HIS:HE1 | 27:LF:235:ASN:H    | 1.62                     | 0.46              |
| 30:LI:187:LYS:HE3 | 30:LI:189:CYS:HB2  | 1.97                     | 0.46              |
| 37:LQ:124:ASP:OD1 | 37:LQ:125:GLN:N    | 2.39                     | 0.46              |
| 38:LR:24:LEU:HA   | 38:LR:50:ILE:HD12  | 1.98                     | 0.46              |
| 40:LT:36:LYS:NZ   | 40:LT:65:TYR:O     | 2.47                     | 0.46              |
| 41:LU:34:MET:SD   | 41:LU:35:ASP:N     | 2.89                     | 0.46              |
| 42:LV:90:ARG:NH2  | 42:LV:140:ALA:O    | 2.49                     | 0.46              |
| 48:Lc:48:LEU:HB3  | 48:Lc:72:HIS:O     | 2.15                     | 0.46              |
| 53:Lh:14:LYS:HE2  | 53:Lh:14:LYS:HB3   | 1.74                     | 0.46              |
| 53:Lh:22:ASP:OD1  | 53:Lh:22:ASP:C     | 2.59                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 64:SR:11:LYS:O     | 64:SR:15:VAL:HG22  | 2.16                     | 0.46              |
| 65:SD:24:PHE:CD2   | 67:SK:63:ALA:HB2   | 2.51                     | 0.46              |
| 65:SD:65:ARG:HA    | 65:SD:68:GLU:OE2   | 2.16                     | 0.46              |
| 66:SF:93:VAL:HG22  | 66:SF:97:PHE:CZ    | 2.51                     | 0.46              |
| 71:ST:85:ASN:CB    | 71:ST:88:MET:HB3   | 2.42                     | 0.46              |
| 72:SU:106:ILE:HG23 | 72:SU:107:GLU:H    | 1.80                     | 0.46              |
| 73:Sc:30:VAL:N     | 73:Sc:44:ARG:O     | 2.47                     | 0.46              |
| 74:Sd:27:ARG:NH1   | 79:S2:1263:U:H4'   | 2.31                     | 0.46              |
| 75:Sg:31:ILE:HG23  | 75:Sg:45:LEU:HD11  | 1.98                     | 0.46              |
| 76:SM:79:VAL:CG2   | 76:SM:88:TRP:CH2   | 2.99                     | 0.46              |
| 79:S2:26:U:H2'     | 79:S2:27:A:C8      | 2.50                     | 0.46              |
| 79:S2:458:A:H2'    | 79:S2:459:C:C6     | 2.49                     | 0.46              |
| 79:S2:734:C:H6     | 79:S2:736:C:H42    | 1.63                     | 0.46              |
| 79:S2:799:U:C4     | 79:S2:867:G:C6     | 3.04                     | 0.46              |
| 79:S2:1091:C:H2'   | 79:S2:1092:G:H8    | 1.80                     | 0.46              |
| 79:S2:1139:C:H2'   | 79:S2:1140:G:O4'   | 2.16                     | 0.46              |
| 79:S2:1446:A:HO2'  | 79:S2:1447:G:H8    | 1.59                     | 0.46              |
| 79:S2:1639:G:N2    | 82:PE:41:U:O2'     | 2.42                     | 0.46              |
| 79:S2:1778:C:H2'   | 79:S2:1779:G:H8    | 1.81                     | 0.46              |
| 81:AP:38:C:C2      | 81:AP:39:G:C8      | 3.04                     | 0.46              |
| 87:LW:86:SER:N     | 87:LW:89:ASP:OD2   | 2.49                     | 0.46              |
| 1:cH:47:GLY:H      | 9:se:55:PRO:CD     | 2.28                     | 0.46              |
| 2:sE:164:LEU:HD23  | 2:sE:164:LEU:H     | 1.80                     | 0.46              |
| 3:sI:31:ARG:NE     | 79:s2:380:G:OP1    | 2.49                     | 0.46              |
| 6:sG:67:VAL:HG11   | 6:sG:99:GLY:HA2    | 1.98                     | 0.46              |
| 7:sJ:59:GLU:O      | 7:sJ:62:THR:HG22   | 2.16                     | 0.46              |
| 10:sA:146:ALA:CB   | 10:sA:157:VAL:HG21 | 2.46                     | 0.46              |
| 11:sB:129:THR:HG22 | 11:sB:133:TYR:O    | 2.15                     | 0.46              |
| 12:sH:122:LEU:HD12 | 12:sH:123:THR:N    | 2.31                     | 0.46              |
| 12:sH:140:VAL:N    | 12:sH:157:HIS:O    | 2.42                     | 0.46              |
| 13:sV:56:CYS:SG    | 13:sV:59:ILE:HG22  | 2.56                     | 0.46              |
| 20:l7:2:U:H2'      | 20:l7:3:C:C6       | 2.50                     | 0.46              |
| 20:l7:2:U:O4       | 20:l7:117:G:O6     | 2.33                     | 0.46              |
| 20:l7:59:G:H2'     | 20:l7:60:G:C8      | 2.51                     | 0.46              |
| 21:l8:55:U:N3      | 21:l8:56:G:N7      | 2.63                     | 0.46              |
| 21:l8:77:A:H2'     | 21:l8:78:G:C8      | 2.50                     | 0.46              |
| 23:lB:77:THR:N     | 23:lB:333:LEU:O    | 2.35                     | 0.46              |
| 24:lC:318:PRO:C    | 24:lC:320:LYS:H    | 2.24                     | 0.46              |
| 24:lC:348:LYS:HA   | 24:lC:351:VAL:HG12 | 1.98                     | 0.46              |
| 30:lI:93:PRO:HB2   | 30:lI:125:THR:HB   | 1.98                     | 0.46              |
| 32:lL:155:MET:O    | 32:lL:155:MET:HG2  | 2.16                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 33:IM:29:ASP:O     | 33:IM:37:LEU:N     | 2.45                     | 0.46              |
| 34:IN:36:LEU:HD13  | 34:IN:37:HIS:N     | 2.31                     | 0.46              |
| 34:IN:172:ARG:HH21 | 85:I5:29:G:P       | 2.39                     | 0.46              |
| 35:IO:3:GLU:HB3    | 35:IO:5:GLN:OE1    | 2.16                     | 0.46              |
| 35:IO:14:HIS:NE2   | 35:IO:120:VAL:O    | 2.47                     | 0.46              |
| 36:IP:86:LYS:HB2   | 85:I5:3857:G:H5''  | 1.98                     | 0.46              |
| 39:IS:83:ARG:HE    | 40:IT:156:TYR:HB2  | 1.81                     | 0.46              |
| 39:IS:143:LYS:HE2  | 39:IS:143:LYS:HB3  | 1.84                     | 0.46              |
| 41:IU:39:PHE:O     | 41:IU:43:LEU:HD12  | 2.16                     | 0.46              |
| 44:IY:24:HIS:NE2   | 44:IY:25:ILE:HG12  | 2.31                     | 0.46              |
| 51:If:65:ASN:ND2   | 51:If:67:THR:HB    | 2.30                     | 0.46              |
| 60:lo:32:SER:OG    | 60:lo:35:ALA:N     | 2.48                     | 0.46              |
| 60:lo:34:TYR:OH    | 85:I5:3729:U:H5''  | 2.16                     | 0.46              |
| 65:sD:217:ILE:HG23 | 65:sD:218:LEU:H    | 1.79                     | 0.46              |
| 71:sT:33:TRP:CZ2   | 71:sT:102:ARG:HG3  | 2.51                     | 0.46              |
| 72:sU:51:LYS:HB3   | 72:sU:90:ASP:O     | 2.16                     | 0.46              |
| 72:sU:66:ARG:NH2   | 72:sU:75:LYS:HA    | 2.30                     | 0.46              |
| 75:sg:251:ALA:HA   | 75:sg:256:ILE:HG13 | 1.98                     | 0.46              |
| 76:sM:95:ASP:O     | 76:sM:97:GLU:N     | 2.49                     | 0.46              |
| 79:s2:12:U:O2'     | 79:s2:1357:A:N3    | 2.49                     | 0.46              |
| 79:s2:26:U:H2'     | 79:s2:27:A:C8      | 2.51                     | 0.46              |
| 79:s2:946:U:C2     | 79:s2:947:G:C8     | 3.04                     | 0.46              |
| 79:s2:982:G:H2'    | 79:s2:983:A:H8     | 1.81                     | 0.46              |
| 79:s2:1374:C:C4    | 79:s2:1375:G:C5    | 3.03                     | 0.46              |
| 79:s2:1472:C:H2'   | 79:s2:1473:G:C8    | 2.51                     | 0.46              |
| 82:pE:9:A:H5'      | 82:pE:11:C:OP2     | 2.16                     | 0.46              |
| 82:pE:12:U:H2'     | 82:pE:13:C:C6      | 2.51                     | 0.46              |
| 85:I5:132:G:H2'    | 85:I5:133:C:H4'    | 1.98                     | 0.46              |
| 85:I5:342:G:H2'    | 85:I5:343:C:H6     | 1.81                     | 0.46              |
| 85:I5:484:U:O4     | 85:I5:665:C:H2'    | 2.16                     | 0.46              |
| 85:I5:739:G:H22    | 85:I5:926:G:H1'    | 1.81                     | 0.46              |
| 85:I5:1253:G:H4'   | 85:I5:1254:A:N7    | 2.30                     | 0.46              |
| 85:I5:1324:A:O2'   | 85:I5:1326:A:OP1   | 2.33                     | 0.46              |
| 85:I5:1797:G:H2'   | 85:I5:1798:G:H8    | 1.81                     | 0.46              |
| 85:I5:2017:A:H2'   | 85:I5:2017:A:OP2   | 2.16                     | 0.46              |
| 85:I5:2465:C:H2'   | 85:I5:2466:G:C8    | 2.51                     | 0.46              |
| 85:I5:3665:G:H2'   | 85:I5:3666:C:C6    | 2.50                     | 0.46              |
| 85:I5:3736:A:O2'   | 85:I5:3933:G:H5'   | 2.16                     | 0.46              |
| 85:I5:4093:G:H8    | 85:I5:4094:G:N7    | 2.14                     | 0.46              |
| 85:I5:4602:A:H3'   | 85:I5:4603:C:H6    | 1.81                     | 0.46              |
| 85:I5:5024:C:C5    | 85:I5:5025:C:H1'   | 2.51                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 80:CB:5:THR:O      | 80:CB:8:GLN:NE2    | 2.48                     | 0.46              |
| 80:CB:129:VAL:HG12 | 80:CB:139:THR:HG21 | 1.98                     | 0.46              |
| 80:CB:170:GLU:O    | 80:CB:174:LEU:HD12 | 2.16                     | 0.46              |
| 80:CB:402:VAL:O    | 80:CB:411:TYR:N    | 2.39                     | 0.46              |
| 80:CB:767:ARG:HH12 | 80:CB:791:ASN:HD21 | 1.64                     | 0.46              |
| 2:SE:137:PRO:HD2   | 2:SE:149:TYR:HD2   | 1.81                     | 0.46              |
| 2:SE:259:LYS:O     | 2:SE:259:LYS:NZ    | 2.42                     | 0.46              |
| 3:SI:124:LYS:HE2   | 3:SI:124:LYS:HB2   | 1.62                     | 0.46              |
| 4:SL:98:LYS:HE3    | 4:SL:99:TYR:CE1    | 2.51                     | 0.46              |
| 5:SX:115:ILE:HG21  | 5:SX:118:VAL:HB    | 1.98                     | 0.46              |
| 8:SY:100:LYS:O     | 8:SY:101:LYS:HD3   | 2.15                     | 0.46              |
| 10:SA:66:VAL:HA    | 10:SA:186:ARG:HH22 | 1.79                     | 0.46              |
| 12:SH:61:ILE:HD11  | 12:SH:95:ILE:HG12  | 1.98                     | 0.46              |
| 12:SH:162:GLN:HB3  | 12:SH:166:VAL:HG22 | 1.98                     | 0.46              |
| 18:SW:28:ARG:O     | 18:SW:60:LYS:HG2   | 2.16                     | 0.46              |
| 85:L5:132:G:C3'    | 85:L5:133:C:H4'    | 2.46                     | 0.46              |
| 85:L5:301:G:H2'    | 85:L5:302:C:C6     | 2.50                     | 0.46              |
| 85:L5:1202:C:H3'   | 85:L5:1203:G:C5'   | 2.45                     | 0.46              |
| 85:L5:1388:A:H2'   | 85:L5:1389:U:C6    | 2.51                     | 0.46              |
| 85:L5:1415:G:H2'   | 85:L5:1416:G:H8    | 1.81                     | 0.46              |
| 85:L5:1821:G:H2'   | 85:L5:1821:G:N3    | 2.31                     | 0.46              |
| 85:L5:2379:A:H2'   | 85:L5:2380:G:O4'   | 2.16                     | 0.46              |
| 85:L5:2754:G:OP2   | 45:LZ:133:LYS:NZ   | 2.42                     | 0.46              |
| 85:L5:2835:A:H2'   | 85:L5:2836:A:H8    | 1.81                     | 0.46              |
| 85:L5:4039:G:N2    | 85:L5:4050:A:HO2'  | 2.14                     | 0.46              |
| 85:L5:4110:C:C2    | 85:L5:4113:U:C2    | 3.04                     | 0.46              |
| 85:L5:4508:C:N3    | 85:L5:4512:U:H5    | 2.14                     | 0.46              |
| 85:L5:4918:C:H2'   | 85:L5:4919:G:C8    | 2.50                     | 0.46              |
| 21:L8:38:U:O3'     | 53:Lh:86:LYS:NZ    | 2.41                     | 0.46              |
| 21:L8:65:A:C4      | 21:L8:66:A:C8      | 3.04                     | 0.46              |
| 21:L8:138:C:C2     | 21:L8:139:G:C8     | 3.03                     | 0.46              |
| 24:LC:29:LYS:O     | 24:LC:282:HIS:NE2  | 2.44                     | 0.46              |
| 27:LF:166:ARG:HD2  | 27:LF:209:TRP:NE1  | 2.31                     | 0.46              |
| 27:LF:203:GLU:OE1  | 27:LF:203:GLU:N    | 2.37                     | 0.46              |
| 28:LG:77:PRO:HG2   | 34:LN:18:VAL:HA    | 1.98                     | 0.46              |
| 30:LI:38:ARG:HG3   | 30:LI:83:ASP:OD1   | 2.15                     | 0.46              |
| 33:LM:47:ARG:CD    | 39:LS:73:LEU:HD11  | 2.44                     | 0.46              |
| 39:LS:4:SER:HB3    | 39:LS:111:ARG:HH12 | 1.81                     | 0.46              |
| 40:LT:11:THR:O     | 40:LT:11:THR:OG1   | 2.32                     | 0.46              |
| 61:Lp:47:MET:HE2   | 61:Lp:57:CYS:HB2   | 1.98                     | 0.46              |
| 61:Lp:52:VAL:O     | 61:Lp:54:ILE:HD12  | 2.16                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 62:Lr:17:LEU:HD12  | 62:Lr:17:LEU:HA    | 1.78                     | 0.46              |
| 65:SD:53:THR:O     | 65:SD:90:LYS:HD3   | 2.15                     | 0.46              |
| 65:SD:113:LEU:HD23 | 65:SD:114:ALA:N    | 2.31                     | 0.46              |
| 68:SP:40:ARG:NH1   | 79:S2:1617:G:O6    | 2.48                     | 0.46              |
| 71:ST:132:ASP:OD1  | 71:ST:133:ARG:N    | 2.47                     | 0.46              |
| 75:Sg:128:THR:HG23 | 75:Sg:130:LYS:NZ   | 2.18                     | 0.46              |
| 78:Sf:93:HIS:CD2   | 79:S2:1305:C:OP1   | 2.68                     | 0.46              |
| 79:S2:637:U:H2'    | 79:S2:638:C:C6     | 2.50                     | 0.46              |
| 82:PE:2:C:H2'      | 82:PE:3:C:C6       | 2.51                     | 0.46              |
| 82:PE:37:A:H3'     | 82:PE:38:A:H8      | 1.80                     | 0.46              |
| 6:sG:134:GLY:N     | 79:s2:65:C:H42     | 2.14                     | 0.46              |
| 10:sA:9:GLN:O      | 10:sA:55:TRP:HH2   | 1.98                     | 0.46              |
| 10:sA:181:GLU:OE1  | 10:sA:181:GLU:C    | 2.59                     | 0.46              |
| 18:sW:101:PHE:CD1  | 18:sW:112:ASP:CG   | 2.91                     | 0.46              |
| 22:lA:40:TYR:HE2   | 22:lA:89:TYR:CE1   | 2.34                     | 0.46              |
| 23:lB:76:VAL:HG23  | 23:lB:333:LEU:C    | 2.41                     | 0.46              |
| 24:lC:285:ILE:HG21 | 37:lQ:125:GLN:HE22 | 1.80                     | 0.46              |
| 27:lF:67:THR:HB    | 27:lF:71:MET:SD    | 2.56                     | 0.46              |
| 28:lG:170:LEU:HD23 | 28:lG:170:LEU:HA   | 1.72                     | 0.46              |
| 31:lJ:163:MET:HB3  | 31:lJ:174:ILE:HG21 | 1.96                     | 0.46              |
| 32:IL:55:ILE:HG22  | 32:IL:95:GLY:O     | 2.16                     | 0.46              |
| 32:IL:59:VAL:HG21  | 32:IL:73:GLY:CA    | 2.46                     | 0.46              |
| 32:IL:171:GLU:OE1  | 32:IL:174:LYS:HD2  | 2.16                     | 0.46              |
| 35:lO:18:ARG:HH12  | 85:l5:2054:U:P     | 2.39                     | 0.46              |
| 35:lO:130:LYS:HG2  | 85:l5:2055:G:C4    | 2.51                     | 0.46              |
| 43:lX:54:LEU:HD12  | 43:lX:55:ARG:H     | 1.81                     | 0.46              |
| 52:lg:59:VAL:HB    | 52:lg:63:VAL:HG11  | 1.97                     | 0.46              |
| 53:lh:27:GLU:OE2   | 53:lh:28:LEU:N     | 2.49                     | 0.46              |
| 57:ll:46:ARG:NH1   | 57:ll:46:ARG:HB2   | 2.30                     | 0.46              |
| 63:lz:59:PRO:CB    | 63:lz:170:GLY:HA3  | 2.46                     | 0.46              |
| 63:lz:148:VAL:HG23 | 63:lz:149:ASP:N    | 2.30                     | 0.46              |
| 64:sR:6:THR:HG23   | 79:s2:1368:U:O2    | 2.16                     | 0.46              |
| 64:sR:7:LYS:HD3    | 79:s2:1367:U:H3    | 1.79                     | 0.46              |
| 64:sR:28:PHE:HD2   | 79:s2:1455:A:N7    | 2.14                     | 0.46              |
| 67:sK:19:GLY:O     | 67:sK:71:LEU:HD23  | 2.16                     | 0.46              |
| 68:sP:82:ASP:OD1   | 68:sP:82:ASP:C     | 2.58                     | 0.46              |
| 72:sU:63:ILE:HG21  | 74:sd:43:PHE:CZ    | 2.51                     | 0.46              |
| 75:sg:42:MET:CE    | 75:sg:57:ARG:HG3   | 2.46                     | 0.46              |
| 79:s2:118:C:H1'    | 79:s2:445:A:C8     | 2.51                     | 0.46              |
| 79:s2:443:U:H2'    | 79:s2:444:G:O4'    | 2.16                     | 0.46              |
| 79:s2:640:A:C6     | 79:s2:641:A:N6     | 2.83                     | 0.46              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 79:s2:929:G:O6    | 79:s2:1012:A:N1    | 2.49                     | 0.46              |
| 79:s2:1466:G:C5   | 79:s2:1467:C:C5    | 3.04                     | 0.46              |
| 80:cB:174:LEU:CD1 | 80:cB:178:PHE:HE1  | 2.28                     | 0.46              |
| 82:pE:35:U:H2'    | 82:pE:36:U:H6      | 1.81                     | 0.46              |
| 85:l5:451:C:O2'   | 85:l5:1293:G:H2'   | 2.16                     | 0.46              |
| 85:l5:482:G:H2'   | 85:l5:485:C:C5     | 2.51                     | 0.46              |
| 85:l5:700:G:N1    | 85:l5:701:G:C6     | 2.84                     | 0.46              |
| 85:l5:1234:G:H2'  | 85:l5:1235:G:H8    | 1.81                     | 0.46              |
| 85:l5:1846:G:H2'  | 85:l5:1847:C:H6    | 1.79                     | 0.46              |
| 85:l5:2634:C:C2   | 85:l5:2635:U:C5    | 3.04                     | 0.46              |
| 85:l5:2714:G:H2'  | 85:l5:2715:G:H8    | 1.80                     | 0.46              |
| 85:l5:2757:A:H2'  | 85:l5:2758:G:C8    | 2.51                     | 0.46              |
| 85:l5:3648:A:C4   | 85:l5:3785:A:C6    | 3.04                     | 0.46              |
| 80:CB:9:ILE:HA    | 80:CB:9:ILE:HD13   | 1.87                     | 0.46              |
| 2:SE:85:GLY:O     | 2:SE:101:LEU:HD22  | 2.16                     | 0.46              |
| 5:SX:10:ALA:HA    | 5:SX:13:LEU:HD21   | 1.98                     | 0.46              |
| 6:SG:234:LEU:HD12 | 6:SG:234:LEU:HA    | 1.80                     | 0.46              |
| 7:SJ:91:LYS:HE3   | 7:SJ:96:TYR:CD1    | 2.51                     | 0.46              |
| 7:SJ:129:LEU:HG   | 7:SJ:135:ILE:HD11  | 1.97                     | 0.46              |
| 10:SA:121:LEU:CD2 | 10:SA:143:PRO:HG2  | 2.46                     | 0.46              |
| 12:SH:159:ASP:O   | 12:SH:160:LYS:HG2  | 2.15                     | 0.46              |
| 12:SH:169:LYS:HE2 | 12:SH:173:PHE:HZ   | 1.81                     | 0.46              |
| 85:L5:4:G:N1      | 21:L8:154:G:C6     | 2.84                     | 0.46              |
| 85:L5:346:G:OP2   | 44:LY:13:LYS:NZ    | 2.25                     | 0.46              |
| 85:L5:989:U:O2    | 85:L5:1064:G:C6    | 2.68                     | 0.46              |
| 85:L5:1354:A:N1   | 85:L5:1385:G:O2'   | 2.39                     | 0.46              |
| 85:L5:1755:C:H42  | 85:L5:1775:A:H61   | 1.63                     | 0.46              |
| 85:L5:1874:A:H2'  | 85:L5:1875:C:C6    | 2.51                     | 0.46              |
| 85:L5:1995:G:C5   | 85:L5:1996:C:C4    | 3.04                     | 0.46              |
| 85:L5:2281:U:C2   | 85:L5:2282:A:C8    | 3.04                     | 0.46              |
| 85:L5:2583:C:N4   | 52:Lg:75:SER:OG    | 2.48                     | 0.46              |
| 85:L5:4208:U:H2'  | 85:L5:4209:G:H8    | 1.81                     | 0.46              |
| 85:L5:4237:C:O3'  | 85:L5:4326:G:N2    | 2.49                     | 0.46              |
| 85:L5:4603:C:H2'  | 85:L5:4604:G:C8    | 2.51                     | 0.46              |
| 85:L5:4993:G:H22  | 85:L5:5058:A:H2    | 1.63                     | 0.46              |
| 85:L5:5040:U:OP2  | 23:LB:396:ARG:NH2  | 2.46                     | 0.46              |
| 20:L7:115:A:H2'   | 20:L7:116:G:H8     | 1.81                     | 0.46              |
| 21:L8:144:U:H2'   | 21:L8:145:C:C6     | 2.51                     | 0.46              |
| 23:LB:307:TYR:CE1 | 23:LB:366:LYS:HD2  | 2.51                     | 0.46              |
| 25:LD:119:TYR:HE1 | 25:LD:134:SER:HA   | 1.80                     | 0.46              |
| 29:LH:92:MET:HG2  | 29:LH:179:ILE:HD11 | 1.98                     | 0.46              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 33:LM:71:LYS:O    | 33:LM:75:GLN:HG2   | 2.15                     | 0.46              |
| 34:LN:119:TYR:CE2 | 34:LN:133:ILE:HD11 | 2.46                     | 0.46              |
| 37:LQ:159:PRO:HA  | 37:LQ:160:HIS:HA   | 1.54                     | 0.46              |
| 50:Le:90:MET:SD   | 62:Lr:113:ARG:HG3  | 2.55                     | 0.46              |
| 51:Lf:8:LYS:HB2   | 51:Lf:100:ARG:CZ   | 2.46                     | 0.46              |
| 56:Lk:51:GLU:OE1  | 56:Lk:51:GLU:N     | 2.45                     | 0.46              |
| 63:Lz:59:PRO:HG2  | 63:Lz:62:LYS:HZ2   | 1.81                     | 0.46              |
| 64:SR:24:LEU:HD12 | 64:SR:34:VAL:HG21  | 1.98                     | 0.46              |
| 66:SF:124:ASP:OD1 | 73:Sc:47:LYS:NZ    | 2.32                     | 0.46              |
| 68:SP:101:THR:OG1 | 68:SP:102:PHE:N    | 2.49                     | 0.46              |
| 75:Sg:106:LYS:HB3 | 75:Sg:125:ARG:HB3  | 1.97                     | 0.46              |
| 79:S2:191:A:H3'   | 79:S2:192:C:C6     | 2.51                     | 0.46              |
| 79:S2:442:C:H2'   | 79:S2:443:U:C6     | 2.50                     | 0.46              |
| 79:S2:1236:G:H2'  | 79:S2:1237:C:H6    | 1.81                     | 0.46              |
| 79:S2:1355:C:C4   | 79:S2:1356:G:C5    | 3.04                     | 0.46              |
| 79:S2:1828:C:H2'  | 79:S2:1829:G:C8    | 2.51                     | 0.46              |
| 81:AP:42:A:H2'    | 81:AP:43:A:H8      | 1.81                     | 0.46              |
| 82:PE:16:C:H5''   | 82:PE:18:U:H5''    | 1.97                     | 0.46              |
| 2:sE:160:ILE:HD12 | 2:sE:160:ILE:O     | 2.16                     | 0.46              |
| 2:sE:178:GLY:O    | 2:sE:231:GLY:HA2   | 2.16                     | 0.46              |
| 2:sE:191:ARG:NH1  | 2:sE:245:ARG:HD2   | 2.30                     | 0.46              |
| 4:sL:94:HIS:O     | 4:sL:103:GLU:N     | 2.49                     | 0.46              |
| 6:sG:23:LYS:HE3   | 6:sG:23:LYS:HB3    | 1.68                     | 0.46              |
| 6:sG:41:LEU:HG    | 6:sG:45:TRP:CD2    | 2.51                     | 0.46              |
| 6:sG:191:ARG:O    | 6:sG:195:LYS:HG2   | 2.16                     | 0.46              |
| 7:sJ:104:ASP:HA   | 7:sJ:107:GLU:HG3   | 1.98                     | 0.46              |
| 11:sB:46:LYS:HB2  | 11:sB:46:LYS:HE3   | 1.61                     | 0.46              |
| 12:sH:130:LEU:O   | 12:sH:134:VAL:HG22 | 2.16                     | 0.46              |
| 15:sC:267:GLN:HA  | 15:sC:270:THR:HB   | 1.98                     | 0.46              |
| 16:sN:55:ARG:NE   | 79:s2:1017:U:H5'   | 2.31                     | 0.46              |
| 20:l7:78:C:O2'    | 85:l5:1736:A:N3    | 2.48                     | 0.46              |
| 22:lA:58:LEU:HA   | 22:lA:58:LEU:HD12  | 1.72                     | 0.46              |
| 22:lA:245:ARG:NE  | 22:lA:245:ARG:HA   | 2.31                     | 0.46              |
| 25:lD:30:TYR:HA   | 25:lD:33:ARG:HB3   | 1.98                     | 0.46              |
| 25:lD:35:ARG:NH1  | 85:l5:4326:G:O2'   | 2.49                     | 0.46              |
| 25:lD:180:PHE:HB2 | 25:lD:190:PHE:HE1  | 1.81                     | 0.46              |
| 25:lD:193:GLU:O   | 25:lD:196:ARG:HG3  | 2.15                     | 0.46              |
| 26:lE:265:PRO:O   | 26:lE:266:GLN:HG2  | 2.15                     | 0.46              |
| 26:lE:278:THR:HB  | 85:l5:4754:G:N7    | 2.31                     | 0.46              |
| 30:lI:15:LYS:HE3  | 85:l5:1863:U:OP1   | 2.16                     | 0.46              |
| 31:lJ:77:ALA:HA   | 31:lJ:80:GLU:OE1   | 2.16                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 32:IL:58:ILE:HD13  | 32:IL:157:VAL:HG12 | 1.98                     | 0.46              |
| 32:IL:129:ARG:NH1  | 85:l5:173:C:H5''   | 2.29                     | 0.46              |
| 45:lZ:3:LYS:HB3    | 45:lZ:6:LYS:NZ     | 2.31                     | 0.46              |
| 48:lc:47:ILE:HD13  | 48:lc:72:HIS:HB3   | 1.96                     | 0.46              |
| 60:lo:61:LYS:HE3   | 60:lo:61:LYS:CA    | 2.32                     | 0.46              |
| 79:s2:96:C:H2'     | 79:s2:97:U:H6      | 1.81                     | 0.46              |
| 79:s2:210:U:C2     | 79:s2:211:G:C8     | 3.03                     | 0.46              |
| 79:s2:467:G:H2'    | 79:s2:468:A:H8     | 1.81                     | 0.46              |
| 79:s2:516:A:N1     | 79:s2:643:A:O2'    | 2.32                     | 0.46              |
| 79:s2:604:A:O2'    | 79:s2:605:A:O4'    | 2.20                     | 0.46              |
| 79:s2:1189:A:H2'   | 79:s2:1190:A:H8    | 1.81                     | 0.46              |
| 79:s2:1538:C:H2'   | 79:s2:1539:U:C6    | 2.51                     | 0.46              |
| 80:cB:265:TYR:HA   | 80:cB:287:ARG:HA   | 1.98                     | 0.46              |
| 80:cB:316:ILE:O    | 80:cB:320:ASP:N    | 2.48                     | 0.46              |
| 80:cB:581:GLU:HB2  | 80:cB:697:MET:HG3  | 1.97                     | 0.46              |
| 80:cB:734:LEU:HA   | 80:cB:738:PRO:HG3  | 1.98                     | 0.46              |
| 83:ls:82:ILE:HG22  | 83:ls:86:VAL:HG21  | 1.98                     | 0.46              |
| 85:l5:664:G:H2'    | 85:l5:665:C:H6     | 1.81                     | 0.46              |
| 85:l5:976:G:H2'    | 85:l5:977:C:O4'    | 2.16                     | 0.46              |
| 85:l5:1563:A:H8    | 85:l5:1563:A:OP1   | 1.99                     | 0.46              |
| 85:l5:1858:A:H2'   | 85:l5:1859:C:H6    | 1.81                     | 0.46              |
| 85:l5:2029:A:H2'   | 85:l5:2030:A:C8    | 2.50                     | 0.46              |
| 85:l5:2273:G:H2'   | 85:l5:2274:C:H6    | 1.81                     | 0.46              |
| 85:l5:2514:G:C2    | 85:l5:2515:G:C8    | 3.04                     | 0.46              |
| 85:l5:2669:C:H2'   | 85:l5:2670:C:O4'   | 2.16                     | 0.46              |
| 85:l5:2780:C:H2'   | 85:l5:2781:G:H8    | 1.80                     | 0.46              |
| 85:l5:2893:U:H2'   | 85:l5:2894:A:H8    | 1.81                     | 0.46              |
| 85:l5:3882:C:C2    | 85:l5:3883:U:C5    | 3.04                     | 0.46              |
| 85:l5:3891:A:H2'   | 85:l5:3892:U:O4'   | 2.16                     | 0.46              |
| 85:l5:4041:C:P     | 85:l5:4042:G:H3'   | 2.55                     | 0.46              |
| 85:l5:4578:G:H2'   | 85:l5:4579:U:C6    | 2.51                     | 0.46              |
| 85:l5:4988:U:O2'   | 85:l5:4989:U:OP2   | 2.31                     | 0.46              |
| 80:CB:475:VAL:HG12 | 80:CB:479:LEU:HD23 | 1.97                     | 0.46              |
| 80:CB:502:SER:O    | 80:CB:504:VAL:HG23 | 2.15                     | 0.46              |
| 5:SX:108:LYS:HD2   | 5:SX:108:LYS:HA    | 1.83                     | 0.46              |
| 7:SJ:6:SER:OG      | 7:SJ:8:VAL:HG22    | 2.15                     | 0.46              |
| 7:SJ:41:ARG:HH12   | 79:S2:644:G:H5''   | 1.81                     | 0.46              |
| 10:SA:110:ASN:ND2  | 10:SA:113:GLN:HE22 | 2.14                     | 0.46              |
| 11:SB:107:ARG:HH12 | 17:SO:133:THR:C    | 2.23                     | 0.46              |
| 11:SB:157:GLN:NE2  | 11:SB:159:GLN:H    | 2.14                     | 0.46              |
| 85:L5:347:A:H2'    | 85:L5:348:G:C8     | 2.51                     | 0.46              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 85:L5:439:G:H2'   | 85:L5:440:U:C6     | 2.50                     | 0.46              |
| 85:L5:461:G:H2'   | 85:L5:462:G:H8     | 1.81                     | 0.46              |
| 85:L5:1384:C:H2'  | 85:L5:1385:G:H8    | 1.81                     | 0.46              |
| 85:L5:1458:C:C2   | 85:L5:1459:A:C8    | 3.04                     | 0.46              |
| 85:L5:1634:A:H62  | 22:LA:3:ARG:HH12   | 1.64                     | 0.46              |
| 85:L5:2259:G:H5'  | 85:L5:2260:C:C5    | 2.51                     | 0.46              |
| 85:L5:2689:C:H2'  | 85:L5:2690:C:C6    | 2.51                     | 0.46              |
| 85:L5:2704:C:H2'  | 85:L5:2705:G:C8    | 2.51                     | 0.46              |
| 85:L5:3642:A:C8   | 55:Lj:3:LYS:HD3    | 2.50                     | 0.46              |
| 85:L5:4108:G:HO2' | 85:L5:4109:G:P     | 2.38                     | 0.46              |
| 85:L5:4244:A:H2'  | 85:L5:4245:G:O4'   | 2.15                     | 0.46              |
| 85:L5:4716:C:H5'' | 23:LB:276:HIS:O    | 2.16                     | 0.46              |
| 85:L5:4761:G:C2   | 85:L5:4762:A:C5    | 3.03                     | 0.46              |
| 85:L5:4889:G:H2'  | 85:L5:4890:G:H8    | 1.81                     | 0.46              |
| 20:L7:11:A:O2'    | 20:L7:12:U:H3'     | 2.16                     | 0.46              |
| 21:L8:20:A:H2'    | 21:L8:21:C:H6      | 1.80                     | 0.46              |
| 21:L8:115:G:H2'   | 21:L8:116:C:H6     | 1.81                     | 0.46              |
| 21:L8:142:U:H2'   | 21:L8:143:G:C8     | 2.51                     | 0.46              |
| 24:LC:242:PRO:HG3 | 24:LC:248:ARG:HD2  | 1.97                     | 0.46              |
| 25:LD:52:ILE:HD13 | 25:LD:63:GLN:HG3   | 1.97                     | 0.46              |
| 25:LD:89:LYS:HE2  | 25:LD:229:ASN:CB   | 2.42                     | 0.46              |
| 26:LE:254:ASP:HA  | 26:LE:257:ILE:HG22 | 1.98                     | 0.46              |
| 29:LH:150:ASP:HB3 | 29:LH:153:LEU:HD23 | 1.98                     | 0.46              |
| 34:LN:96:ARG:HH22 | 34:LN:104:GLU:HG2  | 1.81                     | 0.46              |
| 45:LZ:41:ALA:HB2  | 45:LZ:77:TYR:CE1   | 2.45                     | 0.46              |
| 59:Ln:1:MET:HB3   | 79:S2:1852:C:OP2   | 2.15                     | 0.46              |
| 60:Lo:25:GLN:HE22 | 60:Lo:66:ILE:HG23  | 1.80                     | 0.46              |
| 67:SK:16:PHE:CD1  | 67:SK:79:LEU:HD21  | 2.51                     | 0.46              |
| 67:SK:53:LYS:HG2  | 67:SK:58:VAL:O     | 2.16                     | 0.46              |
| 70:SS:100:ALA:O   | 70:SS:103:LEU:HD23 | 2.16                     | 0.46              |
| 75:Sg:8:ARG:NH2   | 75:Sg:47:ARG:HB3   | 2.31                     | 0.46              |
| 75:Sg:123:GLY:HA2 | 75:Sg:129:ILE:HD13 | 1.98                     | 0.46              |
| 75:Sg:143:GLN:C   | 75:Sg:145:GLU:H    | 2.24                     | 0.46              |
| 79:S2:26:U:H2'    | 79:S2:27:A:H8      | 1.81                     | 0.46              |
| 79:S2:536:A:C5    | 79:S2:537:C:H1'    | 2.50                     | 0.46              |
| 79:S2:734:C:N4    | 79:S2:737:G:H22    | 2.13                     | 0.46              |
| 79:S2:1170:A:H61  | 79:S2:1188:A:H3'   | 1.81                     | 0.46              |
| 79:S2:1264:C:H4'  | 79:S2:1265:A:O4'   | 2.16                     | 0.46              |
| 79:S2:1744:G:H1'  | 79:S2:1790:A:N6    | 2.30                     | 0.46              |
| 79:S2:1860:A:O2'  | 79:S2:1862:G:H8    | 1.98                     | 0.46              |
| 82:PE:10:G:H1     | 82:PE:26:A:H1'     | 1.81                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 87:IW:13:ILE:HD11  | 87:IW:32:LEU:HB2   | 1.98                     | 0.46              |
| 1:cH:78:GLY:HA2    | 1:cH:81:ILE:HD12   | 1.98                     | 0.45              |
| 2:sE:17:HIS:CE1    | 2:sE:18:TRP:CE3    | 3.05                     | 0.45              |
| 2:sE:37:LYS:HB2    | 2:sE:40:GLU:CG     | 2.45                     | 0.45              |
| 3:sI:184:ARG:NH2   | 79:s2:305:U:O4     | 2.50                     | 0.45              |
| 4:sL:31:GLU:H      | 4:sL:31:GLU:CD     | 2.23                     | 0.45              |
| 6:sG:137:ARG:HB2   | 79:s2:170:A:H5'    | 1.96                     | 0.45              |
| 9:se:57:ALA:O      | 9:se:58:ASN:ND2    | 2.47                     | 0.45              |
| 10:sA:207:PRO:HD2  | 10:sA:208:GLU:N    | 2.28                     | 0.45              |
| 11:sB:172:MET:HE1  | 11:sB:173:THR:HG23 | 1.98                     | 0.45              |
| 15:sC:183:LYS:HE3  | 18:sW:95:PRO:HA    | 1.97                     | 0.45              |
| 22:lA:30:ARG:HA    | 22:lA:123:ARG:HH21 | 1.79                     | 0.45              |
| 23:lB:217:ILE:HG23 | 23:lB:284:ILE:HD11 | 1.97                     | 0.45              |
| 25:ID:45:ASN:ND2   | 85:l5:1823:G:O3'   | 2.44                     | 0.45              |
| 26:lE:270:TYR:CD1  | 33:lM:110:PHE:CD1  | 3.04                     | 0.45              |
| 27:lF:155:TYR:OH   | 27:lF:188:GLU:OE1  | 2.30                     | 0.45              |
| 29:lH:188:GLN:O    | 29:lH:188:GLN:HG2  | 2.16                     | 0.45              |
| 30:II:42:LYS:N     | 30:II:45:GLU:OE2   | 2.34                     | 0.45              |
| 30:II:183:ASP:O    | 30:II:186:ALA:N    | 2.50                     | 0.45              |
| 34:lN:120:TRP:HE1  | 34:lN:122:GLY:CA   | 2.28                     | 0.45              |
| 35:lO:78:ARG:HD2   | 35:lO:78:ARG:HA    | 1.67                     | 0.45              |
| 37:lQ:77:ASN:O     | 37:lQ:77:ASN:ND2   | 2.48                     | 0.45              |
| 38:lR:148:ASP:OD1  | 38:lR:151:ARG:NH2  | 2.50                     | 0.45              |
| 49:ld:40:LYS:HB2   | 49:ld:40:LYS:HE2   | 1.78                     | 0.45              |
| 49:ld:118:GLN:NE2  | 85:l5:5055:G:H21   | 2.13                     | 0.45              |
| 50:le:29:VAL:HG23  | 85:l5:1332:C:H5''  | 1.98                     | 0.45              |
| 51:lf:74:VAL:HG13  | 51:lf:84:VAL:CG1   | 2.41                     | 0.45              |
| 54:li:33:LEU:HD11  | 54:li:38:LYS:HB3   | 1.99                     | 0.45              |
| 60:lo:104:ILE:HD13 | 60:lo:104:ILE:HA   | 1.84                     | 0.45              |
| 62:lr:6:GLN:O      | 62:lr:10:VAL:HG22  | 2.17                     | 0.45              |
| 62:lr:56:ASP:OD2   | 62:lr:58:LYS:N     | 2.40                     | 0.45              |
| 63:lz:17:VAL:HG11  | 63:lz:179:LEU:HD22 | 1.98                     | 0.45              |
| 64:sR:11:LYS:HB3   | 64:sR:11:LYS:HE3   | 1.47                     | 0.45              |
| 64:sR:29:HIS:HB2   | 79:s2:1455:A:C8    | 2.51                     | 0.45              |
| 65:sD:21:LEU:O     | 65:sD:25:LEU:HG    | 2.16                     | 0.45              |
| 71:sT:134:ILE:HA   | 71:sT:137:GLN:OE1  | 2.16                     | 0.45              |
| 73:sc:28:THR:O     | 73:sc:45:ASN:HA    | 2.15                     | 0.45              |
| 73:sc:51:ARG:NH2   | 73:sc:54:ASP:OD1   | 2.49                     | 0.45              |
| 74:sd:14:PHE:CZ    | 79:s2:1617:G:H4'   | 2.50                     | 0.45              |
| 74:sd:33:LYS:HG2   | 74:sd:34:TYR:CD2   | 2.51                     | 0.45              |
| 75:sg:42:MET:HE3   | 75:sg:92:LEU:CD1   | 2.46                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 76:sM:19:GLN:HB2   | 76:sM:88:TRP:CH2   | 2.51                     | 0.45              |
| 79:s2:185:G:N1     | 79:s2:214:U:N3     | 2.63                     | 0.45              |
| 79:s2:360:A:H2     | 79:s2:363:A:H5'    | 1.81                     | 0.45              |
| 79:s2:448:A:H4'    | 79:s2:449:A:H5''   | 1.97                     | 0.45              |
| 79:s2:845:G:C6     | 79:s2:846:G:C2     | 3.04                     | 0.45              |
| 79:s2:1243:U:H2'   | 79:s2:1244:U:O4'   | 2.16                     | 0.45              |
| 79:s2:1430:C:H2'   | 79:s2:1431:G:H8    | 1.82                     | 0.45              |
| 79:s2:1466:G:H2'   | 79:s2:1467:C:H6    | 1.80                     | 0.45              |
| 80:cB:333:LYS:HG2  | 80:cB:334:PRO:HD3  | 1.97                     | 0.45              |
| 82:pE:24:G:H2'     | 82:pE:25:C:C6      | 2.51                     | 0.45              |
| 84:lt:67:ARG:HD2   | 84:lt:67:ARG:HA    | 1.75                     | 0.45              |
| 85:l5:11:G:H2'     | 85:l5:12:A:C8      | 2.52                     | 0.45              |
| 85:l5:302:C:H2'    | 85:l5:303:C:C6     | 2.51                     | 0.45              |
| 85:l5:358:C:H2'    | 85:l5:359:A:C8     | 2.50                     | 0.45              |
| 85:l5:1097:C:H2'   | 85:l5:1098:G:C8    | 2.50                     | 0.45              |
| 85:l5:1741:G:O2'   | 85:l5:1781:U:OP2   | 2.31                     | 0.45              |
| 85:l5:2648:G:H2'   | 85:l5:2649:G:H8    | 1.81                     | 0.45              |
| 85:l5:3723:A:H2'   | 85:l5:3724:A:H8    | 1.81                     | 0.45              |
| 85:l5:3787:G:H1'   | 85:l5:3789:C:N4    | 2.31                     | 0.45              |
| 85:l5:3965:A:O2'   | 85:l5:4038:C:N3    | 2.49                     | 0.45              |
| 85:l5:4396:A:C2    | 85:l5:4397:A:C4    | 3.04                     | 0.45              |
| 85:l5:4444:C:H2'   | 85:l5:4445:U:C6    | 2.49                     | 0.45              |
| 85:l5:4991:U:H2'   | 85:l5:4992:G:C8    | 2.51                     | 0.45              |
| 85:l5:5027:C:O2'   | 85:l5:5028:G:H5''  | 2.16                     | 0.45              |
| 85:l5:5043:A:H2'   | 85:l5:5044:A:C8    | 2.51                     | 0.45              |
| 80:CB:22:MET:SD    | 80:CB:102:LEU:HA   | 2.56                     | 0.45              |
| 80:CB:649:ILE:HA   | 80:CB:663:THR:HG22 | 1.97                     | 0.45              |
| 4:SL:77:VAL:HG12   | 4:SL:124:ASP:H     | 1.81                     | 0.45              |
| 5:SX:64:SER:HB3    | 79:S2:614:C:O2     | 2.16                     | 0.45              |
| 10:SA:50:ASN:ND2   | 10:SA:52:LYS:HE3   | 2.31                     | 0.45              |
| 11:SB:85:LYS:HE2   | 11:SB:103:MET:N    | 2.31                     | 0.45              |
| 12:SH:32:MET:O     | 12:SH:32:MET:HG3   | 2.16                     | 0.45              |
| 15:SC:191:VAL:HG11 | 15:SC:236:PHE:HA   | 1.98                     | 0.45              |
| 16:SN:16:LEU:HD11  | 16:SN:62:GLN:HG3   | 1.98                     | 0.45              |
| 18:SW:80:ASP:OD2   | 79:S2:804:U:H5'    | 2.16                     | 0.45              |
| 85:L5:86:U:H2'     | 85:L5:87:A:C8      | 2.52                     | 0.45              |
| 85:L5:180:C:H2'    | 85:L5:181:C:H4'    | 1.97                     | 0.45              |
| 85:L5:408:A:O2'    | 85:L5:411:G:OP2    | 2.21                     | 0.45              |
| 85:L5:716:C:H2'    | 85:L5:717:U:O4'    | 2.16                     | 0.45              |
| 85:L5:978:G:H2'    | 85:L5:979:C:H6     | 1.80                     | 0.45              |
| 85:L5:1307:A:H2'   | 85:L5:1308:C:C6    | 2.50                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 85:L5:1534:A:C1'   | 55:Lj:11:ARG:HH21  | 2.29                     | 0.45              |
| 85:L5:1597:G:P     | 36:LP:131:ARG:HH21 | 2.39                     | 0.45              |
| 85:L5:1687:U:H2'   | 85:L5:1688:G:H8    | 1.78                     | 0.45              |
| 85:L5:1786:A:C6    | 85:L5:1789:C:C2    | 3.04                     | 0.45              |
| 85:L5:1952:G:OP1   | 39:LS:139:ARG:NE   | 2.47                     | 0.45              |
| 85:L5:2055:G:P     | 35:LO:130:LYS:HZ3  | 2.39                     | 0.45              |
| 85:L5:4102:C:H2'   | 85:L5:4106:G:O4'   | 2.16                     | 0.45              |
| 85:L5:4311:A:H2'   | 85:L5:4312:U:H6    | 1.80                     | 0.45              |
| 21:L8:154:G:C6     | 21:L8:155:C:N4     | 2.84                     | 0.45              |
| 24:LC:237:ILE:HA   | 24:LC:240:LEU:HB2  | 1.98                     | 0.45              |
| 25:LD:200:MET:HE1  | 25:LD:240:TYR:CB   | 2.42                     | 0.45              |
| 25:LD:259:LYS:HA   | 25:LD:259:LYS:HD3  | 1.68                     | 0.45              |
| 25:LD:271:MET:HB2  | 25:LD:275:GLN:HG3  | 1.98                     | 0.45              |
| 26:LE:144:ILE:HG13 | 26:LE:196:ALA:HB2  | 1.98                     | 0.45              |
| 27:LF:127:LYS:HE2  | 40:LT:133:ALA:CB   | 2.46                     | 0.45              |
| 28:LG:159:HIS:NE2  | 28:LG:185:LYS:HD3  | 2.30                     | 0.45              |
| 31:LJ:166:PHE:HD1  | 31:LJ:170:TYR:HD1  | 1.64                     | 0.45              |
| 33:LM:37:LEU:HD12  | 39:LS:75:VAL:HG23  | 1.98                     | 0.45              |
| 37:LQ:177:ALA:O    | 46:La:51:GLY:HA2   | 2.16                     | 0.45              |
| 41:LU:66:SER:HB2   | 41:LU:69:LYS:HG2   | 1.97                     | 0.45              |
| 43:LX:116:LEU:HD12 | 43:LX:117:TYR:CD1  | 2.51                     | 0.45              |
| 45:LZ:70:SER:H     | 45:LZ:111:ARG:HH11 | 1.63                     | 0.45              |
| 46:La:93:ASN:ND2   | 46:La:95:THR:O     | 2.49                     | 0.45              |
| 46:La:98:ALA:HB3   | 46:La:123:ILE:HD11 | 1.97                     | 0.45              |
| 46:La:123:ILE:HD12 | 46:La:123:ILE:N    | 2.31                     | 0.45              |
| 50:Le:84:GLU:O     | 50:Le:87:VAL:HG12  | 2.16                     | 0.45              |
| 59:Ln:16:LYS:HG2   | 59:Ln:20:MET:CE    | 2.36                     | 0.45              |
| 67:SK:73:ASN:HA    | 67:SK:76:ILE:HG12  | 1.98                     | 0.45              |
| 69:SQ:33:LYS:NZ    | 79:S2:1425:G:O3'   | 2.49                     | 0.45              |
| 70:SS:64:VAL:O     | 70:SS:68:ILE:HG12  | 2.16                     | 0.45              |
| 70:SS:130:ARG:NH2  | 79:S2:1230:C:OP1   | 2.29                     | 0.45              |
| 74:Sd:19:ARG:NE    | 74:Sd:32:ARG:HH11  | 2.14                     | 0.45              |
| 79:S2:24:C:O2'     | 79:S2:25:A:H8      | 1.99                     | 0.45              |
| 79:S2:462:C:H2'    | 79:S2:463:C:O4'    | 2.16                     | 0.45              |
| 79:S2:617:G:HO2'   | 79:S2:632:C:HO2'   | 1.63                     | 0.45              |
| 79:S2:845:G:H2'    | 79:S2:846:G:O4'    | 2.15                     | 0.45              |
| 79:S2:1054:G:C6    | 79:S2:1065:G:C6    | 3.04                     | 0.45              |
| 79:S2:1417:C:N4    | 79:S2:1424:G:O6    | 2.49                     | 0.45              |
| 79:S2:1420:G:O2'   | 79:S2:1421:A:O5'   | 2.33                     | 0.45              |
| 87:IW:37:GLU:O     | 87:IW:41:LEU:HG    | 2.17                     | 0.45              |
| 5:sX:48:LYS:HG3    | 79:s2:483:C:H5''   | 1.98                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:sJ:16:PRO:HD3    | 7:sJ:44:TRP:CE2    | 2.50                     | 0.45              |
| 11:sB:185:VAL:O    | 11:sB:189:ILE:HG12 | 2.16                     | 0.45              |
| 12:sH:73:GLN:HB3   | 12:sH:135:PHE:CE1  | 2.50                     | 0.45              |
| 12:sH:76:GLN:NE2   | 12:sH:94:PHE:HB2   | 2.31                     | 0.45              |
| 19:sb:46:VAL:HG23  | 19:sb:54:VAL:HG21  | 1.98                     | 0.45              |
| 22:lA:137:ILE:HG13 | 22:lA:148:VAL:HA   | 1.97                     | 0.45              |
| 23:lB:374:PHE:CE2  | 85:l5:5050:C:H1'   | 2.51                     | 0.45              |
| 25:lD:18:VAL:HG23  | 25:lD:24:ARG:HD2   | 1.98                     | 0.45              |
| 26:lE:186:LEU:HD21 | 26:lE:253:VAL:HG11 | 1.98                     | 0.45              |
| 26:lE:265:PRO:O    | 26:lE:267:LEU:HD22 | 2.16                     | 0.45              |
| 27:lF:73:ARG:HD3   | 85:l5:730:G:C5     | 2.51                     | 0.45              |
| 27:lF:215:SER:C    | 27:lF:247:MET:HE1  | 2.41                     | 0.45              |
| 31:lJ:121:PRO:HD3  | 70:sS:101:ASN:CB   | 2.42                     | 0.45              |
| 34:lN:101:VAL:O    | 34:lN:104:GLU:HG2  | 2.17                     | 0.45              |
| 34:lN:176:LYS:NZ   | 85:l5:67:C:H1'     | 2.30                     | 0.45              |
| 35:lO:68:ARG:HH12  | 85:l5:4564:A:H5''  | 1.81                     | 0.45              |
| 35:lO:140:ARG:O    | 35:lO:144:GLU:HG3  | 2.16                     | 0.45              |
| 37:lQ:89:ASP:CG    | 37:lQ:91:ARG:HE    | 2.24                     | 0.45              |
| 38:lR:38:ARG:HD3   | 85:l5:2525:U:OP2   | 2.16                     | 0.45              |
| 40:lT:150:LEU:HA   | 40:lT:150:LEU:HD23 | 1.47                     | 0.45              |
| 52:lg:66:ARG:NH2   | 85:l5:2517:A:O2'   | 2.46                     | 0.45              |
| 54:li:48:CYS:SG    | 54:li:49:GLY:N     | 2.89                     | 0.45              |
| 55:lj:21:ARG:O     | 55:lj:22:CYS:SG    | 2.74                     | 0.45              |
| 55:lj:25:LYS:HZ1   | 85:l5:371:A:P      | 2.40                     | 0.45              |
| 62:lr:67:ARG:NH2   | 85:l5:666:G:OP2    | 2.32                     | 0.45              |
| 64:sR:7:LYS:HD2    | 79:s2:1366:G:N7    | 2.32                     | 0.45              |
| 66:sF:147:VAL:O    | 66:sF:151:ILE:HG22 | 2.16                     | 0.45              |
| 66:sF:174:ALA:O    | 66:sF:178:ILE:HG13 | 2.16                     | 0.45              |
| 69:sQ:32:ILE:O     | 69:sQ:33:LYS:HG3   | 2.17                     | 0.45              |
| 71:sT:14:PHE:HE1   | 71:sT:134:ILE:HG23 | 1.81                     | 0.45              |
| 71:sT:18:LEU:HD12  | 71:sT:134:ILE:HG21 | 1.97                     | 0.45              |
| 75:sg:8:ARG:HB3    | 75:sg:309:VAL:HG12 | 1.98                     | 0.45              |
| 77:sZ:53:ALA:O     | 77:sZ:57:LYS:HG2   | 2.17                     | 0.45              |
| 79:s2:487:U:OP1    | 79:s2:514:U:O2'    | 2.19                     | 0.45              |
| 79:s2:932:G:O6     | 79:s2:1009:A:N1    | 2.49                     | 0.45              |
| 79:s2:1146:C:H2'   | 79:s2:1147:C:C6    | 2.51                     | 0.45              |
| 79:s2:1225:U:H2'   | 79:s2:1226:G:C8    | 2.51                     | 0.45              |
| 79:s2:1352:G:H2'   | 79:s2:1353:A:H8    | 1.80                     | 0.45              |
| 79:s2:1681:U:O2'   | 79:s2:1682:C:O4'   | 2.34                     | 0.45              |
| 80:cB:27:HIS:CE1   | 80:cB:28:VAL:HG22  | 2.51                     | 0.45              |
| 80:cB:160:MET:HE1  | 80:cB:215:GLY:H    | 1.81                     | 0.45              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 80:cB:206:ASP:HB3 | 80:cB:209:LEU:HD21 | 1.98                     | 0.45              |
| 80:cB:479:LEU:C   | 80:cB:529:LYS:HZ3  | 2.24                     | 0.45              |
| 85:l5:446:C:H2'   | 85:l5:447:C:C6     | 2.51                     | 0.45              |
| 85:l5:485:C:O2    | 85:l5:485:C:H2'    | 2.15                     | 0.45              |
| 85:l5:1296:G:O2'  | 85:l5:1297:U:O5'   | 2.31                     | 0.45              |
| 85:l5:1318:C:H2'  | 85:l5:1319:U:O4'   | 2.16                     | 0.45              |
| 85:l5:1812:C:H2'  | 85:l5:1813:U:C6    | 2.52                     | 0.45              |
| 85:l5:1999:A:H2'  | 85:l5:2000:G:C5    | 2.51                     | 0.45              |
| 85:l5:2411:C:H2'  | 85:l5:2412:A:C8    | 2.48                     | 0.45              |
| 85:l5:2431:A:H2'  | 85:l5:2432:U:C6    | 2.51                     | 0.45              |
| 85:l5:2752:G:C6   | 85:l5:2753:G:C6    | 3.04                     | 0.45              |
| 85:l5:2853:C:H2'  | 85:l5:2854:G:O4'   | 2.15                     | 0.45              |
| 85:l5:4705:A:H2'  | 85:l5:4706:G:O4'   | 2.17                     | 0.45              |
| 80:CB:134:GLY:HA2 | 80:CB:181:ILE:HD13 | 1.99                     | 0.45              |
| 8:SY:45:ALA:HA    | 8:SY:50:THR:HG1    | 1.80                     | 0.45              |
| 10:SA:85:ARG:O    | 10:SA:88:LEU:HG    | 2.16                     | 0.45              |
| 17:SO:116:LEU:HA  | 17:SO:119:LEU:HG   | 1.99                     | 0.45              |
| 85:L5:125:C:H2'   | 85:L5:126:C:H6     | 1.80                     | 0.45              |
| 85:L5:759:G:C2    | 85:L5:905:C:C2     | 3.04                     | 0.45              |
| 85:L5:942:G:H4'   | 85:L5:944:A:C6     | 2.51                     | 0.45              |
| 85:L5:1175:A:H5'' | 25:LD:268:ARG:HE   | 1.81                     | 0.45              |
| 85:L5:1202:C:N3   | 85:L5:1203:G:O2'   | 2.49                     | 0.45              |
| 85:L5:1348:U:H2'  | 85:L5:1349:G:C8    | 2.51                     | 0.45              |
| 85:L5:1573:G:OP1  | 85:L5:2667:C:O2'   | 2.30                     | 0.45              |
| 85:L5:1691:G:C6   | 85:L5:1846:G:C6    | 3.04                     | 0.45              |
| 85:L5:1862:U:O3'  | 30:LI:15:LYS:NZ    | 2.36                     | 0.45              |
| 85:L5:1907:A:H3'  | 85:L5:1908:A:H8    | 1.81                     | 0.45              |
| 85:L5:1925:G:H2'  | 85:L5:1926:C:H6    | 1.81                     | 0.45              |
| 85:L5:1978:C:H2'  | 85:L5:1979:A:O4'   | 2.15                     | 0.45              |
| 85:L5:2080:U:H2'  | 85:L5:2081:C:C6    | 2.52                     | 0.45              |
| 85:L5:2467:U:H4'  | 85:L5:2468:U:H5'   | 1.97                     | 0.45              |
| 85:L5:2487:G:H8   | 85:L5:2487:G:OP2   | 1.98                     | 0.45              |
| 85:L5:2898:G:H2'  | 85:L5:2899:C:C6    | 2.51                     | 0.45              |
| 85:L5:3651:A:H5'  | 22:LA:199:VAL:HG12 | 1.98                     | 0.45              |
| 85:L5:3834:C:H2'  | 85:L5:3835:C:C6    | 2.52                     | 0.45              |
| 85:L5:3834:C:C2   | 85:L5:3835:C:C5    | 3.04                     | 0.45              |
| 85:L5:4306:U:H2'  | 85:L5:4307:A:H8    | 1.81                     | 0.45              |
| 85:L5:4311:A:H2'  | 85:L5:4312:U:C6    | 2.51                     | 0.45              |
| 85:L5:4350:C:C2   | 85:L5:4351:U:C5    | 3.04                     | 0.45              |
| 85:L5:4743:G:H2'  | 85:L5:4744:A:H8    | 1.79                     | 0.45              |
| 22:LA:104:VAL:CA  | 22:LA:107:MET:HE3  | 2.38                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:LC:301:ALA:HB1  | 37:LQ:132:LYS:HE2  | 1.98                     | 0.45              |
| 24:LC:302:LEU:HD11 | 37:LQ:38:ARG:CZ    | 2.46                     | 0.45              |
| 27:LF:61:TYR:CD2   | 27:LF:147:LEU:HD21 | 2.51                     | 0.45              |
| 27:LF:127:LYS:HG3  | 27:LF:128:ALA:H    | 1.80                     | 0.45              |
| 28:LG:66:GLN:O     | 28:LG:70:LEU:HG    | 2.17                     | 0.45              |
| 29:LH:93:ARG:NH2   | 29:LH:142:ASP:O    | 2.49                     | 0.45              |
| 31:LJ:63:ARG:HH22  | 60:Lo:103:VAL:HA   | 1.81                     | 0.45              |
| 33:LM:28:VAL:HG22  | 33:LM:67:SER:H     | 1.81                     | 0.45              |
| 33:LM:104:MET:SD   | 33:LM:104:MET:C    | 2.99                     | 0.45              |
| 41:LU:61:VAL:CG2   | 41:LU:74:SER:HB2   | 2.43                     | 0.45              |
| 49:Ld:68:LEU:HD22  | 49:Ld:106:VAL:HG13 | 1.98                     | 0.45              |
| 51:Lf:40:GLU:OE1   | 51:Lf:40:GLU:N     | 2.40                     | 0.45              |
| 54:Li:61:LEU:HD12  | 54:Li:61:LEU:C     | 2.40                     | 0.45              |
| 59:Ln:7:LYS:O      | 59:Ln:11:ARG:HG3   | 2.16                     | 0.45              |
| 64:SR:25:GLY:O     | 64:SR:31:ASN:ND2   | 2.48                     | 0.45              |
| 65:SD:225:GLU:N    | 65:SD:225:GLU:OE1  | 2.49                     | 0.45              |
| 69:SQ:100:VAL:HG22 | 69:SQ:101:ASP:N    | 2.29                     | 0.45              |
| 70:SS:132:ARG:HD3  | 79:S2:1623:A:N6    | 2.30                     | 0.45              |
| 72:SU:35:VAL:HG11  | 72:SU:107:GLU:HG2  | 1.98                     | 0.45              |
| 74:Sd:12:ARG:HA    | 74:Sd:12:ARG:HD3   | 1.52                     | 0.45              |
| 75:Sg:173:LEU:HB2  | 75:Sg:189:ILE:HG22 | 1.98                     | 0.45              |
| 76:SM:106:CYS:SG   | 79:S2:1284:A:O2'   | 2.54                     | 0.45              |
| 79:S2:546:G:C2     | 79:S2:548:C:C4     | 3.03                     | 0.45              |
| 79:S2:693:A:C6     | 79:S2:739:C:H4'    | 2.52                     | 0.45              |
| 79:S2:958:G:C6     | 79:S2:959:G:C6     | 3.04                     | 0.45              |
| 79:S2:1373:C:H2'   | 79:S2:1374:C:H6    | 1.82                     | 0.45              |
| 79:S2:1687:C:C2    | 79:S2:1688:C:C5    | 3.04                     | 0.45              |
| 79:S2:1756:C:P     | 79:S2:1757:G:H21   | 2.37                     | 0.45              |
| 1:cH:84:GLY:CA     | 1:cH:88:LYS:NZ     | 2.80                     | 0.45              |
| 1:cH:85:ARG:NH1    | 1:cH:92:GLN:HG3    | 2.30                     | 0.45              |
| 1:cH:114:ALA:O     | 1:cH:115:ILE:C     | 2.59                     | 0.45              |
| 2:sE:19:MET:HE3    | 79:s2:846:G:H2'    | 1.99                     | 0.45              |
| 2:sE:75:LYS:HB2    | 2:sE:75:LYS:HE3    | 1.64                     | 0.45              |
| 2:sE:141:THR:HG22  | 2:sE:145:ARG:O     | 2.17                     | 0.45              |
| 3:sI:201:LYS:NZ    | 4:sL:8:ARG:HA      | 2.31                     | 0.45              |
| 5:sX:100:VAL:CG2   | 5:sX:122:VAL:HG13  | 2.45                     | 0.45              |
| 6:sG:98:ARG:NH1    | 6:sG:99:GLY:O      | 2.49                     | 0.45              |
| 6:sG:216:ARG:C     | 6:sG:218:LYS:N     | 2.73                     | 0.45              |
| 8:sY:86:GLU:OE2    | 8:sY:90:ARG:HD3    | 2.16                     | 0.45              |
| 15:sC:72:ASP:OD2   | 15:sC:272:HIS:CE1  | 2.69                     | 0.45              |
| 15:sC:116:THR:HG22 | 15:sC:121:ARG:HH11 | 1.82                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 19:sb:36:LYS:NZ    | 19:sb:41:TYR:HA    | 2.32                     | 0.45              |
| 22:lA:211:PHE:HB3  | 22:lA:219:ILE:HG22 | 1.98                     | 0.45              |
| 23:lB:271:GLN:NE2  | 23:lB:272:LYS:O    | 2.50                     | 0.45              |
| 25:lD:216:GLU:O    | 25:lD:219:TYR:HB3  | 2.16                     | 0.45              |
| 26:lE:111:LYS:HD2  | 62:lr:87:ARG:NH1   | 2.32                     | 0.45              |
| 28:lG:91:THR:HA    | 28:lG:94:GLN:CD    | 2.41                     | 0.45              |
| 29:lH:126:VAL:HG11 | 29:lH:161:ILE:HG22 | 1.98                     | 0.45              |
| 29:lH:159:ALA:HA   | 29:lH:162:GLN:HG2  | 1.98                     | 0.45              |
| 30:lI:12:CYS:HB2   | 30:lI:57:TYR:CE1   | 2.52                     | 0.45              |
| 32:lL:77:SER:O     | 32:lL:81:LEU:HD12  | 2.15                     | 0.45              |
| 34:lN:82:GLY:HA2   | 85:l5:4187:G:H4'   | 1.98                     | 0.45              |
| 37:lQ:6:ARG:CZ     | 37:lQ:8:ASN:HD21   | 2.29                     | 0.45              |
| 41:lU:19:LEU:H     | 41:lU:19:LEU:CD2   | 2.29                     | 0.45              |
| 45:lZ:128:LYS:H    | 45:lZ:128:LYS:HG2  | 1.48                     | 0.45              |
| 53:lh:31:LEU:HD12  | 53:lh:31:LEU:HA    | 1.76                     | 0.45              |
| 64:sR:12:ALA:O     | 64:sR:50:ILE:HG23  | 2.16                     | 0.45              |
| 65:sD:35:SER:O     | 65:sD:51:LEU:HB2   | 2.16                     | 0.45              |
| 65:sD:86:LEU:O     | 65:sD:87:TYR:HD2   | 1.99                     | 0.45              |
| 68:sP:129:GLY:HA3  | 79:s2:1237:C:O3'   | 2.17                     | 0.45              |
| 75:sg:262:GLU:CD   | 75:sg:263:GLY:N    | 2.74                     | 0.45              |
| 75:sg:301:GLY:C    | 75:sg:302:TYR:HD1  | 2.24                     | 0.45              |
| 79:s2:63:U:O2'     | 79:s2:170:A:N3     | 2.44                     | 0.45              |
| 79:s2:383:G:H2'    | 79:s2:384:U:C6     | 2.52                     | 0.45              |
| 79:s2:1017:U:H2'   | 79:s2:1018:U:H6    | 1.81                     | 0.45              |
| 79:s2:1064:C:H2'   | 79:s2:1065:G:H8    | 1.82                     | 0.45              |
| 79:s2:1260:A:C5    | 79:s2:1619:A:C6    | 3.04                     | 0.45              |
| 79:s2:1428:G:N1    | 79:s2:1585:U:O4'   | 2.50                     | 0.45              |
| 79:s2:1685:U:C2    | 79:s2:1686:G:C8    | 3.04                     | 0.45              |
| 81:aP:3:C:N4       | 81:aP:70:A:H61     | 2.11                     | 0.45              |
| 85:l5:152:U:H2'    | 85:l5:153:G:H8     | 1.81                     | 0.45              |
| 85:l5:666:G:N7     | 85:l5:668:C:N4     | 2.65                     | 0.45              |
| 85:l5:718:C:H2'    | 85:l5:719:C:O4'    | 2.16                     | 0.45              |
| 85:l5:964:A:C3'    | 85:l5:965:G:H4'    | 2.46                     | 0.45              |
| 85:l5:1578:U:H2'   | 85:l5:1579:C:C6    | 2.52                     | 0.45              |
| 85:l5:2417:A:C4    | 85:l5:2418:A:C8    | 3.04                     | 0.45              |
| 85:l5:2564:G:H2'   | 85:l5:2565:A:C8    | 2.51                     | 0.45              |
| 85:l5:2710:C:C2    | 85:l5:2712:G:C8    | 3.04                     | 0.45              |
| 85:l5:4092:G:C4    | 85:l5:4093:G:C2    | 3.04                     | 0.45              |
| 80:CB:26:ALA:HB2   | 80:CB:128:VAL:HB   | 1.97                     | 0.45              |
| 4:SL:46:THR:HG23   | 4:SL:62:PHE:CD1    | 2.52                     | 0.45              |
| 8:SY:40:ILE:HA     | 8:SY:43:LYS:HB3    | 1.98                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:SA:23:THR:HG22 | 10:SA:170:SER:HA  | 1.99                     | 0.45              |
| 11:SB:63:LYS:HE3  | 11:SB:89:GLU:O    | 2.16                     | 0.45              |
| 11:SB:109:LYS:O   | 11:SB:113:MET:SD  | 2.74                     | 0.45              |
| 15:SC:268:GLU:OE2 | 15:SC:268:GLU:HA  | 2.16                     | 0.45              |
| 19:Sb:7:LEU:H     | 19:Sb:7:LEU:HD12  | 1.81                     | 0.45              |
| 85:L5:78:U:H2'    | 85:L5:79:C:C6     | 2.52                     | 0.45              |
| 85:L5:248:C:H2'   | 85:L5:249:C:C6    | 2.51                     | 0.45              |
| 85:L5:405:U:P     | 44:LY:87:ARG:HH22 | 2.38                     | 0.45              |
| 85:L5:458:C:H2'   | 85:L5:459:C:H6    | 1.81                     | 0.45              |
| 85:L5:1316:G:H2'  | 85:L5:1317:U:H6   | 1.81                     | 0.45              |
| 85:L5:1452:A:C2   | 85:L5:1453:G:H1'  | 2.51                     | 0.45              |
| 85:L5:1473:U:H2'  | 85:L5:1474:C:C6   | 2.51                     | 0.45              |
| 85:L5:1643:A:C4   | 85:L5:1644:C:C5   | 3.05                     | 0.45              |
| 85:L5:1976:G:OP1  | 85:L5:1984:A:H4'  | 2.16                     | 0.45              |
| 85:L5:2055:G:N7   | 35:LO:130:LYS:HA  | 2.31                     | 0.45              |
| 85:L5:2288:G:O2'  | 85:L5:2290:C:O5'  | 2.29                     | 0.45              |
| 85:L5:2821:U:C4   | 85:L5:2822:G:C5   | 3.05                     | 0.45              |
| 85:L5:3805:U:H2'  | 85:L5:3806:G:C8   | 2.46                     | 0.45              |
| 85:L5:3947:A:H2'  | 85:L5:3948:C:C4   | 2.51                     | 0.45              |
| 85:L5:3967:G:H3'  | 85:L5:3968:U:C5   | 2.51                     | 0.45              |
| 85:L5:4176:C:H2'  | 85:L5:4177:C:C6   | 2.51                     | 0.45              |
| 85:L5:4549:G:H2'  | 85:L5:4550:G:C8   | 2.51                     | 0.45              |
| 85:L5:4584:A:H62  | 85:L5:4718:G:H21  | 1.64                     | 0.45              |
| 85:L5:4654:C:H2'  | 85:L5:4655:A:H8   | 1.81                     | 0.45              |
| 85:L5:4954:G:C2   | 85:L5:4955:A:C5   | 3.05                     | 0.45              |
| 24:LC:303:ARG:HG2 | 37:LQ:38:ARG:O    | 2.16                     | 0.45              |
| 29:LH:37:ASP:OD1  | 29:LH:38:PHE:N    | 2.50                     | 0.45              |
| 29:LH:93:ARG:HH22 | 29:LH:140:GLN:HB3 | 1.80                     | 0.45              |
| 29:LH:128:MET:HE3 | 29:LH:128:MET:HB3 | 1.60                     | 0.45              |
| 33:LM:26:ALA:HB3  | 33:LM:39:ASP:O    | 2.17                     | 0.45              |
| 33:LM:29:ASP:O    | 33:LM:37:LEU:N    | 2.40                     | 0.45              |
| 38:LR:171:LYS:HD2 | 38:LR:171:LYS:C   | 2.41                     | 0.45              |
| 40:LT:79:GLN:HB2  | 40:LT:84:ILE:HG22 | 1.98                     | 0.45              |
| 46:La:74:ASN:CG   | 46:La:114:LYS:HB3 | 2.42                     | 0.45              |
| 53:Lh:56:ARG:O    | 53:Lh:59:THR:OG1  | 2.28                     | 0.45              |
| 56:Lk:52:LYS:HA   | 56:Lk:55:LYS:HG2  | 1.97                     | 0.45              |
| 56:Lk:54:GLU:O    | 56:Lk:58:GLN:OE1  | 2.34                     | 0.45              |
| 63:Lz:112:ALA:HB3 | 63:Lz:142:GLU:HA  | 1.98                     | 0.45              |
| 66:SF:88:MET:HB3  | 79:S2:1592:C:OP1  | 2.15                     | 0.45              |
| 66:SF:171:GLU:O   | 66:SF:175:ASP:OD1 | 2.34                     | 0.45              |
| 71:ST:35:ASP:OD1  | 71:ST:35:ASP:N    | 2.48                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 72:SU:46:LYS:HG3   | 72:SU:48:LEU:HD22  | 1.98                     | 0.45              |
| 72:SU:55:ARG:HG3   | 72:SU:87:ARG:NE    | 2.32                     | 0.45              |
| 72:SU:61:LEU:HB2   | 72:SU:82:MET:HB2   | 1.98                     | 0.45              |
| 75:Sg:40:ILE:HB    | 75:Sg:59:LEU:HD22  | 1.98                     | 0.45              |
| 75:Sg:286:CYS:HB3  | 75:Sg:302:TYR:CE1  | 2.52                     | 0.45              |
| 76:SM:51:VAL:HA    | 76:SM:77:ILE:HB    | 1.99                     | 0.45              |
| 76:SM:97:GLU:CD    | 76:SM:97:GLU:H     | 2.24                     | 0.45              |
| 79:S2:85:A:H2'     | 79:S2:86:C:C6      | 2.51                     | 0.45              |
| 79:S2:1867:U:H4'   | 79:S2:1868:U:H5'   | 1.98                     | 0.45              |
| 82:PE:22:G:H2'     | 82:PE:23:A:H8      | 1.80                     | 0.45              |
| 84:Lt:123:ARG:NH2  | 84:Lt:126:SER:HA   | 2.31                     | 0.45              |
| 4:sL:41:GLY:C      | 4:sL:42:LEU:HD12   | 2.42                     | 0.45              |
| 4:sL:82:MET:HE1    | 79:s2:373:G:O2'    | 2.17                     | 0.45              |
| 5:sX:66:ILE:HD11   | 5:sX:68:LYS:HE3    | 1.97                     | 0.45              |
| 6:sG:88:ARG:HG3    | 6:sG:91:GLU:HB2    | 1.98                     | 0.45              |
| 12:sH:82:GLU:O     | 12:sH:86:LYS:HG2   | 2.17                     | 0.45              |
| 12:sH:164:ASN:OD1  | 12:sH:164:ASN:N    | 2.48                     | 0.45              |
| 17:sO:149:ARG:HH12 | 79:s2:1065:G:H5'   | 1.81                     | 0.45              |
| 19:sb:6:ASP:OD1    | 19:sb:8:LEU:HG     | 2.17                     | 0.45              |
| 23:lB:136:LYS:HA   | 23:lB:139:ASP:OD1  | 2.16                     | 0.45              |
| 24:lC:234:LYS:HD2  | 85:l5:1373:A:H2    | 1.81                     | 0.45              |
| 24:lC:303:ARG:HH22 | 85:l5:2087:C:P     | 2.40                     | 0.45              |
| 25:lD:271:MET:HB2  | 25:lD:275:GLN:HG3  | 1.97                     | 0.45              |
| 27:lF:126:ASN:O    | 27:lF:130:ILE:HG12 | 2.15                     | 0.45              |
| 31:lJ:10:ASN:N     | 31:lJ:11:PRO:HD2   | 2.31                     | 0.45              |
| 31:lJ:15:LEU:HD22  | 31:lJ:165:TRP:CD2  | 2.51                     | 0.45              |
| 33:lM:71:LYS:HE3   | 33:lM:71:LYS:HB2   | 1.87                     | 0.45              |
| 45:lZ:81:MET:HE1   | 52:lg:92:LYS:HA    | 1.99                     | 0.45              |
| 47:lb:12:GLN:NE2   | 85:l5:1670:G:OP1   | 2.36                     | 0.45              |
| 52:lg:12:SER:O     | 85:l5:2803:U:O2'   | 2.25                     | 0.45              |
| 56:lk:40:ARG:HD3   | 56:lk:41:TYR:CE2   | 2.52                     | 0.45              |
| 57:ll:29:MET:HB3   | 57:ll:29:MET:HE3   | 1.57                     | 0.45              |
| 64:sR:42:PRO:O     | 64:sR:43:SER:OG    | 2.23                     | 0.45              |
| 65:sD:163:PRO:HD2  | 79:s2:1388:A:H61   | 1.81                     | 0.45              |
| 66:sF:123:GLU:HG3  | 66:sF:200:ALA:CB   | 2.45                     | 0.45              |
| 68:sP:108:LYS:NZ   | 68:sP:110:GLU:H    | 2.15                     | 0.45              |
| 71:sT:112:MET:SD   | 71:sT:112:MET:N    | 2.90                     | 0.45              |
| 71:sT:129:ARG:NH1  | 79:s2:1415:C:O2'   | 2.49                     | 0.45              |
| 72:sU:26:SER:HB2   | 72:sU:110:VAL:HA   | 1.98                     | 0.45              |
| 73:sc:31:ARG:CD    | 73:sc:43:ILE:HG22  | 2.46                     | 0.45              |
| 74:sd:6:LEU:HA     | 74:sd:9:SER:HB3    | 1.99                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 77:sZ:99:LEU:HD12  | 77:sZ:100:VAL:N    | 2.31                     | 0.45              |
| 79:s2:907:G:H2'    | 79:s2:908:A:C8     | 2.51                     | 0.45              |
| 79:s2:1169:G:H3'   | 79:s2:1170:A:H8    | 1.82                     | 0.45              |
| 79:s2:1608:U:H3    | 79:s2:1631:U:H3    | 1.63                     | 0.45              |
| 80:cB:21:ASN:ND2   | 80:cB:101:ASN:HB2  | 2.30                     | 0.45              |
| 80:cB:83:GLU:HA    | 80:cB:86:LEU:HB2   | 1.98                     | 0.45              |
| 80:cB:390:PRO:HB3  | 80:cB:466:CYS:H    | 1.81                     | 0.45              |
| 82:pE:22:G:C2      | 82:pE:23:A:C5      | 3.04                     | 0.45              |
| 85:l5:493:G:O2'    | 85:l5:494:U:OP1    | 2.32                     | 0.45              |
| 85:l5:691:C:H2'    | 85:l5:692:A:H8     | 1.79                     | 0.45              |
| 85:l5:1275:G:H2'   | 85:l5:1276:C:H6    | 1.81                     | 0.45              |
| 85:l5:1578:U:H2'   | 85:l5:1579:C:H6    | 1.81                     | 0.45              |
| 85:l5:1969:G:H2'   | 85:l5:1969:G:N3    | 2.32                     | 0.45              |
| 85:l5:2608:G:H2'   | 85:l5:2609:G:H8    | 1.81                     | 0.45              |
| 85:l5:2751:G:N3    | 85:l5:2752:G:C8    | 2.84                     | 0.45              |
| 85:l5:3956:G:H21   | 85:l5:3963:A:H1'   | 1.81                     | 0.45              |
| 85:l5:4424:A:N7    | 85:l5:4475:G:C6    | 2.85                     | 0.45              |
| 85:l5:4600:G:O2'   | 85:l5:4601:U:P     | 2.74                     | 0.45              |
| 80:CB:143:LEU:HD13 | 80:CB:189:ILE:HG22 | 1.98                     | 0.45              |
| 80:CB:227:GLN:O    | 80:CB:228:PHE:C    | 2.59                     | 0.45              |
| 80:CB:287:ARG:O    | 80:CB:291:GLN:HB2  | 2.16                     | 0.45              |
| 80:CB:462:GLU:CD   | 80:CB:462:GLU:H    | 2.24                     | 0.45              |
| 80:CB:526:ARG:O    | 80:CB:529:LYS:HB3  | 2.17                     | 0.45              |
| 80:CB:611:ASP:OD1  | 80:CB:611:ASP:N    | 2.49                     | 0.45              |
| 80:CB:632:ALA:HB3  | 80:CB:633:ARG:NH1  | 2.32                     | 0.45              |
| 80:CB:685:TRP:CE3  | 80:CB:726:ARG:HD3  | 2.52                     | 0.45              |
| 80:CB:746:LEU:HG   | 80:CB:747:VAL:N    | 2.31                     | 0.45              |
| 2:SE:149:TYR:CD1   | 6:SG:205:GLU:HG2   | 2.51                     | 0.45              |
| 2:SE:255:ARG:HH12  | 2:SE:259:LYS:HB2   | 1.82                     | 0.45              |
| 4:SL:35:ARG:NH1    | 4:SL:55:TYR:O      | 2.48                     | 0.45              |
| 4:SL:84:ARG:O      | 4:SL:112:HIS:ND1   | 2.50                     | 0.45              |
| 5:SX:67:ARG:NH2    | 79:S2:618:C:H41    | 2.12                     | 0.45              |
| 6:SG:45:TRP:HA     | 6:SG:48:TYR:HD2    | 1.82                     | 0.45              |
| 6:SG:170:ARG:HD3   | 79:S2:67:C:H41     | 1.81                     | 0.45              |
| 11:SB:110:MET:HA   | 11:SB:113:MET:HE1  | 1.98                     | 0.45              |
| 12:SH:56:GLY:C     | 12:SH:58:LYS:HE2   | 2.42                     | 0.45              |
| 85:L5:138:G:N1     | 85:L5:139:G:C6     | 2.85                     | 0.45              |
| 85:L5:300:A:H2'    | 85:L5:301:G:C8     | 2.47                     | 0.45              |
| 85:L5:498:C:H2'    | 85:L5:499:G:H4'    | 1.98                     | 0.45              |
| 85:L5:506:C:H2'    | 85:L5:507:G:C8     | 2.51                     | 0.45              |
| 85:L5:976:G:H2'    | 85:L5:977:C:O4'    | 2.16                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 85:L5:1097:C:H2'   | 85:L5:1098:G:C8    | 2.51                     | 0.45              |
| 85:L5:1217:G:N1    | 85:L5:1218:G:C6    | 2.85                     | 0.45              |
| 85:L5:1424:G:H2'   | 85:L5:1425:G:O4'   | 2.16                     | 0.45              |
| 85:L5:1535:C:H5'   | 55:Lj:11:ARG:HD3   | 1.98                     | 0.45              |
| 85:L5:1730:U:H2'   | 85:L5:1731:C:H6    | 1.82                     | 0.45              |
| 85:L5:1748:U:H2'   | 85:L5:1749:A:O4'   | 2.16                     | 0.45              |
| 85:L5:1812:C:H1'   | 47:Lb:57:MET:HE1   | 1.99                     | 0.45              |
| 85:L5:2112:G:H5''  | 85:L5:2251:G:O6    | 2.16                     | 0.45              |
| 85:L5:2270:G:H2'   | 85:L5:2271:C:C6    | 2.52                     | 0.45              |
| 85:L5:2276:A:H2'   | 85:L5:2277:C:C6    | 2.52                     | 0.45              |
| 85:L5:2294:G:C6    | 85:L5:2341:A:C6    | 3.04                     | 0.45              |
| 85:L5:2459:G:H2'   | 85:L5:2461:G:OP2   | 2.16                     | 0.45              |
| 85:L5:2594:C:H5''  | 22:LA:70:LYS:HG2   | 1.97                     | 0.45              |
| 85:L5:2793:G:O2'   | 55:Lj:5:THR:HG23   | 2.16                     | 0.45              |
| 85:L5:2805:C:O2    | 52:Lg:4:ARG:HB3    | 2.16                     | 0.45              |
| 85:L5:2865:U:OP1   | 38:LR:84:THR:OG1   | 2.29                     | 0.45              |
| 85:L5:3859:G:H4'   | 36:LP:139:TYR:CE1  | 2.50                     | 0.45              |
| 85:L5:4156:G:H8    | 85:L5:4156:G:OP2   | 2.00                     | 0.45              |
| 85:L5:4296:U:H2'   | 85:L5:4297:G:O4'   | 2.16                     | 0.45              |
| 85:L5:4888:U:O2'   | 85:L5:4931:G:N2    | 2.50                     | 0.45              |
| 85:L5:4920:C:H2'   | 85:L5:4921:C:C6    | 2.51                     | 0.45              |
| 85:L5:4974:C:H1'   | 85:L5:4985:U:O2    | 2.16                     | 0.45              |
| 20:L7:3:C:H2'      | 20:L7:4:U:C6       | 2.51                     | 0.45              |
| 21:L8:33:G:H4'     | 21:L8:34:U:C5      | 2.52                     | 0.45              |
| 21:L8:36:G:OP2     | 53:Lh:88:THR:HG23  | 2.17                     | 0.45              |
| 21:L8:51:U:O3'     | 57:Ll:21:ARG:NH2   | 2.47                     | 0.45              |
| 21:L8:66:A:H2'     | 21:L8:67:U:H6      | 1.82                     | 0.45              |
| 23:LB:175:GLN:NE2  | 23:LB:177:LYS:O    | 2.49                     | 0.45              |
| 24:LC:62:THR:HB    | 24:LC:92:PHE:HE1   | 1.82                     | 0.45              |
| 25:LD:39:GLN:NE2   | 25:LD:46:THR:OG1   | 2.49                     | 0.45              |
| 26:LE:141:ARG:HB2  | 26:LE:191:GLN:NE2  | 2.31                     | 0.45              |
| 28:LG:136:LEU:HD12 | 28:LG:136:LEU:HA   | 1.78                     | 0.45              |
| 29:LH:23:ARG:HH11  | 29:LH:42:ASN:HA    | 1.81                     | 0.45              |
| 31:LJ:134:LEU:HA   | 31:LJ:134:LEU:HD13 | 1.75                     | 0.45              |
| 34:LN:28:TRP:O     | 34:LN:32:GLN:HG2   | 2.16                     | 0.45              |
| 34:LN:145:ASN:OD1  | 34:LN:148:THR:OG1  | 2.24                     | 0.45              |
| 35:LO:84:VAL:HA    | 35:LO:87:MET:HG2   | 1.98                     | 0.45              |
| 36:LP:122:ALA:HB3  | 36:LP:143:PRO:HG2  | 1.98                     | 0.45              |
| 37:LQ:180:ARG:HA   | 37:LQ:180:ARG:HD2  | 1.85                     | 0.45              |
| 41:LU:74:SER:OG    | 41:LU:75:GLU:N     | 2.48                     | 0.45              |
| 45:LZ:123:LYS:O    | 45:LZ:124:THR:OG1  | 2.30                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 50:Le:69:MET:SD    | 50:Le:70:LEU:O     | 2.74                     | 0.45              |
| 55:Lj:67:LEU:HA    | 55:Lj:70:VAL:HG22  | 1.98                     | 0.45              |
| 61:Lp:11:VAL:HG11  | 61:Lp:23:ARG:HB3   | 1.99                     | 0.45              |
| 62:Lr:63:VAL:HA    | 62:Lr:79:ARG:HA    | 1.98                     | 0.45              |
| 62:Lr:93:ILE:O     | 62:Lr:96:MET:HB2   | 2.16                     | 0.45              |
| 66:SF:78:MET:O     | 66:SF:78:MET:SD    | 2.74                     | 0.45              |
| 66:SF:123:GLU:OE1  | 66:SF:139:VAL:N    | 2.49                     | 0.45              |
| 67:SK:35:LEU:HD23  | 67:SK:36:ALA:H     | 1.82                     | 0.45              |
| 72:SU:34:LYS:HD2   | 72:SU:34:LYS:C     | 2.42                     | 0.45              |
| 72:SU:94:PRO:HD2   | 72:SU:97:ILE:HD11  | 1.98                     | 0.45              |
| 74:Sd:32:ARG:HH22  | 79:S2:1660:C:H3'   | 1.80                     | 0.45              |
| 77:SZ:70:PRO:HD3   | 77:SZ:88:LEU:HD12  | 1.98                     | 0.45              |
| 77:SZ:102:LYS:HA   | 77:SZ:102:LYS:HD2  | 1.64                     | 0.45              |
| 79:S2:752:G:OP2    | 79:S2:752:G:N2     | 2.40                     | 0.45              |
| 79:S2:1397:U:OP2   | 79:S2:1397:U:H3'   | 2.17                     | 0.45              |
| 79:S2:1737:G:H2'   | 79:S2:1738:C:C6    | 2.51                     | 0.45              |
| 79:S2:1805:G:C2    | 79:S2:1806:A:C5    | 3.04                     | 0.45              |
| 87:IW:106:GLU:HA   | 87:IW:109:ILE:HD12 | 1.98                     | 0.45              |
| 87:LW:86:SER:O     | 87:LW:90:ILE:HG12  | 2.17                     | 0.45              |
| 1:CH:73:VAL:HG12   | 1:CH:113:ARG:O     | 2.16                     | 0.45              |
| 1:CH:100:ASN:ND2   | 79:S2:635:G:H21    | 2.15                     | 0.45              |
| 1:cH:141:ILE:HG21  | 1:cH:145:PRO:HD3   | 1.98                     | 0.45              |
| 2:sE:62:LYS:HG3    | 2:sE:63:LYS:N      | 2.31                     | 0.45              |
| 2:sE:122:LYS:N     | 2:sE:162:ILE:O     | 2.50                     | 0.45              |
| 4:sL:87:VAL:HG12   | 4:sL:110:SER:HB3   | 1.98                     | 0.45              |
| 4:sL:126:VAL:HG23  | 4:sL:144:LYS:O     | 2.17                     | 0.45              |
| 6:sG:70:HIS:HB3    | 6:sG:101:ILE:HB    | 1.99                     | 0.45              |
| 8:sY:19:GLN:CG     | 8:sY:81:TYR:HD1    | 2.29                     | 0.45              |
| 8:sY:25:ILE:HD11   | 8:sY:60:PHE:CZ     | 2.50                     | 0.45              |
| 8:sY:105:LYS:HE3   | 79:s2:490:C:P      | 2.56                     | 0.45              |
| 8:sY:106:GLN:HA    | 8:sY:109:GLU:HG2   | 1.97                     | 0.45              |
| 8:sY:111:LYS:NZ    | 79:s2:56:G:OP1     | 2.46                     | 0.45              |
| 10:sA:15:VAL:HA    | 10:sA:18:PHE:HB2   | 1.98                     | 0.45              |
| 11:sB:33:VAL:C     | 11:sB:34:LYS:HD2   | 2.41                     | 0.45              |
| 17:sO:149:ARG:HH22 | 79:s2:960:U:H5''   | 1.81                     | 0.45              |
| 21:l8:110:U:H3     | 85:l5:2510:G:P     | 2.38                     | 0.45              |
| 27:lF:73:ARG:HD3   | 85:l5:730:G:C4     | 2.52                     | 0.45              |
| 28:lG:206:GLN:N    | 28:lG:206:GLN:OE1  | 2.50                     | 0.45              |
| 32:lL:198:ARG:HA   | 32:lL:201:GLU:HG2  | 1.99                     | 0.45              |
| 34:lN:47:LYS:HA    | 34:lN:50:ARG:HD3   | 1.99                     | 0.45              |
| 35:lO:194:GLU:OE2  | 35:lO:195:VAL:N    | 2.49                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 41:IU:82:TYR:OH    | 85:l5:2631:U:C2    | 2.66                     | 0.45              |
| 42:IV:111:GLU:OE1  | 42:IV:111:GLU:N    | 2.24                     | 0.45              |
| 44:IY:84:ARG:HA    | 44:IY:84:ARG:NE    | 2.31                     | 0.45              |
| 55:lj:55:ARG:HA    | 55:lj:58:THR:HG22  | 1.98                     | 0.45              |
| 58:lm:97:ARG:HB2   | 58:lm:120:ASN:HB3  | 1.98                     | 0.45              |
| 66:sF:148:ASN:HD21 | 79:s2:1677:U:P     | 2.40                     | 0.45              |
| 66:sF:164:ARG:NH1  | 79:s2:1533:A:OP1   | 2.50                     | 0.45              |
| 66:sF:187:SER:OG   | 66:sF:190:ILE:HG12 | 2.16                     | 0.45              |
| 70:sS:33:ILE:H     | 70:sS:33:ILE:HD12  | 1.81                     | 0.45              |
| 70:sS:62:ASP:O     | 70:sS:65:GLU:OE1   | 2.34                     | 0.45              |
| 71:sT:113:VAL:HG13 | 71:sT:122:LYS:O    | 2.17                     | 0.45              |
| 73:sc:56:LEU:HD12  | 73:sc:57:THR:N     | 2.32                     | 0.45              |
| 75:sg:19:THR:N     | 75:sg:34:ALA:O     | 2.49                     | 0.45              |
| 75:sg:64:HIS:HB3   | 75:sg:83:TRP:HB2   | 1.98                     | 0.45              |
| 75:sg:196:ASN:ND2  | 75:sg:236:ILE:O    | 2.49                     | 0.45              |
| 78:sf:87:THR:HB    | 78:sf:90:LYS:HD2   | 1.98                     | 0.45              |
| 79:s2:420:G:HO2'   | 79:s2:421:G:P      | 2.40                     | 0.45              |
| 79:s2:559:G:N3     | 79:s2:560:A:C8     | 2.84                     | 0.45              |
| 79:s2:863:U:H2'    | 79:s2:864:A:H8     | 1.81                     | 0.45              |
| 79:s2:1733:U:H2'   | 79:s2:1734:G:O4'   | 2.15                     | 0.45              |
| 80:cB:609:PHE:HD1  | 80:cB:613:LEU:HB2  | 1.82                     | 0.45              |
| 85:l5:507:G:C2     | 85:l5:652:G:C2     | 3.05                     | 0.45              |
| 85:l5:1351:G:H2'   | 85:l5:1352:C:H6    | 1.81                     | 0.45              |
| 85:l5:1414:C:H2'   | 85:l5:1415:G:C8    | 2.39                     | 0.45              |
| 85:l5:2588:C:OP1   | 85:l5:2768:C:O2'   | 2.25                     | 0.45              |
| 85:l5:2659:A:C6    | 85:l5:2673:G:C2    | 3.04                     | 0.45              |
| 85:l5:3690:U:H2'   | 85:l5:3691:G:O4'   | 2.15                     | 0.45              |
| 85:l5:4040:C:P     | 85:l5:4045:G:H22   | 2.39                     | 0.45              |
| 85:l5:4041:C:O5'   | 85:l5:4042:G:H5''  | 2.16                     | 0.45              |
| 85:l5:4262:C:H2'   | 85:l5:4263:C:C6    | 2.50                     | 0.45              |
| 85:l5:4438:U:H2'   | 85:l5:4439:U:O4'   | 2.16                     | 0.45              |
| 85:l5:4551:U:H2'   | 85:l5:4552:U:C6    | 2.52                     | 0.45              |
| 85:l5:4573:G:H8    | 85:l5:4573:G:O5'   | 2.00                     | 0.45              |
| 80:CB:333:LYS:O    | 80:CB:337:LYS:HG3  | 2.16                     | 0.45              |
| 80:CB:666:THR:HG22 | 80:CB:706:ASP:HA   | 1.98                     | 0.45              |
| 2:SE:19:MET:HE1    | 79:S2:846:G:C4     | 2.52                     | 0.45              |
| 3:SI:8:TRP:HA      | 3:SI:18:ARG:HE     | 1.81                     | 0.45              |
| 3:SI:100:CYS:O     | 3:SI:175:ILE:HG22  | 2.16                     | 0.45              |
| 6:SG:147:LEU:HB3   | 6:SG:151:ASP:HB2   | 1.99                     | 0.45              |
| 7:SJ:40:LYS:HG3    | 86:Se:34:ARG:NH2   | 2.32                     | 0.45              |
| 10:SA:8:LEU:HD13   | 10:SA:59:LEU:CD1   | 2.47                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:SA:173:LEU:O    | 10:SA:177:MET:SD   | 2.75                     | 0.45              |
| 10:SA:185:MET:O    | 10:SA:185:MET:HE3  | 2.16                     | 0.45              |
| 12:SH:153:LEU:HD11 | 12:SH:186:ASN:OD1  | 2.17                     | 0.45              |
| 85:L5:84:A:OP1     | 85:L5:84:A:H8      | 2.00                     | 0.45              |
| 85:L5:171:U:H6     | 85:L5:172:C:H5     | 1.65                     | 0.45              |
| 85:L5:304:C:H2'    | 85:L5:305:A:O4'    | 2.17                     | 0.45              |
| 85:L5:381:U:H4'    | 85:L5:415:G:H5'    | 1.98                     | 0.45              |
| 85:L5:396:A:OP2    | 85:L5:396:A:H8     | 2.00                     | 0.45              |
| 85:L5:413:G:N3     | 57:L1:36:ARG:NH2   | 2.64                     | 0.45              |
| 85:L5:446:C:H2'    | 85:L5:447:C:C6     | 2.52                     | 0.45              |
| 85:L5:1374:G:H2'   | 85:L5:1375:C:H6    | 1.81                     | 0.45              |
| 85:L5:1389:U:H2'   | 85:L5:1390:G:C8    | 2.52                     | 0.45              |
| 85:L5:1540:C:OP1   | 22:LA:190:LYS:HD2  | 2.17                     | 0.45              |
| 85:L5:1693:U:OP2   | 37:LQ:49:LYS:NZ    | 2.33                     | 0.45              |
| 85:L5:2046:G:OP1   | 35:LO:60:LYS:NZ    | 2.46                     | 0.45              |
| 85:L5:2072:C:O2'   | 27:LF:213:LEU:O    | 2.31                     | 0.45              |
| 85:L5:2690:C:H2'   | 85:L5:2691:U:C6    | 2.51                     | 0.45              |
| 85:L5:2811:G:N2    | 85:L5:2813:A:H3'   | 2.32                     | 0.45              |
| 85:L5:2846:G:C4    | 85:L5:2847:G:C8    | 3.04                     | 0.45              |
| 85:L5:3753:G:N7    | 85:L5:3776:G:H2'   | 2.31                     | 0.45              |
| 85:L5:4075:U:OP1   | 28:LG:249:ARG:NH2  | 2.46                     | 0.45              |
| 85:L5:4096:C:OP1   | 85:L5:4108:G:C4    | 2.69                     | 0.45              |
| 85:L5:4561:C:H2'   | 85:L5:4562:C:C6    | 2.52                     | 0.45              |
| 85:L5:4768:G:O3'   | 85:L5:4873:G:N2    | 2.50                     | 0.45              |
| 85:L5:4975:G:O2'   | 85:L5:4977:A:N6    | 2.38                     | 0.45              |
| 85:L5:5066:U:H2'   | 85:L5:5067:U:C6    | 2.51                     | 0.45              |
| 22:LA:37:ARG:HG3   | 22:LA:38:HIS:ND1   | 2.31                     | 0.45              |
| 24:LC:122:TYR:HA   | 24:LC:125:CYS:SG   | 2.57                     | 0.45              |
| 24:LC:200:ARG:HG3  | 24:LC:201:ARG:HG3  | 1.98                     | 0.45              |
| 26:LE:67:ALA:O     | 26:LE:71:ARG:HG2   | 2.17                     | 0.45              |
| 26:LE:178:PRO:HG2  | 26:LE:181:LEU:HD12 | 1.99                     | 0.45              |
| 27:LF:226:HIS:ND1  | 27:LF:234:GLY:HA3  | 2.31                     | 0.45              |
| 28:LG:30:PRO:HD2   | 45:LZ:123:LYS:HZ1  | 1.80                     | 0.45              |
| 29:LH:34:LEU:HD11  | 29:LH:150:ASP:HB2  | 1.99                     | 0.45              |
| 29:LH:72:THR:O     | 29:LH:76:HIS:ND1   | 2.50                     | 0.45              |
| 31:LJ:41:GLU:N     | 31:LJ:41:GLU:OE1   | 2.49                     | 0.45              |
| 31:LJ:87:LEU:HD12  | 31:LJ:92:TYR:HA    | 1.98                     | 0.45              |
| 36:LP:15:CYS:SG    | 36:LP:102:ALA:HB2  | 2.56                     | 0.45              |
| 38:LR:176:ARG:HH12 | 38:LR:177:LEU:HG   | 1.80                     | 0.45              |
| 39:LS:54:MET:HA    | 39:LS:54:MET:HE3   | 1.98                     | 0.45              |
| 40:LT:31:MET:SD    | 40:LT:31:MET:N     | 2.81                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 47:Lb:90:SER:OG    | 47:Lb:91:ARG:N     | 2.50                     | 0.45              |
| 54:Li:86:LYS:HG3   | 54:Li:90:LEU:HD11  | 1.97                     | 0.45              |
| 63:Lz:33:GLU:H     | 63:Lz:206:ILE:CG2  | 2.28                     | 0.45              |
| 69:SQ:112:LEU:HA   | 69:SQ:112:LEU:HD12 | 1.78                     | 0.45              |
| 72:SU:116:ILE:HG23 | 72:SU:119:ALA:H    | 1.81                     | 0.45              |
| 74:Sd:13:LYS:CG    | 74:Sd:14:PHE:H     | 2.30                     | 0.45              |
| 75:Sg:43:TRP:N     | 75:Sg:43:TRP:CD1   | 2.85                     | 0.45              |
| 77:SZ:101:SER:OG   | 77:SZ:102:LYS:N    | 2.49                     | 0.45              |
| 78:Sf:92:LYS:HD2   | 78:Sf:92:LYS:HA    | 1.67                     | 0.45              |
| 78:Sf:138:ARG:H    | 78:Sf:138:ARG:HG3  | 1.61                     | 0.45              |
| 79:S2:35:C:H2'     | 79:S2:36:U:C6      | 2.52                     | 0.45              |
| 79:S2:963:A:H2'    | 79:S2:964:A:H8     | 1.82                     | 0.45              |
| 79:S2:1144:A:H2'   | 79:S2:1145:A:H8    | 1.80                     | 0.45              |
| 79:S2:1592:C:H2'   | 79:S2:1593:C:C6    | 2.51                     | 0.45              |
| 1:CH:70:HIS:NE2    | 65:SD:107:TYR:O    | 2.39                     | 0.45              |
| 5:sX:15:SER:HA     | 5:sX:18:ARG:CZ     | 2.47                     | 0.45              |
| 6:sG:69:THR:O      | 6:sG:99:GLY:HA3    | 2.16                     | 0.45              |
| 6:sG:136:LYS:O     | 6:sG:176:ILE:HD12  | 2.16                     | 0.45              |
| 6:sG:178:ARG:NH2   | 79:s2:145:G:N7     | 2.63                     | 0.45              |
| 10:sA:17:LYS:NZ    | 64:sR:91:LEU:O     | 2.34                     | 0.45              |
| 10:sA:70:ASN:OD1   | 10:sA:72:ALA:N     | 2.50                     | 0.45              |
| 11:sB:114:VAL:HA   | 11:sB:142:PHE:HE1  | 1.82                     | 0.45              |
| 11:sB:144:LYS:CE   | 11:sB:208:HIS:HB3  | 2.47                     | 0.45              |
| 12:sH:163:GLN:O    | 12:sH:167:GLU:HB3  | 2.17                     | 0.45              |
| 13:sV:3:ASN:O      | 13:sV:6:GLY:N      | 2.47                     | 0.45              |
| 15:sC:117:ARG:HH11 | 15:sC:117:ARG:C    | 2.20                     | 0.45              |
| 15:sC:130:ILE:HG13 | 15:sC:162:ILE:HD11 | 1.98                     | 0.45              |
| 21:l8:70:G:C2      | 21:l8:87:G:N3      | 2.84                     | 0.45              |
| 22:lA:34:PHE:CZ    | 85:l5:4087:G:C4    | 3.05                     | 0.45              |
| 23:lB:219:VAL:HG11 | 23:lB:337:VAL:HG21 | 1.98                     | 0.45              |
| 25:lD:181:PRO:HD2  | 25:lD:195:HIS:HD1  | 1.80                     | 0.45              |
| 27:lF:60:GLU:O     | 27:lF:64:MET:HE1   | 2.17                     | 0.45              |
| 27:lF:90:ALA:HB3   | 27:lF:125:LEU:HD21 | 1.99                     | 0.45              |
| 27:lF:196:THR:O    | 27:lF:196:THR:OG1  | 2.33                     | 0.45              |
| 35:lO:62:MET:HG2   | 35:lO:69:GLY:CA    | 2.40                     | 0.45              |
| 36:lP:7:ASP:C      | 36:lP:7:ASP:OD1    | 2.59                     | 0.45              |
| 36:lP:127:ARG:O    | 36:lP:139:TYR:N    | 2.47                     | 0.45              |
| 37:lQ:93:GLN:N     | 37:lQ:93:GLN:CD    | 2.75                     | 0.45              |
| 38:lR:81:ARG:HB3   | 38:lR:88:ARG:NH1   | 2.31                     | 0.45              |
| 38:lR:97:ARG:O     | 38:lR:101:ILE:HG12 | 2.17                     | 0.45              |
| 41:lU:64:GLU:OE2   | 41:lU:71:THR:HB    | 2.17                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 46:la:65:ARG:NH2   | 85:l5:84:A:OP1     | 2.50                     | 0.45              |
| 51:lf:110:ILE:HD13 | 51:lf:110:ILE:HA   | 1.86                     | 0.45              |
| 53:lh:88:THR:HB    | 53:lh:91:MET:SD    | 2.57                     | 0.45              |
| 55:lj:49:TRP:CE3   | 85:l5:1646:A:H1'   | 2.51                     | 0.45              |
| 60:lo:3:ASN:O      | 85:l5:4232:U:H5''  | 2.17                     | 0.45              |
| 63:lz:174:MET:HE3  | 63:lz:175:THR:N    | 2.32                     | 0.45              |
| 64:sR:28:PHE:C     | 64:sR:29:HIS:HD1   | 2.15                     | 0.45              |
| 66:sF:82:ASN:OD1   | 66:sF:82:ASN:N     | 2.45                     | 0.45              |
| 69:sQ:10:VAL:HG12  | 69:sQ:95:TYR:CD2   | 2.47                     | 0.45              |
| 69:sQ:101:ASP:OD2  | 69:sQ:102:GLU:N    | 2.50                     | 0.45              |
| 71:sT:78:ILE:HD11  | 79:s2:1587:G:C4    | 2.52                     | 0.45              |
| 72:sU:61:LEU:HD23  | 72:sU:82:MET:CB    | 2.47                     | 0.45              |
| 72:sU:97:ILE:O     | 72:sU:100:GLN:NE2  | 2.36                     | 0.45              |
| 73:sc:13:ARG:CZ    | 73:sc:55:VAL:HB    | 2.46                     | 0.45              |
| 77:sZ:47:LEU:HA    | 77:sZ:78:LYS:NZ    | 2.32                     | 0.45              |
| 77:sZ:98:LYS:CE    | 77:sZ:111:ARG:O    | 2.65                     | 0.45              |
| 79:s2:43:U:H2'     | 79:s2:44:U:H5      | 1.81                     | 0.45              |
| 79:s2:89:C:O2      | 79:s2:499:G:H4'    | 2.16                     | 0.45              |
| 79:s2:1188:A:H2'   | 79:s2:1189:A:O4'   | 2.17                     | 0.45              |
| 79:s2:1264:C:H4'   | 79:s2:1265:A:O4'   | 2.16                     | 0.45              |
| 79:s2:1274:G:H5'   | 79:s2:1274:G:N3    | 2.32                     | 0.45              |
| 85:l5:497:G:H22    | 85:l5:658:C:N4     | 2.15                     | 0.45              |
| 85:l5:750:U:H2'    | 85:l5:751:G:O4'    | 2.17                     | 0.45              |
| 85:l5:947:C:H2'    | 85:l5:948:C:H6     | 1.81                     | 0.45              |
| 85:l5:959:G:O2'    | 85:l5:2263:A:N6    | 2.50                     | 0.45              |
| 85:l5:993:G:H22    | 85:l5:1050:C:H2'   | 1.80                     | 0.45              |
| 85:l5:1955:G:H2'   | 85:l5:1956:A:H8    | 1.80                     | 0.45              |
| 85:l5:1998:A:H1'   | 85:l5:2019:C:O2'   | 2.17                     | 0.45              |
| 85:l5:2394:G:O4'   | 85:l5:2397:G:N2    | 2.50                     | 0.45              |
| 85:l5:2885:A:H2'   | 85:l5:2886:U:C6    | 2.51                     | 0.45              |
| 85:l5:3651:A:H3'   | 85:l5:3652:A:H8    | 1.81                     | 0.45              |
| 85:l5:3759:A:H5'   | 85:l5:3765:G:H22   | 1.81                     | 0.45              |
| 85:l5:4348:A:C6    | 85:l5:4350:C:N3    | 2.85                     | 0.45              |
| 85:l5:4412:C:H2'   | 85:l5:4413:C:H6    | 1.80                     | 0.45              |
| 85:l5:4548:A:H5'   | 85:l5:4549:G:C5'   | 2.47                     | 0.45              |
| 85:l5:4622:A:H2'   | 85:l5:4623:G:C8    | 2.51                     | 0.45              |
| 85:l5:4998:G:H2'   | 85:l5:4999:G:C8    | 2.52                     | 0.45              |
| 80:CB:601:ARG:NH2  | 80:CB:708:THR:HG21 | 2.32                     | 0.45              |
| 3:SI:5:ARG:N       | 3:SI:28:GLU:O      | 2.38                     | 0.45              |
| 3:SI:139:LYS:C     | 3:SI:140:LYS:HG3   | 2.42                     | 0.45              |
| 6:SG:131:ARG:O     | 87:LW:82:ILE:HD12  | 2.17                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:SJ:35:TYR:CE1    | 7:SJ:112:THR:HG21  | 2.52                     | 0.45              |
| 12:SH:184:ASP:OD1  | 12:SH:184:ASP:C    | 2.60                     | 0.45              |
| 14:Sa:15:ARG:HG3   | 79:S2:993:G:O6     | 2.16                     | 0.45              |
| 15:SC:210:PRO:HD3  | 15:SC:236:PHE:CE2  | 2.52                     | 0.45              |
| 15:SC:272:HIS:HA   | 15:SC:275:LYS:HG3  | 1.99                     | 0.45              |
| 16:SN:61:ALA:HB1   | 79:S2:1016:U:H6    | 1.81                     | 0.45              |
| 17:SO:59:GLY:HA3   | 79:S2:957:A:OP1    | 2.16                     | 0.45              |
| 85:L5:47:A:OP1     | 85:L5:49:U:H1'     | 2.16                     | 0.45              |
| 85:L5:78:U:H2'     | 85:L5:79:C:H6      | 1.82                     | 0.45              |
| 85:L5:249:C:H2'    | 85:L5:250:C:C6     | 2.51                     | 0.45              |
| 85:L5:256:G:H2'    | 85:L5:257:C:H6     | 1.82                     | 0.45              |
| 85:L5:304:C:O2'    | 54:Li:76:ARG:HD3   | 2.16                     | 0.45              |
| 85:L5:441:G:H2'    | 85:L5:442:G:H8     | 1.80                     | 0.45              |
| 85:L5:447:C:H2'    | 85:L5:448:G:C8     | 2.52                     | 0.45              |
| 85:L5:986:C:H2'    | 85:L5:987:C:H6     | 1.82                     | 0.45              |
| 85:L5:1387:A:N7    | 46:La:74:ASN:ND2   | 2.64                     | 0.45              |
| 85:L5:1603:C:H2'   | 85:L5:1604:G:H8    | 1.81                     | 0.45              |
| 85:L5:2362:U:H2'   | 85:L5:2363:A:H8    | 1.81                     | 0.45              |
| 85:L5:2784:C:H2'   | 85:L5:2785:C:C6    | 2.47                     | 0.45              |
| 85:L5:3650:C:H2'   | 85:L5:3651:A:C8    | 2.51                     | 0.45              |
| 85:L5:3661:G:N1    | 85:L5:3682:A:OP2   | 2.47                     | 0.45              |
| 85:L5:3783:A:C2    | 85:L5:3787:G:C6    | 3.04                     | 0.45              |
| 85:L5:3808:C:H3'   | 85:L5:3809:G:N2    | 2.31                     | 0.45              |
| 85:L5:4180:G:H2'   | 85:L5:4181:U:C6    | 2.52                     | 0.45              |
| 85:L5:4242:U:N3    | 85:L5:4281:A:H2    | 2.15                     | 0.45              |
| 85:L5:4299:U:H2'   | 85:L5:4300:U:H6    | 1.80                     | 0.45              |
| 85:L5:4529:G:H2'   | 85:L5:4530:U:C6    | 2.52                     | 0.45              |
| 85:L5:4977:A:H2'   | 85:L5:4978:G:C8    | 2.51                     | 0.45              |
| 85:L5:5056:A:H2'   | 85:L5:5057:C:C6    | 2.51                     | 0.45              |
| 21:L8:142:U:P      | 34:LN:38:ARG:HH22  | 2.39                     | 0.45              |
| 23:LB:94:GLU:N     | 23:LB:158:GLN:OE1  | 2.32                     | 0.45              |
| 25:LD:51:MET:CE    | 25:LD:146:LEU:HB2  | 2.47                     | 0.45              |
| 27:LF:92:VAL:HG23  | 27:LF:114:LEU:HD11 | 1.98                     | 0.45              |
| 29:LH:17:ASP:N     | 29:LH:17:ASP:OD2   | 2.47                     | 0.45              |
| 33:LM:70:GLN:O     | 33:LM:74:ARG:HG3   | 2.16                     | 0.45              |
| 35:LO:109:PRO:C    | 35:LO:111:PRO:HD2  | 2.42                     | 0.45              |
| 35:LO:173:GLN:NE2  | 35:LO:177:LEU:HD11 | 2.31                     | 0.45              |
| 37:LQ:76:GLU:OE1   | 37:LQ:76:GLU:N     | 2.43                     | 0.45              |
| 37:LQ:109:ALA:O    | 37:LQ:113:ILE:HG22 | 2.16                     | 0.45              |
| 38:LR:115:ILE:HD12 | 38:LR:120:TYR:HB2  | 1.98                     | 0.45              |
| 38:LR:149:LYS:O    | 38:LR:149:LYS:HD3  | 2.16                     | 0.45              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 45:LZ:10:VAL:HG13 | 45:LZ:83:THR:HB    | 1.99                     | 0.45              |
| 47:Lb:12:GLN:HB3  | 47:Lb:16:TRP:CH2   | 2.51                     | 0.45              |
| 47:Lb:54:LEU:CA   | 47:Lb:57:MET:HG2   | 2.25                     | 0.45              |
| 49:Ld:29:ILE:H    | 49:Ld:29:ILE:HD12  | 1.81                     | 0.45              |
| 54:Li:25:ARG:NH1  | 54:Li:25:ARG:HA    | 2.32                     | 0.45              |
| 58:Lm:94:MET:CE   | 58:Lm:123:PRO:HA   | 2.47                     | 0.45              |
| 60:Lo:11:PHE:CE1  | 60:Lo:13:LYS:HA    | 2.52                     | 0.45              |
| 60:Lo:31:ASP:OD1  | 60:Lo:38:LYS:HE3   | 2.17                     | 0.45              |
| 63:Lz:48:ARG:HD3  | 63:Lz:48:ARG:HA    | 1.79                     | 0.45              |
| 64:SR:7:LYS:N     | 79:S2:1373:C:OP1   | 2.45                     | 0.45              |
| 64:SR:101:ASP:OD1 | 64:SR:101:ASP:N    | 2.50                     | 0.45              |
| 66:SF:48:TYR:CE2  | 69:SQ:56:LEU:HD13  | 2.48                     | 0.45              |
| 67:SK:76:ILE:CG2  | 67:SK:80:ARG:HH12  | 2.30                     | 0.45              |
| 70:SS:17:ASN:CG   | 70:SS:101:ASN:HD21 | 2.24                     | 0.45              |
| 70:SS:34:LYS:O    | 70:SS:99:LEU:HG    | 2.16                     | 0.45              |
| 71:ST:44:GLU:OE1  | 71:ST:45:LEU:HG    | 2.16                     | 0.45              |
| 75:Sg:60:ARG:NH2  | 79:S2:1397:U:O2'   | 2.50                     | 0.45              |
| 75:Sg:113:PHE:N   | 75:Sg:113:PHE:CD1  | 2.85                     | 0.45              |
| 79:S2:90:G:H2'    | 79:S2:91:A:O4'     | 2.16                     | 0.45              |
| 79:S2:194:C:H2'   | 79:S2:195:C:H6     | 1.80                     | 0.45              |
| 79:S2:303:C:H2'   | 79:S2:304:C:O4'    | 2.17                     | 0.45              |
| 79:S2:1032:C:H2'  | 79:S2:1033:G:O4'   | 2.17                     | 0.45              |
| 79:S2:1180:C:H2'  | 79:S2:1181:A:C8    | 2.52                     | 0.45              |
| 79:S2:1301:A:H2'  | 79:S2:1303:C:C5    | 2.52                     | 0.45              |
| 79:S2:1504:U:H2'  | 79:S2:1505:U:C6    | 2.51                     | 0.45              |
| 79:S2:1597:C:H4'  | 79:S2:1603:G:O6    | 2.16                     | 0.45              |
| 79:S2:1688:C:C2   | 79:S2:1689:C:C5    | 3.04                     | 0.45              |
| 87:IW:4:GLU:CD    | 87:IW:4:GLU:H      | 2.23                     | 0.45              |
| 6:sG:8:PRO:HA     | 79:s2:167:G:H5'    | 1.97                     | 0.45              |
| 6:sG:21:GLU:O     | 6:sG:25:ARG:HG2    | 2.16                     | 0.45              |
| 8:sY:18:LEU:HD12  | 8:sY:85:ASN:HD22   | 1.82                     | 0.45              |
| 8:sY:118:ARG:HH12 | 79:s2:86:C:P       | 2.40                     | 0.45              |
| 10:sA:21:ALA:HB3  | 10:sA:173:LEU:HD22 | 1.97                     | 0.45              |
| 10:sA:37:TYR:HA   | 10:sA:53:ARG:HD3   | 1.99                     | 0.45              |
| 11:sB:203:SER:OG  | 79:s2:1113:A:N3    | 2.43                     | 0.45              |
| 13:sV:7:GLU:OE2   | 13:sV:9:VAL:HB     | 2.17                     | 0.45              |
| 15:sC:60:TRP:HH2  | 15:sC:93:ILE:HG22  | 1.82                     | 0.45              |
| 15:sC:199:PRO:O   | 15:sC:202:THR:HG23 | 2.17                     | 0.45              |
| 17:sO:42:VAL:HG22 | 17:sO:42:VAL:O     | 2.17                     | 0.45              |
| 18:sW:81:VAL:HG21 | 18:sW:104:LEU:HD22 | 1.98                     | 0.45              |
| 20:l7:39:C:C6     | 31:lJ:49:VAL:HG21  | 2.51                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:1A:192:LYS:HB3  | 22:1A:193:ARG:CZ   | 2.47                     | 0.45              |
| 23:1B:40:PRO:O     | 23:1B:42:HIS:HD2   | 2.00                     | 0.45              |
| 23:1B:53:MET:HB3   | 23:1B:77:THR:HA    | 1.99                     | 0.45              |
| 24:1C:289:LEU:HD23 | 24:1C:289:LEU:HA   | 1.83                     | 0.45              |
| 28:1G:34:LYS:HA    | 28:1G:34:LYS:CE    | 2.43                     | 0.45              |
| 28:1G:34:LYS:CE    | 85:15:4129:G:H1'   | 2.44                     | 0.45              |
| 28:1G:143:VAL:O    | 28:1G:147:VAL:HG23 | 2.16                     | 0.45              |
| 33:1M:64:PHE:HB2   | 33:1M:65:PRO:HD2   | 1.98                     | 0.45              |
| 33:1M:100:ARG:HA   | 33:1M:103:LYS:HD3  | 1.98                     | 0.45              |
| 41:1U:70:ILE:HD12  | 41:1U:70:ILE:N     | 2.31                     | 0.45              |
| 41:1U:111:GLU:OE1  | 41:1U:112:LEU:N    | 2.50                     | 0.45              |
| 42:1V:84:GLN:NE2   | 42:1V:86:LYS:O     | 2.27                     | 0.45              |
| 42:1V:112:MET:HE1  | 42:1V:135:ASN:ND2  | 2.31                     | 0.45              |
| 44:1Y:1:MET:HE1    | 85:15:227:A:O5'    | 2.17                     | 0.45              |
| 44:1Y:37:GLU:HG2   | 44:1Y:38:LEU:HD22  | 1.98                     | 0.45              |
| 46:1a:98:ALA:HB1   | 46:1a:122:VAL:HA   | 1.98                     | 0.45              |
| 52:1g:83:CYS:O     | 52:1g:87:VAL:HG23  | 2.17                     | 0.45              |
| 56:1k:51:GLU:N     | 56:1k:51:GLU:OE1   | 2.50                     | 0.45              |
| 57:1l:38:ASN:O     | 57:1l:41:ARG:HG3   | 2.17                     | 0.45              |
| 63:1z:62:LYS:HD2   | 63:1z:62:LYS:HA    | 1.64                     | 0.45              |
| 65:sD:90:LYS:HD3   | 65:sD:91:VAL:N     | 2.31                     | 0.45              |
| 66:sF:168:THR:HG22 | 79:s2:1535:U:OP2   | 2.17                     | 0.45              |
| 68:sP:118:GLU:HA   | 68:sP:118:GLU:OE2  | 2.16                     | 0.45              |
| 70:sS:70:ILE:HG23  | 70:sS:77:TYR:CE2   | 2.52                     | 0.45              |
| 74:sd:8:TRP:HZ3    | 74:sd:12:ARG:CZ    | 2.30                     | 0.45              |
| 76:sM:82:ASN:OD1   | 76:sM:82:ASN:N     | 2.49                     | 0.45              |
| 76:sM:106:CYS:HG   | 79:s2:1284:A:HO2'  | 1.62                     | 0.45              |
| 79:s2:72:C:N4      | 79:s2:74:G:H22     | 2.14                     | 0.45              |
| 79:s2:535:G:H5''   | 79:s2:536:A:OP2    | 2.17                     | 0.45              |
| 79:s2:943:U:H2'    | 79:s2:944:A:O4'    | 2.17                     | 0.45              |
| 79:s2:1329:U:O2'   | 79:s2:1332:A:OP2   | 2.28                     | 0.45              |
| 79:s2:1642:U:H2'   | 79:s2:1643:U:C6    | 2.51                     | 0.45              |
| 80:cB:100:ILE:HD11 | 80:cB:354:ILE:HD11 | 1.98                     | 0.45              |
| 80:cB:141:THR:C    | 80:cB:145:GLN:HE22 | 2.23                     | 0.45              |
| 80:cB:183:GLU:O    | 80:cB:187:VAL:HG23 | 2.16                     | 0.45              |
| 80:cB:259:LYS:HA   | 80:cB:264:ARG:HH11 | 1.81                     | 0.45              |
| 80:cB:456:ARG:HD3  | 80:cB:456:ARG:N    | 2.32                     | 0.45              |
| 80:cB:730:TYR:HA   | 80:cB:733:VAL:HG12 | 1.98                     | 0.45              |
| 82:pE:39:U:H2'     | 82:pE:40:C:C6      | 2.52                     | 0.45              |
| 83:ls:64:ALA:HA    | 83:ls:68:HIS:ND1   | 2.32                     | 0.45              |
| 83:ls:125:ALA:HA   | 83:ls:154:ILE:HG23 | 1.98                     | 0.45              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 85:l5:106:A:H2'   | 85:l5:107:G:O4'    | 2.16                     | 0.45              |
| 85:l5:120:A:H2'   | 85:l5:149:A:H61    | 1.82                     | 0.45              |
| 85:l5:318:A:H2'   | 85:l5:319:A:C8     | 2.52                     | 0.45              |
| 85:l5:505:G:C6    | 85:l5:654:C:C2     | 3.05                     | 0.45              |
| 85:l5:1405:C:N3   | 85:l5:1413:C:N4    | 2.65                     | 0.45              |
| 85:l5:1406:G:N1   | 85:l5:1411:C:O2'   | 2.38                     | 0.45              |
| 85:l5:1459:A:H2'  | 85:l5:1460:C:O4'   | 2.17                     | 0.45              |
| 85:l5:1644:C:C2   | 85:l5:1645:C:C5    | 3.04                     | 0.45              |
| 85:l5:1833:G:C2   | 85:l5:1835:G:C4    | 3.05                     | 0.45              |
| 85:l5:1914:C:OP2  | 85:l5:1915:C:O2'   | 2.28                     | 0.45              |
| 85:l5:2532:C:H2'  | 85:l5:2533:C:C6    | 2.52                     | 0.45              |
| 85:l5:2610:G:H2'  | 85:l5:2611:A:C8    | 2.51                     | 0.45              |
| 85:l5:3762:U:C2   | 85:l5:3763:A:C8    | 3.05                     | 0.45              |
| 85:l5:3953:G:H8   | 85:l5:3953:G:OP2   | 2.00                     | 0.45              |
| 85:l5:3972:A:H2'  | 85:l5:4041:C:N4    | 2.31                     | 0.45              |
| 85:l5:4171:C:C2   | 85:l5:4172:A:C8    | 3.04                     | 0.45              |
| 80:CB:48:SER:C    | 80:CB:55:ARG:HH22  | 2.24                     | 0.45              |
| 3:SI:41:ARG:HA    | 3:SI:59:ARG:O      | 2.15                     | 0.45              |
| 3:SI:162:LEU:HD12 | 3:SI:162:LEU:HA    | 1.79                     | 0.45              |
| 6:SG:129:VAL:HG13 | 87:LW:80:ARG:HH22  | 1.82                     | 0.45              |
| 7:SJ:114:VAL:HG13 | 7:SJ:126:ALA:HB1   | 1.98                     | 0.45              |
| 8:SY:93:ARG:NE    | 79:S2:575:A:OP1    | 2.50                     | 0.45              |
| 11:SB:70:SER:O    | 11:SB:74:LEU:HB2   | 2.16                     | 0.45              |
| 11:SB:103:MET:HB3 | 11:SB:215:VAL:CG1  | 2.47                     | 0.45              |
| 12:SH:70:LYS:HA   | 12:SH:70:LYS:HD2   | 1.83                     | 0.45              |
| 12:SH:172:THR:O   | 12:SH:176:VAL:HG12 | 2.16                     | 0.45              |
| 16:SN:105:ASN:OD1 | 79:S2:936:G:O2'    | 2.19                     | 0.45              |
| 18:SW:83:LEU:HD11 | 18:SW:120:HIS:HA   | 1.99                     | 0.45              |
| 85:L5:269:G:H2'   | 85:L5:270:U:C6     | 2.51                     | 0.45              |
| 85:L5:370:U:C4    | 85:L5:1637:A:C5    | 3.04                     | 0.45              |
| 85:L5:1315:C:H2'  | 85:L5:1316:G:C8    | 2.51                     | 0.45              |
| 85:L5:1350:C:H2'  | 85:L5:1351:G:H8    | 1.81                     | 0.45              |
| 85:L5:1449:C:H2'  | 85:L5:1450:C:H6    | 1.81                     | 0.45              |
| 85:L5:1600:A:C6   | 85:L5:1638:A:C5    | 3.05                     | 0.45              |
| 85:L5:1719:A:H2'  | 85:L5:1720:C:C6    | 2.51                     | 0.45              |
| 85:L5:1741:G:O2'  | 85:L5:1781:U:OP2   | 2.26                     | 0.45              |
| 85:L5:2033:A:O2'  | 85:L5:2034:G:O5'   | 2.29                     | 0.45              |
| 85:L5:2293:U:H2'  | 85:L5:2294:G:H8    | 1.82                     | 0.45              |
| 85:L5:2319:C:OP2  | 50:Le:62:SER:OG    | 2.27                     | 0.45              |
| 85:L5:2608:G:H2'  | 85:L5:2609:G:C8    | 2.50                     | 0.45              |
| 85:L5:2616:C:C2   | 85:L5:2722:G:N2    | 2.85                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 85:L5:2874:U:O2'   | 85:L5:2876:G:N7    | 2.46                     | 0.45              |
| 85:L5:4091:G:N2    | 85:L5:4159:C:C2    | 2.84                     | 0.45              |
| 85:L5:4092:G:H3'   | 85:L5:4093:G:H21   | 1.81                     | 0.45              |
| 85:L5:4596:C:C4    | 85:L5:4597:U:C4    | 3.05                     | 0.45              |
| 85:L5:4768:G:H5''  | 35:LO:172:LYS:HE3  | 1.98                     | 0.45              |
| 21:L8:75:G:H2'     | 21:L8:76:C:H6      | 1.82                     | 0.45              |
| 24:LC:182:LYS:HD3  | 24:LC:204:ARG:NH1  | 2.31                     | 0.45              |
| 24:LC:267:TRP:NE1  | 24:LC:279:LEU:HB3  | 2.32                     | 0.45              |
| 25:LD:80:ALA:HB1   | 25:LD:92:LEU:HD23  | 1.98                     | 0.45              |
| 25:LD:256:LYS:HA   | 25:LD:256:LYS:HD2  | 1.64                     | 0.45              |
| 32:LL:57:PRO:HG3   | 32:LL:75:GLY:C     | 2.41                     | 0.45              |
| 32:LL:198:ARG:HA   | 32:LL:201:GLU:HG3  | 1.98                     | 0.45              |
| 37:LQ:18:PRO:HB3   | 37:LQ:52:PHE:HA    | 1.99                     | 0.45              |
| 37:LQ:66:MET:SD    | 37:LQ:67:ILE:N     | 2.89                     | 0.45              |
| 37:LQ:187:LYS:C    | 37:LQ:188:ASN:HD22 | 2.24                     | 0.45              |
| 38:LR:99:MET:SD    | 38:LR:99:MET:C     | 3.00                     | 0.45              |
| 38:LR:99:MET:HE3   | 38:LR:99:MET:HB3   | 1.74                     | 0.45              |
| 39:LS:29:ARG:HH21  | 40:LT:150:LEU:HB2  | 1.82                     | 0.45              |
| 40:LT:111:GLU:O    | 40:LT:114:GLN:HG2  | 2.16                     | 0.45              |
| 41:LU:24:ASP:OD1   | 41:LU:26:THR:HG23  | 2.16                     | 0.45              |
| 42:LV:20:LEU:HD23  | 42:LV:20:LEU:HA    | 1.65                     | 0.45              |
| 51:Lf:46:ARG:HD3   | 51:Lf:71:TRP:CE3   | 2.52                     | 0.45              |
| 58:Lm:94:MET:HA    | 58:Lm:94:MET:CE    | 2.38                     | 0.45              |
| 62:Lr:97:ILE:HD11  | 62:Lr:104:PRO:HA   | 1.99                     | 0.45              |
| 65:SD:24:PHE:CE2   | 67:SK:68:TYR:CE1   | 3.05                     | 0.45              |
| 67:SK:3:MET:HG2    | 67:SK:44:HIS:CD2   | 2.51                     | 0.45              |
| 70:SS:71:MET:SD    | 70:SS:99:LEU:HD13  | 2.56                     | 0.45              |
| 71:ST:29:LYS:HG2   | 71:ST:106:ALA:HA   | 1.98                     | 0.45              |
| 71:ST:110:LEU:O    | 71:ST:111:LYS:HG2  | 2.15                     | 0.45              |
| 71:ST:134:ILE:CA   | 71:ST:137:GLN:OE1  | 2.59                     | 0.45              |
| 73:Sc:24:GLN:HA    | 79:S2:1681:U:H1'   | 1.99                     | 0.45              |
| 75:Sg:85:GLY:N     | 75:Sg:107:ASP:HA   | 2.31                     | 0.45              |
| 78:Sf:108:VAL:HG13 | 78:Sf:112:GLY:HA2  | 1.99                     | 0.45              |
| 79:S2:561:A:H2'    | 79:S2:562:U:O4'    | 2.16                     | 0.45              |
| 79:S2:610:G:C4     | 79:S2:611:G:C8     | 3.05                     | 0.45              |
| 79:S2:1395:C:H1'   | 79:S2:1474:A:C5    | 2.51                     | 0.45              |
| 79:S2:1749:G:H2'   | 79:S2:1750:C:C6    | 2.51                     | 0.45              |
| 81:AP:60:A:P       | 81:AP:61:C:H41     | 2.39                     | 0.45              |
| 87:LW:57:ARG:O     | 87:LW:60:LYS:HD2   | 2.16                     | 0.45              |
| 1:CH:121:LEU:HD21  | 1:CH:132:LEU:CD2   | 2.47                     | 0.45              |
| 3:sI:83:TYR:HD2    | 3:sI:101:ILE:HD13  | 1.81                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:sJ:46:VAL:HG21   | 7:sJ:106:LEU:HD11  | 1.97                     | 0.45              |
| 8:sY:43:LYS:HE2    | 8:sY:43:LYS:HB3    | 1.72                     | 0.45              |
| 8:sY:103:SER:N     | 8:sY:106:GLN:OE1   | 2.49                     | 0.45              |
| 9:se:11:LYS:HE2    | 9:se:15:GLN:NE2    | 2.28                     | 0.45              |
| 10:sA:90:PHE:C     | 10:sA:90:PHE:HD1   | 2.25                     | 0.45              |
| 11:sB:108:ASP:O    | 14:sa:68:TYR:HE2   | 2.00                     | 0.45              |
| 12:sH:18:GLU:OE2   | 12:sH:18:GLU:N     | 2.39                     | 0.45              |
| 12:sH:119:SER:O    | 79:s2:913:A:N6     | 2.50                     | 0.45              |
| 13:sV:21:ASN:HD21  | 18:sW:67:GLY:C     | 2.24                     | 0.45              |
| 13:sV:38:GLU:OE1   | 13:sV:47:ASN:ND2   | 2.39                     | 0.45              |
| 13:sV:46:PHE:HD1   | 13:sV:48:GLY:N     | 2.15                     | 0.45              |
| 13:sV:66:ASP:HA    | 13:sV:69:ILE:HD11  | 1.99                     | 0.45              |
| 16:sN:18:TYR:CD1   | 16:sN:18:TYR:O     | 2.70                     | 0.45              |
| 16:sN:123:HIS:ND1  | 85:l5:1563:A:O2'   | 2.50                     | 0.45              |
| 20:l7:60:G:C2      | 20:l7:61:G:C8      | 3.05                     | 0.45              |
| 20:l7:64:G:H2'     | 20:l7:65:G:C8      | 2.51                     | 0.45              |
| 20:l7:75:G:N2      | 20:l7:100:A:OP2    | 2.49                     | 0.45              |
| 22:lA:132:ASN:O    | 22:lA:169:VAL:HG12 | 2.16                     | 0.45              |
| 25:ID:289:ARG:CZ   | 85:l5:1179:U:H5'   | 2.47                     | 0.45              |
| 26:lE:223:ARG:HA   | 26:lE:224:LYS:HA   | 1.62                     | 0.45              |
| 27:lF:96:ARG:NH1   | 27:lF:224:THR:HA   | 2.31                     | 0.45              |
| 29:lH:12:ILE:HG22  | 29:lH:16:VAL:HG23  | 1.99                     | 0.45              |
| 29:lH:107:GLU:OE1  | 29:lH:107:GLU:N    | 2.49                     | 0.45              |
| 34:lN:172:ARG:NH2  | 85:l5:28:C:O3'     | 2.49                     | 0.45              |
| 34:lN:185:GLY:H    | 34:lN:191:ALA:HB2  | 1.81                     | 0.45              |
| 37:lQ:113:ILE:HG21 | 37:lQ:120:ILE:HD11 | 1.99                     | 0.45              |
| 38:lR:38:ARG:O     | 38:lR:39:GLN:HG3   | 2.17                     | 0.45              |
| 44:lY:54:GLU:N     | 44:lY:54:GLU:OE1   | 2.50                     | 0.45              |
| 47:lb:101:HIS:CD2  | 47:lb:104:LEU:HD22 | 2.52                     | 0.45              |
| 53:lh:3:LYS:NZ     | 53:lh:4:ILE:O      | 2.49                     | 0.45              |
| 53:lh:98:HIS:HA    | 53:lh:101:ASN:HD21 | 1.81                     | 0.45              |
| 61:lp:80:LYS:O     | 61:lp:83:ILE:HG22  | 2.17                     | 0.45              |
| 62:lr:58:LYS:HG3   | 62:lr:83:ASN:OD1   | 2.17                     | 0.45              |
| 63:lz:198:TRP:CG   | 63:lz:199:GLN:N    | 2.85                     | 0.45              |
| 65:sD:162:ASP:N    | 65:sD:163:PRO:HD2  | 2.32                     | 0.45              |
| 68:sP:34:MET:O     | 68:sP:42:ARG:HD3   | 2.16                     | 0.45              |
| 68:sP:40:ARG:NH2   | 79:s2:1616:U:O4    | 2.34                     | 0.45              |
| 69:sQ:104:SER:O    | 69:sQ:107:GLU:HG2  | 2.17                     | 0.45              |
| 70:sS:51:ASP:OD2   | 70:sS:54:LYS:HE3   | 2.16                     | 0.45              |
| 71:sT:33:TRP:HZ3   | 79:s2:1567:G:OP2   | 1.99                     | 0.45              |
| 79:s2:318:A:C6     | 79:s2:333:G:C6     | 3.05                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 79:s2:644:G:H2'    | 79:s2:645:C:C6     | 2.51                     | 0.45              |
| 79:s2:976:G:H2'    | 79:s2:977:C:C6     | 2.52                     | 0.45              |
| 79:s2:1165:G:H4'   | 79:s2:1166:G:H5''  | 1.99                     | 0.45              |
| 79:s2:1263:U:H5''  | 79:s2:1264:C:H2'   | 1.99                     | 0.45              |
| 79:s2:1354:G:OP1   | 79:s2:1354:G:H4'   | 2.17                     | 0.45              |
| 80:cB:226:LYS:HG2  | 80:cB:227:GLN:HE22 | 1.81                     | 0.45              |
| 83:ls:23:ASP:O     | 83:ls:92:LYS:NZ    | 2.49                     | 0.45              |
| 85:l5:223:G:H4'    | 85:l5:225:G:C8     | 2.52                     | 0.45              |
| 85:l5:1460:C:H2'   | 85:l5:1461:C:H6    | 1.82                     | 0.45              |
| 85:l5:1666:C:H2'   | 85:l5:1667:G:O4'   | 2.17                     | 0.45              |
| 85:l5:1995:G:C5    | 85:l5:1996:C:C4    | 3.04                     | 0.45              |
| 85:l5:2638:G:O2'   | 85:l5:2639:U:O4'   | 2.32                     | 0.45              |
| 85:l5:4208:U:H2'   | 85:l5:4209:G:C8    | 2.52                     | 0.45              |
| 85:l5:4629:U:H2'   | 85:l5:4630:G:C8    | 2.50                     | 0.45              |
| 85:l5:4752:U:H2'   | 85:l5:4753:U:C6    | 2.52                     | 0.45              |
| 85:l5:4890:G:C4    | 85:l5:4891:G:C8    | 3.05                     | 0.45              |
| 85:l5:4899:G:C6    | 85:l5:4922:C:N4    | 2.84                     | 0.45              |
| 85:l5:4901:G:H2'   | 85:l5:4902:C:O4'   | 2.17                     | 0.45              |
| 80:CB:378:ASP:HA   | 80:CB:383:MET:HE1  | 1.99                     | 0.45              |
| 2:SE:31:PRO:HA     | 2:SE:81:THR:HB     | 1.98                     | 0.45              |
| 2:SE:192:ILE:HD11  | 2:SE:242:LYS:O     | 2.17                     | 0.45              |
| 3:SI:19:LYS:NZ     | 79:S2:101:U:H5''   | 2.31                     | 0.45              |
| 3:SI:124:LYS:HB3   | 3:SI:125:LYS:NZ    | 2.32                     | 0.45              |
| 4:SL:32:LYS:HD3    | 4:SL:33:LEU:O      | 2.15                     | 0.45              |
| 6:SG:200:LYS:HZ2   | 6:SG:204:GLU:HG2   | 1.82                     | 0.45              |
| 7:SJ:45:ARG:O      | 7:SJ:49:THR:HG23   | 2.17                     | 0.45              |
| 11:SB:157:GLN:HE22 | 11:SB:159:GLN:CG   | 2.29                     | 0.45              |
| 11:SB:171:ILE:CD1  | 11:SB:197:ILE:HG13 | 2.47                     | 0.45              |
| 15:SC:96:PHE:C     | 15:SC:96:PHE:CD1   | 2.94                     | 0.45              |
| 17:SO:38:ASN:O     | 17:SO:68:GLU:HB2   | 2.17                     | 0.45              |
| 17:SO:64:ALA:HB3   | 17:SO:67:ASP:OD1   | 2.17                     | 0.45              |
| 18:SW:23:ARG:C     | 18:SW:23:ARG:CD    | 2.90                     | 0.45              |
| 18:SW:115:GLU:O    | 18:SW:119:LYS:N    | 2.38                     | 0.45              |
| 85:L5:280:G:N2     | 85:L5:305:A:H2'    | 2.31                     | 0.45              |
| 85:L5:700:G:N1     | 85:L5:701:G:C6     | 2.84                     | 0.45              |
| 85:L5:751:G:H2'    | 85:L5:752:G:O4'    | 2.17                     | 0.45              |
| 85:L5:926:G:H2'    | 85:L5:927:G:C8     | 2.51                     | 0.45              |
| 85:L5:986:C:H2'    | 85:L5:987:C:C6     | 2.52                     | 0.45              |
| 85:L5:1294:A:H1'   | 85:L5:1296:G:N1    | 2.31                     | 0.45              |
| 85:L5:1458:C:H2'   | 85:L5:1459:A:O4'   | 2.17                     | 0.45              |
| 85:L5:1839:U:H2'   | 85:L5:1840:G:C8    | 2.52                     | 0.45              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 85:L5:2045:G:O6   | 35:LO:62:MET:HB2   | 2.17                     | 0.45              |
| 85:L5:2372:U:H2'  | 85:L5:2373:C:H6    | 1.82                     | 0.45              |
| 85:L5:2710:C:N3   | 85:L5:2712:G:C8    | 2.85                     | 0.45              |
| 85:L5:3700:C:O2'  | 85:L5:3774:A:H1'   | 2.17                     | 0.45              |
| 85:L5:4102:C:C2   | 85:L5:4102:C:C1'   | 2.94                     | 0.45              |
| 85:L5:4146:G:H2'  | 85:L5:4147:G:C8    | 2.51                     | 0.45              |
| 85:L5:4299:U:H2'  | 85:L5:4300:U:C6    | 2.52                     | 0.45              |
| 85:L5:4578:G:C6   | 85:L5:4726:G:C6    | 3.05                     | 0.45              |
| 85:L5:4619:U:H2'  | 85:L5:4620:U:C6    | 2.51                     | 0.45              |
| 85:L5:4968:A:H2'  | 85:L5:4969:C:H6    | 1.82                     | 0.45              |
| 20:L7:63:C:N4     | 30:LI:202:SER:HA   | 2.32                     | 0.45              |
| 21:L8:60:G:C8     | 53:Lh:58:LEU:HD13  | 2.52                     | 0.45              |
| 23:LB:216:MET:HE3 | 23:LB:350:SER:HB2  | 1.99                     | 0.45              |
| 24:LC:117:THR:HA  | 24:LC:120:LYS:HD3  | 1.99                     | 0.45              |
| 24:LC:211:TYR:CE1 | 24:LC:229:LEU:HB3  | 2.51                     | 0.45              |
| 28:LG:50:ASP:HB2  | 43:LX:40:ILE:HD11  | 1.99                     | 0.45              |
| 31:LJ:18:ARG:HG3  | 31:LJ:134:LEU:C    | 2.42                     | 0.45              |
| 33:LM:46:ARG:O    | 33:LM:48:GLN:NE2   | 2.33                     | 0.45              |
| 36:LP:92:LEU:HD23 | 36:LP:92:LEU:HA    | 1.78                     | 0.45              |
| 43:LX:91:GLU:HA   | 43:LX:147:LEU:HD21 | 1.99                     | 0.45              |
| 44:LY:24:HIS:NE2  | 44:LY:25:ILE:HG23  | 2.32                     | 0.45              |
| 50:Le:43:ASN:OD1  | 50:Le:46:ARG:N     | 2.34                     | 0.45              |
| 52:Lg:20:THR:OG1  | 52:Lg:21:ARG:N     | 2.50                     | 0.45              |
| 54:Li:84:LYS:O    | 54:Li:87:ARG:HG2   | 2.17                     | 0.45              |
| 66:SF:20:PHE:HE2  | 66:SF:94:LYS:HB2   | 1.82                     | 0.45              |
| 66:SF:101:HIS:CD2 | 66:SF:105:GLY:HA2  | 2.48                     | 0.45              |
| 70:SS:113:ARG:O   | 70:SS:117:ILE:HB   | 2.17                     | 0.45              |
| 73:Sc:28:THR:O    | 73:Sc:45:ASN:HA    | 2.17                     | 0.45              |
| 76:SM:45:ARG:CZ   | 76:SM:72:HIS:ND1   | 2.80                     | 0.45              |
| 79:S2:105:U:H2'   | 79:S2:106:C:O4'    | 2.16                     | 0.45              |
| 79:S2:859:G:H2'   | 79:S2:860:G:C8     | 2.52                     | 0.45              |
| 79:S2:870:A:H5'   | 79:S2:915:G:H22    | 1.82                     | 0.45              |
| 79:S2:872:A:C6    | 79:S2:915:G:C5     | 3.05                     | 0.45              |
| 79:S2:1030:A:H2'  | 79:S2:1031:A:H8    | 1.81                     | 0.45              |
| 79:S2:1134:G:H2'  | 79:S2:1135:C:C6    | 2.52                     | 0.45              |
| 79:S2:1207:G:C6   | 79:S2:1837:G:C6    | 3.05                     | 0.45              |
| 79:S2:1393:G:H2'  | 79:S2:1394:G:C8    | 2.51                     | 0.45              |
| 79:S2:1616:U:O2'  | 79:S2:1661:A:N3    | 2.45                     | 0.45              |
| 82:PE:25:C:C5     | 82:PE:26:A:C8      | 3.05                     | 0.45              |
| 1:cH:147:ALA:O    | 79:s2:553:U:H4'    | 2.17                     | 0.45              |
| 2:sE:66:MET:HE1   | 79:s2:502:C:C6     | 2.51                     | 0.45              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 5:sX:58:GLU:HG2   | 5:sX:59:ALA:O      | 2.17                     | 0.45              |
| 5:sX:60:LYS:HD2   | 5:sX:60:LYS:HA     | 1.74                     | 0.45              |
| 6:sG:85:ARG:O     | 6:sG:87:ARG:NH1    | 2.48                     | 0.45              |
| 10:sA:184:ARG:HB2 | 10:sA:191:ARG:NH1  | 2.32                     | 0.45              |
| 11:sB:40:ASN:OD1  | 11:sB:75:GLN:HA    | 2.17                     | 0.45              |
| 11:sB:187:LYS:O   | 11:sB:190:PRO:HD2  | 2.16                     | 0.45              |
| 12:sH:50:GLU:HG3  | 12:sH:60:ILE:HD12  | 1.99                     | 0.45              |
| 12:sH:154:ILE:HB  | 12:sH:185:VAL:HG13 | 1.98                     | 0.45              |
| 15:sC:139:LEU:N   | 15:sC:161:SER:OG   | 2.49                     | 0.45              |
| 18:sW:107:SER:HA  | 79:s2:862:A:C8     | 2.52                     | 0.45              |
| 20:l7:3:C:H2'     | 20:l7:4:U:C6       | 2.52                     | 0.45              |
| 24:lC:116:ASN:ND2 | 85:l5:1506:G:N3    | 2.58                     | 0.45              |
| 25:lD:40:ASP:OD2  | 40:lT:69:GLN:HG3   | 2.17                     | 0.45              |
| 26:lE:203:ILE:CD1 | 26:lE:206:VAL:HG11 | 2.47                     | 0.45              |
| 29:lH:51:LYS:HE3  | 29:lH:52:LYS:HG3   | 1.99                     | 0.45              |
| 29:lH:137:SER:HB3 | 29:lH:143:GLU:HB2  | 1.99                     | 0.45              |
| 32:lL:8:MET:HB2   | 85:l5:1344:C:O2'   | 2.17                     | 0.45              |
| 32:lL:123:LYS:O   | 53:lh:122:LYS:HG2  | 2.17                     | 0.45              |
| 33:lM:13:ALA:HB1  | 33:lM:55:MET:HB2   | 1.99                     | 0.45              |
| 34:lN:195:ARG:NH1 | 34:lN:195:ARG:HB3  | 2.32                     | 0.45              |
| 39:lS:111:ARG:NH2 | 85:l5:2062:C:O2'   | 2.50                     | 0.45              |
| 40:lT:158:PHE:HE1 | 40:lT:160:ALA:O    | 2.00                     | 0.45              |
| 43:lX:89:LYS:HE3  | 85:l5:2437:C:N3    | 2.32                     | 0.45              |
| 43:lX:117:TYR:CE2 | 43:lX:153:ILE:HD12 | 2.52                     | 0.45              |
| 51:lf:28:LEU:O    | 51:lf:83:MET:HA    | 2.15                     | 0.45              |
| 55:lj:34:CYS:SG   | 55:lj:35:GLY:N     | 2.89                     | 0.45              |
| 56:lk:25:ILE:HG13 | 56:lk:68:GLU:HG3   | 1.99                     | 0.45              |
| 60:lo:27:LYS:HE2  | 60:lo:27:LYS:HB3   | 1.73                     | 0.45              |
| 60:lo:36:GLN:HA   | 60:lo:39:ARG:NH1   | 2.32                     | 0.45              |
| 60:lo:41:TYR:OH   | 60:lo:45:GLN:NE2   | 2.49                     | 0.45              |
| 68:sP:115:TYR:OH  | 79:s2:1620:A:OP1   | 2.35                     | 0.45              |
| 69:sQ:44:PRO:HB3  | 79:s2:1592:C:O2'   | 2.16                     | 0.45              |
| 69:sQ:85:ARG:O    | 69:sQ:88:ILE:HG13  | 2.17                     | 0.45              |
| 70:sS:47:LYS:NZ   | 70:sS:77:TYR:O     | 2.42                     | 0.45              |
| 71:sT:121:ARG:NH2 | 79:s2:1563:G:O3'   | 2.50                     | 0.45              |
| 72:sU:56:MET:HG3  | 72:sU:57:PRO:HD2   | 1.99                     | 0.45              |
| 75:sg:17:TRP:CZ3  | 75:sg:303:THR:HG22 | 2.52                     | 0.45              |
| 75:sg:36:ARG:HD3  | 75:sg:65:PHE:CG    | 2.52                     | 0.45              |
| 75:sg:114:SER:CB  | 75:sg:119:GLN:H    | 2.30                     | 0.45              |
| 76:sM:18:LEU:O    | 76:sM:21:VAL:HG12  | 2.16                     | 0.45              |
| 76:sM:96:ARG:HA   | 76:sM:96:ARG:NE    | 2.31                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 79:s2:328:U:H5''   | 87:1W:113:LYS:NZ   | 2.32                     | 0.45              |
| 79:s2:480:G:H5'    | 80:cB:407:LYS:HZ2  | 1.82                     | 0.45              |
| 79:s2:694:G:N7     | 79:s2:696:G:N2     | 2.65                     | 0.45              |
| 79:s2:818:A:H2'    | 79:s2:819:G:C8     | 2.51                     | 0.45              |
| 79:s2:1100:A:H61   | 79:s2:1132:C:N4    | 2.14                     | 0.45              |
| 79:s2:1102:G:C6    | 79:s2:1131:G:C6    | 3.05                     | 0.45              |
| 79:s2:1770:G:O3'   | 79:s2:1771:G:N2    | 2.42                     | 0.45              |
| 80:cB:394:LEU:N    | 80:cB:487:THR:OG1  | 2.50                     | 0.45              |
| 85:l5:27:C:C2      | 85:l5:56:A:N1      | 2.85                     | 0.45              |
| 85:l5:248:C:H2'    | 85:l5:249:C:H6     | 1.81                     | 0.45              |
| 85:l5:455:C:O2'    | 85:l5:456:C:H5'    | 2.17                     | 0.45              |
| 85:l5:710:G:H2'    | 85:l5:711:A:C8     | 2.52                     | 0.45              |
| 85:l5:1340:C:H2'   | 85:l5:1341:U:H6    | 1.80                     | 0.45              |
| 85:l5:1719:A:H2'   | 85:l5:1720:C:C6    | 2.52                     | 0.45              |
| 85:l5:2329:U:H2'   | 85:l5:2330:G:C8    | 2.52                     | 0.45              |
| 85:l5:2535:G:H2'   | 85:l5:2536:A:C8    | 2.51                     | 0.45              |
| 85:l5:2602:G:O4'   | 85:l5:2742:G:H2'   | 2.17                     | 0.45              |
| 85:l5:2804:C:H2'   | 85:l5:2805:C:C6    | 2.51                     | 0.45              |
| 85:l5:3671:G:H2'   | 85:l5:3672:G:C2    | 2.52                     | 0.45              |
| 85:l5:3795:A:H2'   | 85:l5:3796:U:C6    | 2.52                     | 0.45              |
| 85:l5:4989:U:H1'   | 85:l5:4990:C:C5    | 2.46                     | 0.45              |
| 80:CB:44:GLY:HA2   | 80:CB:77:LEU:HD22  | 1.99                     | 0.45              |
| 80:CB:58:ASP:HB3   | 80:CB:63:GLU:HB3   | 1.98                     | 0.45              |
| 80:CB:62:ASP:H     | 80:CB:64:GLN:HE22  | 1.64                     | 0.45              |
| 80:CB:289:PHE:HA   | 80:CB:293:ILE:HD13 | 1.98                     | 0.45              |
| 80:CB:649:ILE:HG21 | 80:CB:652:PHE:CE1  | 2.52                     | 0.45              |
| 4:SL:36:TYR:OH     | 79:S2:294:U:OP1    | 2.30                     | 0.45              |
| 5:SX:17:ARG:O      | 5:SX:21:LYS:N      | 2.49                     | 0.45              |
| 7:SJ:17:ARG:HH22   | 7:SJ:18:ARG:HB2    | 1.80                     | 0.45              |
| 7:SJ:136:ARG:HG2   | 7:SJ:140:GLN:O     | 2.17                     | 0.45              |
| 10:SA:8:LEU:O      | 10:SA:8:LEU:HD12   | 2.16                     | 0.45              |
| 10:SA:33:GLN:NE2   | 13:SV:64:GLU:CD    | 2.74                     | 0.45              |
| 10:SA:108:PHE:HB2  | 10:SA:136:GLU:OE1  | 2.16                     | 0.45              |
| 11:SB:73:ASP:OD2   | 17:SO:128:ARG:NH2  | 2.50                     | 0.45              |
| 11:SB:222:LYS:HZ3  | 11:SB:224:GLU:HA   | 1.82                     | 0.45              |
| 12:SH:135:PHE:HD2  | 12:SH:136:PRO:HD3  | 1.82                     | 0.45              |
| 12:SH:139:ILE:HD12 | 12:SH:156:VAL:HG21 | 1.99                     | 0.45              |
| 16:SN:4:MET:SD     | 16:SN:5:HIS:CE1    | 3.10                     | 0.45              |
| 85:L5:370:U:O2'    | 55:Lj:16:HIS:ND1   | 2.27                     | 0.45              |
| 85:L5:474:C:H2'    | 85:L5:475:G:C8     | 2.52                     | 0.45              |
| 85:L5:705:G:H2'    | 85:L5:706:C:H6     | 1.81                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 85:L5:1170:G:O6    | 85:L5:1192:C:N4    | 2.49                     | 0.45              |
| 85:L5:1327:C:H2'   | 85:L5:1328:G:C8    | 2.52                     | 0.45              |
| 85:L5:1338:G:H4'   | 85:L5:1339:U:H6    | 1.82                     | 0.45              |
| 85:L5:1609:U:H2'   | 85:L5:1610:C:O4'   | 2.17                     | 0.45              |
| 85:L5:1726:U:H4'   | 27:LF:132:MET:HE1  | 1.99                     | 0.45              |
| 85:L5:1795:A:H2'   | 85:L5:1796:U:O4'   | 2.16                     | 0.45              |
| 85:L5:1797:G:H2'   | 85:L5:1798:G:H8    | 1.81                     | 0.45              |
| 85:L5:1946:G:O2'   | 85:L5:1948:G:OP2   | 2.30                     | 0.45              |
| 85:L5:2318:G:N1    | 85:L5:2322:G:C6    | 2.85                     | 0.45              |
| 85:L5:2556:G:H2'   | 85:L5:2557:G:H8    | 1.82                     | 0.45              |
| 85:L5:2615:C:H2'   | 85:L5:2616:C:H6    | 1.80                     | 0.45              |
| 85:L5:3600:G:H2'   | 85:L5:3601:C:C6    | 2.51                     | 0.45              |
| 85:L5:4411:G:H2'   | 85:L5:4412:C:H6    | 1.81                     | 0.45              |
| 85:L5:5024:C:N4    | 85:L5:5028:G:N3    | 2.42                     | 0.45              |
| 20:L7:7:G:C8       | 25:LD:22:ARG:HD2   | 2.52                     | 0.45              |
| 21:L8:6:C:C2       | 21:L8:7:U:C5       | 3.05                     | 0.45              |
| 24:LC:281:MET:N    | 24:LC:281:MET:SD   | 2.89                     | 0.45              |
| 25:LD:234:ASP:O    | 25:LD:235:MET:SD   | 2.74                     | 0.45              |
| 29:LH:105:ILE:HG23 | 29:LH:112:VAL:HG12 | 1.98                     | 0.45              |
| 31:LJ:39:VAL:HA    | 31:LJ:42:GLN:OE1   | 2.17                     | 0.45              |
| 37:LQ:149:TYR:CD1  | 37:LQ:152:PHE:HD2  | 2.34                     | 0.45              |
| 39:LS:95:ARG:HD2   | 39:LS:113:MET:CE   | 2.47                     | 0.45              |
| 40:LT:14:MET:HE1   | 40:LT:58:HIS:HD1   | 1.82                     | 0.45              |
| 43:LX:84:GLU:HA    | 43:LX:87:MET:CE    | 2.46                     | 0.45              |
| 43:LX:148:ASP:OD2  | 43:LX:149:VAL:N    | 2.50                     | 0.45              |
| 48:Lc:47:ILE:HB    | 48:Lc:94:LEU:HD21  | 1.99                     | 0.45              |
| 63:Lz:1:MET:HB2    | 63:Lz:2:SER:H      | 1.55                     | 0.45              |
| 65:SD:161:GLY:CA   | 79:S2:1388:A:H61   | 2.30                     | 0.45              |
| 65:SD:193:ASP:O    | 65:SD:195:THR:HG23 | 2.17                     | 0.45              |
| 66:SF:77:MET:CE    | 79:S2:1674:G:H4'   | 2.47                     | 0.45              |
| 67:SK:67:PHE:HB2   | 67:SK:69:TRP:CZ2   | 2.51                     | 0.45              |
| 69:SQ:78:VAL:HG21  | 79:S2:1674:G:OP2   | 2.17                     | 0.45              |
| 69:SQ:82:TYR:O     | 69:SQ:85:ARG:HG2   | 2.16                     | 0.45              |
| 71:ST:100:ALA:O    | 71:ST:103:VAL:HG12 | 2.16                     | 0.45              |
| 72:SU:55:ARG:HE    | 72:SU:87:ARG:CZ    | 2.29                     | 0.45              |
| 74:Sd:15:GLY:H     | 74:Sd:19:ARG:NH2   | 2.15                     | 0.45              |
| 79:S2:106:C:H5''   | 79:S2:431:G:O2'    | 2.17                     | 0.45              |
| 79:S2:964:A:H2'    | 79:S2:965:U:H6     | 1.81                     | 0.45              |
| 79:S2:1284:A:H5'   | 79:S2:1284:A:N3    | 2.32                     | 0.45              |
| 79:S2:1472:C:O2    | 79:S2:1476:A:N6    | 2.50                     | 0.45              |
| 81:AP:43:A:H2'     | 81:AP:44:A:C8      | 2.52                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 87:LW:77:LYS:HB3   | 87:LW:79:GLN:HE22  | 1.81                     | 0.45              |
| 1:cH:75:LEU:HG     | 1:cH:79:LYS:NZ     | 2.31                     | 0.45              |
| 1:cH:121:LEU:CD1   | 1:cH:133:ARG:HD3   | 2.41                     | 0.45              |
| 2:sE:230:LYS:HA    | 2:sE:230:LYS:HD2   | 1.79                     | 0.45              |
| 4:sL:128:VAL:O     | 4:sL:140:PHE:HE1   | 1.95                     | 0.45              |
| 7:sJ:88:ASP:OD1    | 7:sJ:88:ASP:C      | 2.60                     | 0.45              |
| 10:sA:27:GLY:HA3   | 10:sA:28:THR:HA    | 1.80                     | 0.45              |
| 11:sB:62:LEU:CA    | 11:sB:65:ARG:HD2   | 2.42                     | 0.45              |
| 18:sW:101:PHE:CD1  | 18:sW:112:ASP:OD1  | 2.69                     | 0.45              |
| 20:l7:99:G:OP2     | 39:lS:55:LYS:NZ    | 2.36                     | 0.45              |
| 21:l8:140:C:H4'    | 34:lN:110:CYS:SG   | 2.57                     | 0.45              |
| 24:lC:10:VAL:HG23  | 24:lC:153:VAL:HG23 | 1.99                     | 0.45              |
| 25:lD:32:ALA:HA    | 25:lD:35:ARG:HB3   | 1.99                     | 0.45              |
| 25:lD:239:MET:HE1  | 25:lD:240:TYR:CG   | 2.52                     | 0.45              |
| 27:lF:197:VAL:HG13 | 27:lF:201:PHE:CG   | 2.52                     | 0.45              |
| 28:lG:100:HIS:O    | 28:lG:100:HIS:ND1  | 2.49                     | 0.45              |
| 29:lH:65:LYS:NZ    | 85:l5:1949:U:O5'   | 2.47                     | 0.45              |
| 30:lI:79:SER:OG    | 30:lI:147:HIS:CE1  | 2.70                     | 0.45              |
| 31:lJ:99:PHE:HD2   | 31:lJ:105:PHE:HB3  | 1.81                     | 0.45              |
| 32:lL:201:GLU:O    | 32:lL:205:GLN:NE2  | 2.46                     | 0.45              |
| 33:lM:126:GLU:CD   | 33:lM:126:GLU:C    | 2.85                     | 0.45              |
| 34:lN:145:ASN:OD1  | 34:lN:145:ASN:C    | 2.60                     | 0.45              |
| 36:lP:25:HIS:CD2   | 85:l5:2361:G:C5    | 3.05                     | 0.45              |
| 36:lP:50:ASP:OD1   | 36:lP:56:GLN:HG3   | 2.16                     | 0.45              |
| 39:lS:46:TYR:CD2   | 39:lS:46:TYR:C     | 2.95                     | 0.45              |
| 40:lT:126:VAL:O    | 85:l5:1834:U:N3    | 2.40                     | 0.45              |
| 41:lU:45:GLU:OE1   | 41:lU:45:GLU:N     | 2.44                     | 0.45              |
| 45:lZ:57:MET:HE2   | 45:lZ:62:ILE:HD11  | 1.99                     | 0.45              |
| 45:lZ:99:ASP:O     | 45:lZ:102:ARG:HG2  | 2.17                     | 0.45              |
| 47:lb:51:LYS:NZ    | 85:l5:1401:C:OP1   | 2.37                     | 0.45              |
| 58:lm:96:CYS:HB2   | 58:lm:110:CYS:SG   | 2.57                     | 0.45              |
| 62:lr:6:GLN:HA     | 62:lr:9:VAL:HG12   | 1.97                     | 0.45              |
| 63:lz:62:LYS:NZ    | 63:lz:155:ILE:HD12 | 2.32                     | 0.45              |
| 63:lz:206:ILE:HD11 | 63:lz:214:GLN:HB3  | 1.99                     | 0.45              |
| 64:sR:116:ASN:C    | 64:sR:117:LEU:HD23 | 2.42                     | 0.45              |
| 65:sD:75:LYS:NZ    | 67:sK:21:MET:HA    | 2.32                     | 0.45              |
| 65:sD:141:LYS:HB3  | 65:sD:147:ALA:HB2  | 1.99                     | 0.45              |
| 66:sF:20:PHE:HD2   | 66:sF:23:TRP:HZ3   | 1.64                     | 0.45              |
| 66:sF:103:LEU:HA   | 77:sZ:66:LYS:NZ    | 2.25                     | 0.45              |
| 69:sQ:104:SER:HA   | 69:sQ:107:GLU:CG   | 2.47                     | 0.45              |
| 69:sQ:130:LYS:NZ   | 69:sQ:131:LYS:O    | 2.42                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 70:sS:121:ARG:HH22 | 79:s2:1611:G:P     | 2.39                     | 0.45              |
| 71:sT:33:TRP:CH2   | 79:s2:1567:G:H5'   | 2.52                     | 0.45              |
| 75:sg:31:ILE:HA    | 75:sg:31:ILE:HD13  | 1.75                     | 0.45              |
| 75:sg:165:ILE:N    | 75:sg:177:TRP:O    | 2.31                     | 0.45              |
| 76:sM:51:VAL:O     | 76:sM:108:CYS:HA   | 2.16                     | 0.45              |
| 77:sZ:77:LEU:HD13  | 77:sZ:79:ILE:HD13  | 1.99                     | 0.45              |
| 79:s2:302:A:C6     | 79:s2:303:C:N4     | 2.85                     | 0.45              |
| 79:s2:836:G:H5''   | 28:LG:255:LYS:HD3  | 1.98                     | 0.45              |
| 79:s2:1060:A:H1'   | 79:s2:1062:A:N7    | 2.32                     | 0.45              |
| 79:s2:1073:U:C2    | 79:s2:1074:C:C5    | 3.04                     | 0.45              |
| 79:s2:1560:U:C2    | 79:s2:1575:G:O6    | 2.69                     | 0.45              |
| 80:cB:123:ASP:OD1  | 80:cB:415:ARG:NH2  | 2.40                     | 0.45              |
| 80:cB:174:LEU:HD13 | 80:cB:178:PHE:HE1  | 1.82                     | 0.45              |
| 80:cB:457:TYR:N    | 80:cB:457:TYR:CD1  | 2.85                     | 0.45              |
| 81:aP:35:A:H2'     | 81:aP:36:C:H6      | 1.82                     | 0.45              |
| 85:l5:372:A:N3     | 85:l5:1531:U:H1'   | 2.32                     | 0.45              |
| 85:l5:1091:C:H2'   | 85:l5:1092:G:H8    | 1.79                     | 0.45              |
| 85:l5:1293:G:OP2   | 85:l5:1293:G:N2    | 2.42                     | 0.45              |
| 85:l5:1327:C:H2'   | 85:l5:1328:G:H8    | 1.82                     | 0.45              |
| 85:l5:1586:G:H2'   | 85:l5:1587:G:C8    | 2.52                     | 0.45              |
| 85:l5:1614:C:H2'   | 85:l5:1615:C:H6    | 1.81                     | 0.45              |
| 85:l5:1989:G:H2'   | 85:l5:1990:A:C8    | 2.51                     | 0.45              |
| 85:l5:3650:C:H2'   | 85:l5:3651:A:H8    | 1.80                     | 0.45              |
| 85:l5:3695:U:H2'   | 85:l5:3696:C:C6    | 2.52                     | 0.45              |
| 85:l5:3735:G:O2'   | 85:l5:3736:A:OP2   | 2.35                     | 0.45              |
| 85:l5:3762:U:H2'   | 85:l5:3763:A:O4'   | 2.17                     | 0.45              |
| 85:l5:4141:G:H5'   | 85:l5:4142:C:H5    | 1.82                     | 0.45              |
| 85:l5:4460:U:H2'   | 85:l5:4461:C:C6    | 2.52                     | 0.45              |
| 85:l5:4537:C:C2    | 85:l5:4538:G:C8    | 3.05                     | 0.45              |
| 85:l5:4862:G:H2'   | 85:l5:4863:G:C8    | 2.52                     | 0.45              |
| 80:CB:402:VAL:HG23 | 80:CB:411:TYR:HD2  | 1.82                     | 0.45              |
| 80:CB:616:ASP:OD2  | 80:CB:634:TYR:OH   | 2.35                     | 0.45              |
| 2:SE:124:CYS:HB3   | 2:SE:141:THR:OG1   | 2.17                     | 0.45              |
| 4:SL:28:THR:N      | 4:SL:29:GLY:HA2    | 2.30                     | 0.45              |
| 5:SX:49:GLY:O      | 5:SX:100:VAL:N     | 2.39                     | 0.45              |
| 5:SX:107:ARG:NH2   | 79:S2:18:C:O3'     | 2.50                     | 0.45              |
| 8:SY:47:MET:O      | 8:SY:47:MET:HE2    | 2.17                     | 0.45              |
| 11:SB:159:GLN:O    | 11:SB:163:GLN:HG3  | 2.17                     | 0.45              |
| 11:SB:161:VAL:O    | 11:SB:164:ILE:HG12 | 2.16                     | 0.45              |
| 19:Sb:70:LYS:NZ    | 79:S2:1106:C:H5''  | 2.28                     | 0.45              |
| 85:L5:40:G:N2      | 85:L5:4380:A:N7    | 2.65                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 85:L5:417:G:H1'    | 21:L8:17:A:N6      | 2.32                     | 0.45              |
| 85:L5:418:A:OP2    | 21:L8:16:G:N2      | 2.49                     | 0.45              |
| 85:L5:441:G:H2'    | 85:L5:442:G:C8     | 2.51                     | 0.45              |
| 85:L5:743:G:H2'    | 85:L5:744:G:O4'    | 2.17                     | 0.45              |
| 85:L5:1320:U:H2'   | 85:L5:1321:G:O4'   | 2.17                     | 0.45              |
| 85:L5:1727:U:H2'   | 85:L5:1728:U:H6    | 1.80                     | 0.45              |
| 85:L5:2000:G:H5''  | 85:L5:2001:G:H5'   | 1.99                     | 0.45              |
| 85:L5:2269:C:N4    | 62:Lr:11:ARG:HH22  | 2.15                     | 0.45              |
| 85:L5:2436:U:O4    | 43:LX:130:PRO:HG3  | 2.17                     | 0.45              |
| 85:L5:2464:C:O2'   | 85:L5:2465:C:H6    | 2.00                     | 0.45              |
| 85:L5:2505:C:N4    | 85:L5:4085:A:OP2   | 2.50                     | 0.45              |
| 85:L5:3611:A:O2'   | 85:L5:5016:A:O2'   | 2.32                     | 0.45              |
| 85:L5:3689:G:OP1   | 22:LA:202:VAL:HG23 | 2.16                     | 0.45              |
| 85:L5:3721:U:H2'   | 85:L5:3722:G:H8    | 1.82                     | 0.45              |
| 85:L5:4101:C:C2    | 85:L5:4104:G:C5'   | 3.00                     | 0.45              |
| 85:L5:4101:C:H5'   | 85:L5:4107:G:O4'   | 2.16                     | 0.45              |
| 85:L5:4112:C:H3'   | 85:L5:4115:G:OP2   | 2.16                     | 0.45              |
| 85:L5:4232:U:OP1   | 60:Lo:98:LYS:NZ    | 2.49                     | 0.45              |
| 85:L5:4287:G:H2'   | 85:L5:4288:C:C6    | 2.52                     | 0.45              |
| 21:L8:25:G:H2'     | 21:L8:26:C:C6      | 2.52                     | 0.45              |
| 21:L8:120:G:C6     | 21:L8:131:G:C6     | 3.05                     | 0.45              |
| 28:LG:145:THR:HA   | 28:LG:148:GLU:OE2  | 2.17                     | 0.45              |
| 29:LH:7:ASN:OD1    | 29:LH:7:ASN:N      | 2.49                     | 0.45              |
| 29:LH:133:ALA:O    | 29:LH:147:GLU:N    | 2.40                     | 0.45              |
| 32:LL:194:ILE:HG13 | 32:LL:198:ARG:NH1  | 2.33                     | 0.45              |
| 37:LQ:76:GLU:HG2   | 37:LQ:77:ASN:OD1   | 2.17                     | 0.45              |
| 37:LQ:181:ARG:HA   | 37:LQ:187:LYS:HD3  | 1.99                     | 0.45              |
| 40:LT:88:ARG:NH2   | 47:Lb:30:GLU:OE2   | 2.49                     | 0.45              |
| 42:LV:94:VAL:HG21  | 87:LW:20:ARG:NH2   | 2.32                     | 0.45              |
| 45:LZ:54:THR:O     | 45:LZ:57:MET:HE1   | 2.17                     | 0.45              |
| 45:LZ:91:LEU:HD23  | 45:LZ:117:LYS:HD2  | 1.98                     | 0.45              |
| 48:Lc:77:ASN:H     | 48:Lc:80:GLU:HG2   | 1.82                     | 0.45              |
| 49:Ld:117:LEU:HD23 | 49:Ld:117:LEU:HA   | 1.70                     | 0.45              |
| 56:Lk:52:LYS:HA    | 56:Lk:55:LYS:CG    | 2.46                     | 0.45              |
| 64:SR:4:VAL:HA     | 79:S2:1466:G:O5'   | 2.17                     | 0.45              |
| 65:SD:142:LEU:HD21 | 65:SD:148:LYS:NZ   | 2.32                     | 0.45              |
| 71:ST:113:VAL:HA   | 71:ST:123:LEU:HA   | 1.98                     | 0.45              |
| 73:Sc:55:VAL:C     | 73:Sc:56:LEU:HD12  | 2.41                     | 0.45              |
| 76:SM:12:MET:SD    | 76:SM:16:THR:OG1   | 2.75                     | 0.45              |
| 76:SM:29:ASP:CB    | 76:SM:113:ASP:HB2  | 2.47                     | 0.45              |
| 79:S2:40:A:H3'     | 79:S2:486:A:H62    | 1.81                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 79:S2:1170:A:N6    | 79:S2:1189:A:OP2   | 2.45                     | 0.45              |
| 79:S2:1406:G:H2'   | 79:S2:1407:U:C6    | 2.52                     | 0.45              |
| 79:S2:1558:C:H2'   | 79:S2:1559:C:H6    | 1.82                     | 0.45              |
| 79:S2:1681:U:H2'   | 79:S2:1682:C:C6    | 2.52                     | 0.45              |
| 79:S2:1739:C:H2'   | 79:S2:1740:C:H6    | 1.82                     | 0.45              |
| 83:Ls:137:PHE:CZ   | 83:Ls:174:LEU:HB2  | 2.52                     | 0.45              |
| 84:Lt:53:TRP:CZ2   | 84:Lt:56:LEU:HD22  | 2.52                     | 0.45              |
| 87:LW:82:ILE:HG23  | 87:LW:85:ALA:HB3   | 1.98                     | 0.45              |
| 1:CH:28:ALA:HA     | 1:CH:31:ARG:HD2    | 1.98                     | 0.44              |
| 1:cH:61:LEU:HD22   | 65:sD:107:TYR:HE2  | 1.82                     | 0.44              |
| 3:sI:83:TYR:OH     | 4:sL:8:ARG:HB3     | 2.17                     | 0.44              |
| 10:sA:144:THR:CG2  | 10:sA:157:VAL:HA   | 2.47                     | 0.44              |
| 12:sH:70:LYS:HE3   | 12:sH:70:LYS:HB2   | 1.64                     | 0.44              |
| 12:sH:145:ARG:CZ   | 18:sW:51:GLU:HA    | 2.47                     | 0.44              |
| 17:sO:32:HIS:N     | 17:sO:43:HIS:O     | 2.50                     | 0.44              |
| 17:sO:94:HIS:CE1   | 17:sO:128:ARG:H    | 2.34                     | 0.44              |
| 17:sO:96:LYS:HD3   | 17:sO:132:VAL:HG11 | 1.99                     | 0.44              |
| 20:l7:7:G:N2       | 25:lD:70:GLU:O     | 2.44                     | 0.44              |
| 23:lB:29:VAL:HG12  | 23:lB:31:SER:H     | 1.81                     | 0.44              |
| 24:lC:242:PRO:O    | 85:l5:2296:G:O2'   | 2.23                     | 0.44              |
| 24:lC:268:ARG:HH11 | 24:lC:268:ARG:HG3  | 1.81                     | 0.44              |
| 25:lD:68:ARG:CG    | 25:lD:73:MET:HG2   | 2.45                     | 0.44              |
| 25:lD:257:PRO:HA   | 25:lD:259:LYS:HZ1  | 1.82                     | 0.44              |
| 28:lG:120:LYS:HZ2  | 28:lG:125:LYS:HB3  | 1.83                     | 0.44              |
| 30:lI:3:ARG:HD2    | 30:lI:63:GLU:OE2   | 2.17                     | 0.44              |
| 31:lJ:22:LEU:HD11  | 31:lJ:128:LEU:HD22 | 1.99                     | 0.44              |
| 34:lN:33:LEU:HD13  | 34:lN:37:HIS:CD2   | 2.52                     | 0.44              |
| 34:lN:50:ARG:HH22  | 85:l5:278:G:H1'    | 1.81                     | 0.44              |
| 35:lO:81:TRP:CZ2   | 35:lO:99:LEU:HD11  | 2.52                     | 0.44              |
| 41:lU:38:ASN:O     | 41:lU:41:GLN:NE2   | 2.29                     | 0.44              |
| 42:lV:91:LYS:HD3   | 42:lV:91:LYS:HA    | 1.73                     | 0.44              |
| 48:lc:11:LEU:HB3   | 79:s2:1006:C:O3'   | 2.16                     | 0.44              |
| 49:ld:64:ILE:HG22  | 49:ld:106:VAL:HG11 | 1.99                     | 0.44              |
| 52:lg:97:ILE:HD11  | 85:l5:4122:G:C6    | 2.51                     | 0.44              |
| 52:lg:105:LYS:NZ   | 52:lg:108:LYS:HD2  | 2.33                     | 0.44              |
| 55:lj:3:LYS:HB3    | 85:l5:3642:A:C4    | 2.52                     | 0.44              |
| 61:lp:64:VAL:HG21  | 61:lp:71:TYR:CE2   | 2.52                     | 0.44              |
| 66:sF:112:LEU:HA   | 66:sF:177:LEU:HD12 | 1.99                     | 0.44              |
| 66:sF:127:ARG:HH12 | 73:sc:66:ARG:NH2   | 2.16                     | 0.44              |
| 67:sK:8:ARG:HH22   | 79:s2:1314:U:H4'   | 1.82                     | 0.44              |
| 68:sP:128:HIS:CD2  | 79:s2:1522:A:C5    | 3.05                     | 0.44              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 70:sS:88:LYS:HB3  | 70:sS:95:TYR:CE1   | 2.52                     | 0.44              |
| 71:sT:105:GLN:HA  | 71:sT:108:GLU:HG2  | 1.99                     | 0.44              |
| 79:s2:24:C:O2'    | 79:s2:25:A:O5'     | 2.35                     | 0.44              |
| 79:s2:50:A:OP2    | 79:s2:472:C:N4     | 2.50                     | 0.44              |
| 79:s2:329:G:C4    | 79:s2:330:G:C8     | 3.05                     | 0.44              |
| 79:s2:444:G:N1    | 79:s2:447:A:OP2    | 2.50                     | 0.44              |
| 79:s2:456:C:H2'   | 79:s2:457:C:C6     | 2.51                     | 0.44              |
| 79:s2:558:G:O2'   | 79:s2:559:G:OP2    | 2.34                     | 0.44              |
| 79:s2:1349:G:H2'  | 79:s2:1350:U:C6    | 2.52                     | 0.44              |
| 79:s2:1620:A:H1'  | 79:s2:1624:U:OP2   | 2.18                     | 0.44              |
| 80:cB:514:PRO:O   | 80:cB:517:LEU:HD23 | 2.18                     | 0.44              |
| 83:ls:97:GLU:OE2  | 83:ls:98:ILE:N     | 2.50                     | 0.44              |
| 85:l5:146:G:H2'   | 85:l5:147:A:H8     | 1.82                     | 0.44              |
| 85:l5:370:U:C4    | 85:l5:1637:A:C4    | 3.06                     | 0.44              |
| 85:l5:1633:G:N7   | 85:l5:1641:G:C5    | 2.86                     | 0.44              |
| 85:l5:3650:C:H2'  | 85:l5:3651:A:C8    | 2.51                     | 0.44              |
| 85:l5:3878:C:N4   | 85:l5:4518:A:O4'   | 2.50                     | 0.44              |
| 85:l5:3951:G:H8   | 85:l5:3951:G:OP2   | 1.99                     | 0.44              |
| 85:l5:3967:G:H5'' | 85:l5:3969:G:N2    | 2.32                     | 0.44              |
| 85:l5:4133:C:C2'  | 85:l5:4134:C:H5'   | 2.47                     | 0.44              |
| 85:l5:4411:G:C2   | 85:l5:4432:C:C2    | 3.05                     | 0.44              |
| 85:l5:4595:G:H2'  | 85:l5:4596:C:C6    | 2.52                     | 0.44              |
| 85:l5:4652:G:H2'  | 85:l5:4653:C:C6    | 2.52                     | 0.44              |
| 85:l5:4771:C:H2'  | 85:l5:4772:C:H6    | 1.81                     | 0.44              |
| 85:l5:4868:G:O2'  | 85:l5:4872:G:OP1   | 2.34                     | 0.44              |
| 85:l5:4988:U:H4'  | 85:l5:4989:U:H5    | 1.81                     | 0.44              |
| 80:CB:192:TYR:CE2 | 80:CB:780:PRO:HG2  | 2.52                     | 0.44              |
| 80:CB:224:THR:H   | 80:CB:227:GLN:NE2  | 2.15                     | 0.44              |
| 80:CB:824:PRO:HA  | 80:CB:831:PRO:HB2  | 1.99                     | 0.44              |
| 4:SL:47:PRO:HG2   | 4:SL:50:ALA:HB2    | 2.00                     | 0.44              |
| 4:SL:153:LYS:HA   | 4:SL:153:LYS:HD3   | 1.66                     | 0.44              |
| 5:SX:4:CYS:HB3    | 79:S2:1161:U:OP2   | 2.18                     | 0.44              |
| 5:SX:13:LEU:HD12  | 5:SX:14:ARG:H      | 1.80                     | 0.44              |
| 6:SG:44:GLU:HG2   | 6:SG:45:TRP:CD1    | 2.53                     | 0.44              |
| 6:SG:131:ARG:NH1  | 87:LW:80:ARG:HD3   | 2.24                     | 0.44              |
| 7:SJ:2:PRO:O      | 79:S2:509:G:H5''   | 2.17                     | 0.44              |
| 7:SJ:5:ARG:HG2    | 79:S2:38:A:OP1     | 2.17                     | 0.44              |
| 10:SA:50:ASN:CG   | 10:SA:53:ARG:HG3   | 2.43                     | 0.44              |
| 10:SA:128:ARG:NH1 | 10:SA:128:ARG:HB2  | 2.31                     | 0.44              |
| 11:SB:27:LYS:O    | 11:SB:51:ARG:HG3   | 2.17                     | 0.44              |
| 11:SB:65:ARG:HB3  | 11:SB:67:PHE:CE1   | 2.52                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 12:SH:145:ARG:NH1  | 12:SH:145:ARG:HA   | 2.32                     | 0.44              |
| 18:SW:37:PHE:O     | 18:SW:41:MET:HG2   | 2.17                     | 0.44              |
| 85:L5:274:C:O2'    | 85:L5:275:C:H5'    | 2.17                     | 0.44              |
| 85:L5:308:G:C2     | 54:Li:41:ARG:CZ    | 3.00                     | 0.44              |
| 85:L5:684:G:O2'    | 26:LE:101:ASN:OD1  | 2.31                     | 0.44              |
| 85:L5:1294:A:H1'   | 85:L5:1296:G:C2    | 2.52                     | 0.44              |
| 85:L5:1332:C:OP2   | 50:Le:30:LYS:HD3   | 2.17                     | 0.44              |
| 85:L5:1397:A:OP2   | 46:La:113:GLY:N    | 2.48                     | 0.44              |
| 85:L5:1993:C:H4'   | 84:Lt:149:HIS:NE2  | 2.32                     | 0.44              |
| 85:L5:2067:C:H2'   | 85:L5:2068:C:C6    | 2.52                     | 0.44              |
| 85:L5:2309:G:H1    | 85:L5:2329:U:H3    | 1.64                     | 0.44              |
| 85:L5:2685:C:H2'   | 85:L5:2686:G:O4'   | 2.16                     | 0.44              |
| 85:L5:2744:A:H2'   | 85:L5:2745:A:H8    | 1.81                     | 0.44              |
| 85:L5:4089:G:C6    | 85:L5:4161:G:N1    | 2.85                     | 0.44              |
| 85:L5:4092:G:C4    | 85:L5:4093:G:C2    | 3.05                     | 0.44              |
| 85:L5:4116:C:O2'   | 85:L5:4117:U:H5'   | 2.17                     | 0.44              |
| 85:L5:4640:C:H2'   | 85:L5:4641:U:C6    | 2.52                     | 0.44              |
| 23:LB:248:LEU:HD23 | 23:LB:248:LEU:H    | 1.82                     | 0.44              |
| 23:LB:286:LYS:HG2  | 23:LB:332:MET:HE1  | 2.00                     | 0.44              |
| 27:LF:213:LEU:HB3  | 27:LF:247:MET:SD   | 2.57                     | 0.44              |
| 28:LG:116:ALA:O    | 28:LG:119:GLU:HG2  | 2.17                     | 0.44              |
| 28:LG:173:LEU:O    | 28:LG:177:MET:HG2  | 2.17                     | 0.44              |
| 28:LG:175:ARG:NH2  | 28:LG:230:TYR:HB3  | 2.32                     | 0.44              |
| 32:LL:110:LEU:HB3  | 32:LL:111:GLN:NE2  | 2.32                     | 0.44              |
| 32:LL:158:ARG:NH1  | 32:LL:158:ARG:HA   | 2.32                     | 0.44              |
| 33:LM:33:GLN:HG2   | 33:LM:33:GLN:O     | 2.17                     | 0.44              |
| 33:LM:110:PHE:O    | 33:LM:113:MET:SD   | 2.75                     | 0.44              |
| 34:LN:94:PHE:CE2   | 34:LN:96:ARG:HB2   | 2.52                     | 0.44              |
| 39:LS:16:CYS:HA    | 39:LS:59:GLY:HA2   | 1.99                     | 0.44              |
| 44:LY:34:LEU:HA    | 44:LY:106:ILE:HG22 | 1.98                     | 0.44              |
| 48:Lc:55:LEU:HD23  | 48:Lc:55:LEU:HA    | 1.77                     | 0.44              |
| 53:Lh:14:LYS:O     | 53:Lh:18:LEU:HG    | 2.17                     | 0.44              |
| 55:Lj:72:ARG:HA    | 55:Lj:75:ARG:NH2   | 2.32                     | 0.44              |
| 62:Lr:82:ILE:HD13  | 62:Lr:82:ILE:N     | 2.32                     | 0.44              |
| 64:SR:15:VAL:HA    | 64:SR:18:GLU:HG2   | 1.99                     | 0.44              |
| 65:SD:142:LEU:HD23 | 65:SD:142:LEU:H    | 1.82                     | 0.44              |
| 66:SF:33:ILE:HG13  | 73:Sc:11:LEU:CD1   | 2.47                     | 0.44              |
| 68:SP:52:LYS:HG2   | 68:SP:53:GLN:OE1   | 2.17                     | 0.44              |
| 74:Sd:8:TRP:CZ3    | 79:S2:1512:C:H5''  | 2.51                     | 0.44              |
| 79:S2:201:C:H5''   | 79:S2:202:G:H21    | 1.81                     | 0.44              |
| 79:S2:215:G:H2'    | 79:S2:216:C:H6     | 1.81                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 79:S2:1531:A:H2'   | 79:S2:1532:C:C6    | 2.52                     | 0.44              |
| 79:S2:1633:A:H2'   | 79:S2:1634:A:H8    | 1.79                     | 0.44              |
| 81:AP:12:G:N1      | 81:AP:24:A:C6      | 2.85                     | 0.44              |
| 84:Lt:16:ARG:HB2   | 84:Lt:61:LYS:NZ    | 2.33                     | 0.44              |
| 84:Lt:16:ARG:NH1   | 84:Lt:32:ILE:HD13  | 2.32                     | 0.44              |
| 84:Lt:33:GLY:N     | 84:Lt:34:PRO:HD2   | 2.32                     | 0.44              |
| 87:IW:37:GLU:HG2   | 87:IW:37:GLU:H     | 1.59                     | 0.44              |
| 87:LW:19:ARG:HD3   | 87:LW:37:GLU:OE2   | 2.16                     | 0.44              |
| 87:LW:109:ILE:HG13 | 87:LW:110:ARG:HD2  | 1.98                     | 0.44              |
| 1:CH:136:ASP:OD1   | 1:CH:137:ILE:N     | 2.50                     | 0.44              |
| 2:sE:91:SER:OG     | 2:sE:93:ASP:OD1    | 2.31                     | 0.44              |
| 4:sL:103:GLU:OE2   | 5:sX:11:ARG:HB2    | 2.18                     | 0.44              |
| 4:sL:136:LYS:HB2   | 79:s2:373:G:OP2    | 2.18                     | 0.44              |
| 5:sX:77:ASN:O      | 5:sX:79:LYS:HG2    | 2.17                     | 0.44              |
| 8:sY:39:GLU:H      | 8:sY:39:GLU:CD     | 2.26                     | 0.44              |
| 10:sA:83:GLY:O     | 10:sA:87:VAL:HG13  | 2.17                     | 0.44              |
| 10:sA:219:GLU:O    | 10:sA:223:THR:OG1  | 2.22                     | 0.44              |
| 11:sB:28:LYS:HG3   | 11:sB:48:LEU:HD13  | 1.98                     | 0.44              |
| 11:sB:49:VAL:HG11  | 11:sB:62:LEU:HD11  | 1.99                     | 0.44              |
| 11:sB:144:LYS:HG3  | 64:sR:135:VAL:HG21 | 1.98                     | 0.44              |
| 12:sH:145:ARG:NE   | 18:sW:51:GLU:HG3   | 2.32                     | 0.44              |
| 26:IE:173:LEU:HA   | 26:IE:173:LEU:HD12 | 1.72                     | 0.44              |
| 32:IL:149:GLN:OE1  | 32:IL:150:LEU:N    | 2.50                     | 0.44              |
| 33:IM:23:LYS:NZ    | 33:IM:44:GLN:O     | 2.50                     | 0.44              |
| 36:IP:72:GLN:NE2   | 85:l5:4971:A:H5'   | 2.31                     | 0.44              |
| 37:lQ:30:LYS:HE2   | 85:l5:2268:A:O2'   | 2.16                     | 0.44              |
| 38:IR:117:ARG:CD   | 85:l5:2663:G:H4'   | 2.47                     | 0.44              |
| 40:IT:17:ARG:NH1   | 40:IT:17:ARG:HA    | 2.32                     | 0.44              |
| 51:lf:45:LYS:HD3   | 51:lf:106:TYR:O    | 2.17                     | 0.44              |
| 63:lz:198:TRP:NE1  | 63:lz:199:GLN:HG3  | 2.31                     | 0.44              |
| 66:sF:190:ILE:O    | 66:sF:194:ASP:OD2  | 2.34                     | 0.44              |
| 68:sP:64:LYS:HA    | 68:sP:64:LYS:HD2   | 1.80                     | 0.44              |
| 71:sT:104:LEU:HD11 | 71:sT:121:ARG:HD2  | 1.98                     | 0.44              |
| 75:sg:89:LEU:HD12  | 75:sg:89:LEU:O     | 2.18                     | 0.44              |
| 75:sg:100:ARG:NH1  | 79:s2:1399:C:OP1   | 2.50                     | 0.44              |
| 79:s2:113:G:N2     | 79:s2:293:C:O4'    | 2.51                     | 0.44              |
| 79:s2:155:G:C6     | 79:s2:164:A:C6     | 3.05                     | 0.44              |
| 79:s2:434:G:O2'    | 79:s2:473:A:N1     | 2.45                     | 0.44              |
| 79:s2:566:U:H3'    | 79:s2:567:C:H6     | 1.82                     | 0.44              |
| 79:s2:808:A:C4     | 79:s2:809:A:C8     | 3.05                     | 0.44              |
| 79:s2:958:G:C6     | 79:s2:959:G:C6     | 3.04                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 79:s2:1112:U:O2'  | 79:s2:1113:A:H5'  | 2.17                     | 0.44              |
| 79:s2:1310:U:C2   | 79:s2:1311:C:C5   | 3.05                     | 0.44              |
| 79:s2:1468:C:H2'  | 79:s2:1469:A:C8   | 2.52                     | 0.44              |
| 79:s2:1736:G:H2'  | 79:s2:1737:G:H8   | 1.82                     | 0.44              |
| 80:cB:69:THR:HB   | 80:cB:106:PRO:HB3 | 1.99                     | 0.44              |
| 80:cB:594:LYS:NZ  | 80:cB:596:PRO:HA  | 2.31                     | 0.44              |
| 80:cB:631:ARG:O   | 80:cB:635:LEU:HG  | 2.17                     | 0.44              |
| 81:aP:39:G:H2'    | 81:aP:40:C:C6     | 2.52                     | 0.44              |
| 82:pE:36:U:C4     | 82:pE:37:A:C5     | 3.05                     | 0.44              |
| 84:lt:33:GLY:N    | 84:lt:34:PRO:HD3  | 2.32                     | 0.44              |
| 85:l5:208:A:N3    | 85:l5:232:G:O2'   | 2.48                     | 0.44              |
| 85:l5:710:G:H2'   | 85:l5:711:A:H8    | 1.81                     | 0.44              |
| 85:l5:1519:C:H2'  | 85:l5:1520:C:H6   | 1.82                     | 0.44              |
| 85:l5:1887:G:H21  | 85:l5:1938:C:N4   | 2.15                     | 0.44              |
| 85:l5:2066:C:C2   | 85:l5:2067:C:C5   | 3.05                     | 0.44              |
| 85:l5:2586:G:H4'  | 85:l5:2587:A:OP1  | 2.17                     | 0.44              |
| 85:l5:2700:G:C6   | 85:l5:2701:U:C4   | 3.05                     | 0.44              |
| 85:l5:4058:U:H4'  | 85:l5:4059:C:C5   | 2.52                     | 0.44              |
| 85:l5:4400:G:C6   | 85:l5:4401:G:C8   | 3.06                     | 0.44              |
| 85:l5:4877:G:H2'  | 85:l5:4878:C:H6   | 1.82                     | 0.44              |
| 80:CB:325:SER:HA  | 80:CB:328:LYS:NZ  | 2.33                     | 0.44              |
| 6:SG:131:ARG:O    | 87:LW:83:THR:HG23 | 2.17                     | 0.44              |
| 7:SJ:131:ARG:NH1  | 7:SJ:145:PRO:HD3  | 2.32                     | 0.44              |
| 7:SJ:137:VAL:HG22 | 7:SJ:138:ARG:N    | 2.33                     | 0.44              |
| 14:Sa:5:ARG:NH2   | 79:S2:1864:U:H3'  | 2.28                     | 0.44              |
| 14:Sa:89:ARG:HA   | 14:Sa:92:ARG:HB3  | 1.99                     | 0.44              |
| 17:SO:134:PRO:HB3 | 79:S2:944:A:H5''  | 1.98                     | 0.44              |
| 85:L5:470:A:C4    | 85:L5:471:A:C8    | 3.06                     | 0.44              |
| 85:L5:700:G:C6    | 85:L5:701:G:C6    | 3.05                     | 0.44              |
| 85:L5:958:G:N2    | 26:LE:125:LEU:H   | 2.13                     | 0.44              |
| 85:L5:1847:C:H4'  | 37:LQ:152:PHE:CZ  | 2.52                     | 0.44              |
| 85:L5:1907:A:H3'  | 85:L5:1908:A:C8   | 2.52                     | 0.44              |
| 85:L5:2292:C:H2'  | 85:L5:2293:U:H6   | 1.81                     | 0.44              |
| 85:L5:2369:U:H5'  | 85:L5:4656:A:C2   | 2.53                     | 0.44              |
| 85:L5:2461:G:OP1  | 34:LN:105:ARG:NE  | 2.36                     | 0.44              |
| 85:L5:2501:C:N4   | 85:L5:2502:G:O6   | 2.50                     | 0.44              |
| 85:L5:2599:G:C6   | 85:L5:2600:A:C6   | 3.06                     | 0.44              |
| 85:L5:2691:U:H2'  | 85:L5:2692:U:H6   | 1.82                     | 0.44              |
| 85:L5:2759:G:O2'  | 85:L5:2760:G:O4'  | 2.25                     | 0.44              |
| 85:L5:2772:C:C2   | 85:L5:2773:G:C8   | 3.05                     | 0.44              |
| 85:L5:2898:G:H2'  | 85:L5:2899:C:H6   | 1.81                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 85:L5:3835:C:H2'  | 85:L5:3836:A:H8   | 1.82                     | 0.44              |
| 85:L5:3932:U:H2'  | 85:L5:3933:G:C8   | 2.53                     | 0.44              |
| 85:L5:4039:G:H21  | 85:L5:4050:A:HO2' | 1.60                     | 0.44              |
| 85:L5:4096:C:C5   | 85:L5:4110:C:H5   | 2.35                     | 0.44              |
| 85:L5:4097:G:C8   | 85:L5:4111:U:C5   | 3.05                     | 0.44              |
| 85:L5:4679:G:H2'  | 85:L5:4680:G:C8   | 2.52                     | 0.44              |
| 85:L5:4684:A:H2'  | 85:L5:4685:U:O4'  | 2.16                     | 0.44              |
| 21:L8:5:U:C2      | 21:L8:6:C:C5      | 3.05                     | 0.44              |
| 22:LA:46:LYS:HB3  | 22:LA:60:LYS:CD   | 2.47                     | 0.44              |
| 22:LA:142:GLU:CD  | 22:LA:143:THR:H   | 2.25                     | 0.44              |
| 23:LB:59:GLU:OE1  | 23:LB:70:LYS:N    | 2.50                     | 0.44              |
| 26:LE:68:MET:CE   | 26:LE:71:ARG:HG3  | 2.48                     | 0.44              |
| 28:LG:225:ASN:O   | 28:LG:229:ARG:HD3 | 2.17                     | 0.44              |
| 30:LI:66:GLU:O    | 30:LI:70:ILE:HG12 | 2.17                     | 0.44              |
| 31:LJ:139:PHE:HE2 | 31:LJ:155:HIS:CD2 | 2.35                     | 0.44              |
| 32:LL:9:VAL:HG23  | 46:La:49:HIS:CD2  | 2.52                     | 0.44              |
| 32:LL:87:HIS:HB3  | 32:LL:90:VAL:HG12 | 1.99                     | 0.44              |
| 42:LV:64:THR:HG22 | 42:LV:76:VAL:HA   | 1.98                     | 0.44              |
| 48:Lc:81:LEU:CD2  | 48:Lc:91:VAL:HG23 | 2.47                     | 0.44              |
| 53:Lh:23:ASP:HA   | 53:Lh:26:VAL:HG12 | 1.98                     | 0.44              |
| 67:SK:6:LYS:NZ    | 67:SK:38:LYS:O    | 2.50                     | 0.44              |
| 72:SU:60:THR:HA   | 72:SU:82:MET:O    | 2.17                     | 0.44              |
| 78:Sf:138:ARG:NH2 | 79:S2:1293:A:N3   | 2.65                     | 0.44              |
| 79:S2:94:G:C4     | 79:S2:95:G:C8     | 3.05                     | 0.44              |
| 79:S2:192:C:H2'   | 79:S2:193:C:C6    | 2.52                     | 0.44              |
| 79:S2:649:U:H2'   | 79:S2:650:A:C8    | 2.50                     | 0.44              |
| 79:S2:1135:C:H2'  | 79:S2:1136:U:H6   | 1.83                     | 0.44              |
| 79:S2:1499:U:H2'  | 79:S2:1500:G:C8   | 2.52                     | 0.44              |
| 79:S2:1548:G:H1   | 79:S2:1584:G:H1   | 1.65                     | 0.44              |
| 79:S2:1650:A:H3'  | 79:S2:1651:A:H8   | 1.81                     | 0.44              |
| 79:S2:1756:C:OP2  | 79:S2:1757:G:N2   | 2.34                     | 0.44              |
| 81:AP:4:U:H2'     | 81:AP:5:C:H6      | 1.82                     | 0.44              |
| 83:Ls:101:MET:HE3 | 83:Ls:102:LEU:N   | 2.33                     | 0.44              |
| 1:cH:26:ILE:HG22  | 1:cH:30:ARG:HD2   | 2.00                     | 0.44              |
| 2:sE:201:HIS:NE2  | 79:s2:857:U:H4'   | 2.32                     | 0.44              |
| 3:sI:153:LYS:HA   | 3:sI:156:ALA:HB3  | 1.99                     | 0.44              |
| 6:sG:132:ARG:CZ   | 79:s2:168:C:C1'   | 2.95                     | 0.44              |
| 6:sG:132:ARG:NH2  | 79:s2:167:G:C4    | 2.85                     | 0.44              |
| 6:sG:221:LYS:HE3  | 6:sG:221:LYS:HB3  | 1.79                     | 0.44              |
| 6:sG:231:ARG:HE   | 6:sG:231:ARG:C    | 2.26                     | 0.44              |
| 8:sY:26:ASP:CG    | 8:sY:68:LYS:HZ2   | 2.25                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:sA:125:THR:HG22 | 10:sA:175:TRP:HZ2  | 1.82                     | 0.44              |
| 14:sa:78:ALA:O     | 14:sa:83:VAL:HG22  | 2.18                     | 0.44              |
| 15:sC:105:GLU:N    | 15:sC:105:GLU:OE2  | 2.50                     | 0.44              |
| 17:sO:116:LEU:HD23 | 17:sO:116:LEU:HA   | 1.72                     | 0.44              |
| 21:l8:86:U:H3'     | 53:lh:5:LYS:NZ     | 2.32                     | 0.44              |
| 21:l8:114:G:H2'    | 21:l8:115:G:C8     | 2.51                     | 0.44              |
| 21:l8:150:C:N4     | 28:lG:53:ARG:HA    | 2.32                     | 0.44              |
| 22:lA:228:ASP:OD2  | 22:lA:228:ASP:O    | 2.36                     | 0.44              |
| 25:lD:60:ILE:HG13  | 25:lD:93:THR:HA    | 2.00                     | 0.44              |
| 26:lE:105:ARG:HH21 | 85:l5:469:C:H42    | 1.64                     | 0.44              |
| 28:lG:87:LEU:HD12  | 28:lG:87:LEU:HA    | 1.85                     | 0.44              |
| 28:lG:117:ARG:HG3  | 28:lG:121:LYS:NZ   | 2.33                     | 0.44              |
| 29:lH:117:PHE:CZ   | 29:lH:118:LEU:HD13 | 2.53                     | 0.44              |
| 31:lJ:165:TRP:HA   | 31:lJ:168:GLN:HB2  | 2.00                     | 0.44              |
| 32:lL:91:ALA:HB1   | 32:lL:96:ILE:HB    | 2.00                     | 0.44              |
| 34:lN:49:ARG:HH12  | 85:l5:151:G:H3'    | 1.83                     | 0.44              |
| 35:lO:193:THR:O    | 35:lO:197:LYS:HG3  | 2.17                     | 0.44              |
| 36:lP:3:ARG:HD2    | 36:lP:3:ARG:HA     | 1.85                     | 0.44              |
| 39:lS:80:ILE:CG2   | 39:lS:126:ILE:HD11 | 2.46                     | 0.44              |
| 43:lX:106:LYS:HG2  | 85:l5:2779:C:P     | 2.57                     | 0.44              |
| 43:lX:118:ASP:C    | 43:lX:119:ILE:HD13 | 2.42                     | 0.44              |
| 44:lY:28:LYS:NZ    | 85:l5:240:G:O3'    | 2.50                     | 0.44              |
| 48:lc:20:LEU:HD23  | 48:lc:20:LEU:HA    | 1.87                     | 0.44              |
| 49:ld:69:ASN:ND2   | 85:l5:2373:C:O4'   | 2.50                     | 0.44              |
| 56:lk:9:LYS:O      | 56:lk:9:LYS:HD2    | 2.17                     | 0.44              |
| 56:lk:27:LYS:H     | 56:lk:70:LYS:HZ2   | 1.65                     | 0.44              |
| 62:lr:41:ASN:OD1   | 62:lr:44:ILE:HG23  | 2.17                     | 0.44              |
| 62:lr:90:LEU:HD12  | 62:lr:111:ILE:HG23 | 1.99                     | 0.44              |
| 65:sD:150:MET:HE1  | 65:sD:152:PHE:CZ   | 2.52                     | 0.44              |
| 69:sQ:113:ILE:HD13 | 69:sQ:120:LEU:HB2  | 2.00                     | 0.44              |
| 71:sT:64:LEU:HD11  | 71:sT:121:ARG:O    | 2.16                     | 0.44              |
| 75:sg:159:ASN:HD21 | 75:sg:162:ASN:ND2  | 2.03                     | 0.44              |
| 76:sM:52:LEU:HD22  | 76:sM:65:VAL:HG21  | 2.00                     | 0.44              |
| 77:sZ:46:ASN:OD1   | 77:sZ:46:ASN:N     | 2.50                     | 0.44              |
| 79:s2:821:G:H21    | 79:s2:824:C:H4'    | 1.81                     | 0.44              |
| 79:s2:1121:G:C5    | 79:s2:1122:A:N7    | 2.86                     | 0.44              |
| 79:s2:1133:A:C4    | 79:s2:1134:G:C8    | 3.06                     | 0.44              |
| 79:s2:1451:G:H1'   | 79:s2:1474:A:N6    | 2.32                     | 0.44              |
| 79:s2:1523:C:H2'   | 79:s2:1524:G:C8    | 2.50                     | 0.44              |
| 79:s2:1528:G:H2'   | 79:s2:1529:C:C6    | 2.52                     | 0.44              |
| 79:s2:1592:C:H2'   | 79:s2:1593:C:C6    | 2.53                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 80:cB:416:VAL:HG12 | 80:cB:468:ASN:O    | 2.17                     | 0.44              |
| 80:cB:652:PHE:HB2  | 80:cB:656:GLY:O    | 2.18                     | 0.44              |
| 80:cB:655:ASP:H    | 80:cB:684:GLN:HE22 | 1.64                     | 0.44              |
| 83:ls:162:LYS:HA   | 83:ls:162:LYS:HD2  | 1.72                     | 0.44              |
| 84:lt:15:LEU:H     | 84:lt:15:LEU:CD2   | 2.28                     | 0.44              |
| 85:l5:928:C:H2'    | 85:l5:929:A:C8     | 2.52                     | 0.44              |
| 85:l5:1854:G:N2    | 85:l5:4394:A:O4'   | 2.50                     | 0.44              |
| 85:l5:1952:G:H2'   | 85:l5:1953:U:H6    | 1.82                     | 0.44              |
| 85:l5:2376:A:H2'   | 85:l5:2377:C:C6    | 2.52                     | 0.44              |
| 85:l5:2498:C:H2'   | 85:l5:2499:C:C6    | 2.47                     | 0.44              |
| 85:l5:4134:C:C2    | 85:l5:4151:G:C2    | 3.04                     | 0.44              |
| 85:l5:4159:C:H2'   | 85:l5:4160:C:H6    | 1.82                     | 0.44              |
| 85:l5:4378:A:O2'   | 85:l5:4379:A:H2'   | 2.18                     | 0.44              |
| 85:l5:4524:G:H4'   | 85:l5:4524:G:OP2   | 2.16                     | 0.44              |
| 85:l5:4652:G:H2'   | 85:l5:4653:C:H6    | 1.82                     | 0.44              |
| 85:l5:4907:G:C6    | 85:l5:4915:G:C6    | 3.05                     | 0.44              |
| 80:CB:188:ILE:HA   | 80:CB:191:THR:HG22 | 1.98                     | 0.44              |
| 80:CB:256:MET:C    | 80:CB:256:MET:HE3  | 2.42                     | 0.44              |
| 80:CB:351:LEU:HA   | 80:CB:354:ILE:HG22 | 1.99                     | 0.44              |
| 80:CB:594:LYS:HD2  | 80:CB:594:LYS:HA   | 1.80                     | 0.44              |
| 80:CB:629:LYS:O    | 80:CB:633:ARG:HG2  | 2.16                     | 0.44              |
| 6:SG:174:PRO:O     | 79:S2:77:A:O2'     | 2.29                     | 0.44              |
| 86:Se:8:ARG:O      | 79:S2:616:A:H4'    | 2.17                     | 0.44              |
| 15:SC:182:CYS:HB2  | 18:SW:95:PRO:HB2   | 1.99                     | 0.44              |
| 15:SC:215:MET:SD   | 15:SC:216:MET:N    | 2.91                     | 0.44              |
| 19:Sb:49:HIS:HA    | 19:Sb:70:LYS:HA    | 1.99                     | 0.44              |
| 85:L5:55:G:P       | 55:Lj:43:ARG:HH22  | 2.40                     | 0.44              |
| 85:L5:486:C:H2'    | 85:L5:487:G:H8     | 1.82                     | 0.44              |
| 85:L5:671:G:H2'    | 85:L5:672:C:C6     | 2.52                     | 0.44              |
| 85:L5:1094:G:C5    | 85:L5:1203:G:C2    | 3.05                     | 0.44              |
| 85:L5:1266:G:C8    | 47:Lb:95:ARG:HG3   | 2.52                     | 0.44              |
| 85:L5:1628:C:H42   | 22:LA:3:ARG:NH1    | 2.16                     | 0.44              |
| 85:L5:1705:G:H3'   | 85:L5:1705:G:N3    | 2.31                     | 0.44              |
| 85:L5:1840:G:H2'   | 85:L5:1841:C:C6    | 2.53                     | 0.44              |
| 85:L5:2573:A:H2'   | 85:L5:2574:G:O4'   | 2.18                     | 0.44              |
| 85:L5:2659:A:N6    | 85:L5:2673:G:C4    | 2.86                     | 0.44              |
| 85:L5:2823:G:OP2   | 38:LR:20:LYS:HE3   | 2.17                     | 0.44              |
| 85:L5:3593:C:H1'   | 85:L5:3595:U:O4    | 2.17                     | 0.44              |
| 85:L5:3710:G:N2    | 85:L5:3711:A:N7    | 2.64                     | 0.44              |
| 85:L5:4055:U:H1'   | 63:Lz:164:CYS:SG   | 2.57                     | 0.44              |
| 85:L5:4091:G:C6    | 85:L5:4114:C:N4    | 2.85                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 85:L5:4102:C:H2'   | 85:L5:4106:G:H5''  | 1.99                     | 0.44              |
| 85:L5:4252:C:H3'   | 85:L5:4253:A:C8    | 2.52                     | 0.44              |
| 85:L5:4258:C:C2    | 85:L5:4259:C:C5    | 3.05                     | 0.44              |
| 85:L5:4389:C:H2'   | 85:L5:4390:A:C8    | 2.52                     | 0.44              |
| 85:L5:4664:A:H3'   | 85:L5:4665:A:H8    | 1.81                     | 0.44              |
| 85:L5:4968:A:H2'   | 85:L5:4969:C:C6    | 2.53                     | 0.44              |
| 85:L5:5018:C:H2'   | 85:L5:5019:A:H8    | 1.83                     | 0.44              |
| 21:L8:75:G:H2'     | 21:L8:76:C:C6      | 2.52                     | 0.44              |
| 21:L8:82:A:N7      | 21:L8:84:A:H5''    | 2.32                     | 0.44              |
| 24:LC:361:LEU:HA   | 24:LC:364:LYS:HG2  | 1.98                     | 0.44              |
| 25:LD:51:MET:HB2   | 25:LD:144:CYS:SG   | 2.58                     | 0.44              |
| 27:LF:28:LEU:HD12  | 27:LF:29:LYS:N     | 2.33                     | 0.44              |
| 31:LJ:19:LYS:HG3   | 31:LJ:21:CYS:SG    | 2.57                     | 0.44              |
| 32:LL:30:ALA:HA    | 32:LL:33:ILE:HG22  | 1.99                     | 0.44              |
| 34:LN:80:THR:OG1   | 34:LN:81:TYR:N     | 2.50                     | 0.44              |
| 37:LQ:97:LYS:C     | 37:LQ:98:LEU:HD22  | 2.43                     | 0.44              |
| 38:LR:99:MET:SD    | 38:LR:103:ARG:CZ   | 3.06                     | 0.44              |
| 39:LS:81:TRP:CD1   | 39:LS:94:TYR:HB2   | 2.53                     | 0.44              |
| 42:LV:61:VAL:N     | 42:LV:79:ALA:O     | 2.33                     | 0.44              |
| 43:LX:109:ILE:HD12 | 43:LX:124:VAL:HG21 | 2.00                     | 0.44              |
| 45:LZ:50:PRO:HG3   | 45:LZ:122:TYR:CE1  | 2.52                     | 0.44              |
| 48:Lc:29:LEU:HD12  | 48:Lc:30:GLY:N     | 2.32                     | 0.44              |
| 54:Li:54:GLU:O     | 54:Li:58:MET:HG3   | 2.17                     | 0.44              |
| 55:Lj:72:ARG:HA    | 55:Lj:75:ARG:HH21  | 1.83                     | 0.44              |
| 64:SR:34:VAL:O     | 64:SR:38:ILE:HG12  | 2.17                     | 0.44              |
| 64:SR:95:ILE:O     | 64:SR:95:ILE:HG23  | 2.17                     | 0.44              |
| 70:SS:123:LEU:HD12 | 70:SS:127:TRP:CZ2  | 2.52                     | 0.44              |
| 71:ST:10:ASN:CG    | 71:ST:13:GLU:HG2   | 2.42                     | 0.44              |
| 71:ST:60:THR:HG22  | 71:ST:75:MET:SD    | 2.57                     | 0.44              |
| 79:S2:71:G:H3'     | 79:S2:72:C:H4'     | 1.98                     | 0.44              |
| 79:S2:497:C:H2'    | 79:S2:498:C:C6     | 2.52                     | 0.44              |
| 79:S2:834:C:H42    | 79:S2:839:C:H42    | 1.64                     | 0.44              |
| 79:S2:1040:G:C6    | 79:S2:1076:G:C6    | 3.05                     | 0.44              |
| 79:S2:1458:G:H2'   | 79:S2:1459:G:C8    | 2.51                     | 0.44              |
| 79:S2:1607:A:N6    | 79:S2:1632:G:H1'   | 2.31                     | 0.44              |
| 79:S2:1777:G:H8    | 79:S2:1777:G:OP2   | 2.00                     | 0.44              |
| 81:AP:26:G:C6      | 81:AP:27:U:C4      | 3.05                     | 0.44              |
| 87:IW:101:ARG:HB2  | 87:IW:102:LYS:NZ   | 2.33                     | 0.44              |
| 3:sI:125:LYS:H     | 3:sI:128:LYS:NZ    | 2.16                     | 0.44              |
| 4:sL:112:HIS:O     | 4:sL:142:VAL:HG23  | 2.17                     | 0.44              |
| 6:sG:133:LEU:HD12  | 79:s2:65:C:C4      | 2.53                     | 0.44              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 6:sG:221:LYS:O    | 6:sG:224:ARG:HG3   | 2.18                     | 0.44              |
| 10:sA:195:TRP:CE3 | 10:sA:197:VAL:HB   | 2.52                     | 0.44              |
| 11:sB:62:LEU:HA   | 11:sB:65:ARG:CD    | 2.42                     | 0.44              |
| 11:sB:63:LYS:HA   | 11:sB:88:THR:HG22  | 1.99                     | 0.44              |
| 11:sB:146:ARG:HB2 | 11:sB:149:GLN:NE2  | 2.33                     | 0.44              |
| 12:sH:37:LYS:NZ   | 12:sH:40:LEU:HB2   | 2.32                     | 0.44              |
| 20:l7:64:G:H2'    | 20:l7:65:G:H8      | 1.81                     | 0.44              |
| 23:lB:51:ALA:HA   | 23:lB:323:TYR:CD1  | 2.53                     | 0.44              |
| 23:lB:394:LYS:O   | 23:lB:397:ILE:HG13 | 2.17                     | 0.44              |
| 24:lC:31:PRO:HG3  | 24:lC:282:HIS:CD2  | 2.53                     | 0.44              |
| 24:lC:256:ALA:O   | 24:lC:260:LEU:HG   | 2.17                     | 0.44              |
| 26:lE:68:MET:SD   | 26:lE:68:MET:N     | 2.91                     | 0.44              |
| 27:lF:46:ARG:NE   | 85:l5:1705:G:H21   | 2.16                     | 0.44              |
| 28:lG:104:PRO:HG3 | 28:lG:194:VAL:HG23 | 2.00                     | 0.44              |
| 28:lG:249:ARG:NH1 | 85:l5:4075:U:OP1   | 2.27                     | 0.44              |
| 29:lH:18:ILE:CD1  | 29:lH:27:VAL:HG22  | 2.47                     | 0.44              |
| 32:lL:76:PHE:O    | 32:lL:99:ASP:N     | 2.39                     | 0.44              |
| 35:lO:171:LYS:HA  | 35:lO:174:LEU:HG   | 1.99                     | 0.44              |
| 43:lX:65:ALA:HB2  | 53:lh:69:LEU:HD21  | 2.00                     | 0.44              |
| 47:lb:53:GLY:HA3  | 47:lb:56:LYS:NZ    | 2.32                     | 0.44              |
| 63:lz:139:THR:OG1 | 63:lz:156:LYS:HE2  | 2.17                     | 0.44              |
| 68:sP:127:LYS:O   | 68:sP:128:HIS:HB2  | 2.16                     | 0.44              |
| 69:sQ:110:ASP:O   | 69:sQ:114:GLN:HB2  | 2.18                     | 0.44              |
| 71:sT:144:LYS:HD3 | 71:sT:144:LYS:HA   | 1.85                     | 0.44              |
| 72:sU:51:LYS:HG2  | 72:sU:90:ASP:OD1   | 2.16                     | 0.44              |
| 73:sc:14:VAL:HG12 | 73:sc:54:ASP:O     | 2.17                     | 0.44              |
| 75:sg:202:PRO:HD3 | 75:sg:241:PHE:HB3  | 1.99                     | 0.44              |
| 75:sg:241:PHE:CD2 | 75:sg:248:LEU:HD13 | 2.52                     | 0.44              |
| 76:sM:59:PRO:C    | 76:sM:63:LYS:HZ2   | 2.26                     | 0.44              |
| 78:sf:107:LYS:NZ  | 78:sf:108:VAL:H    | 2.14                     | 0.44              |
| 79:s2:74:G:H5''   | 79:s2:76:U:C4      | 2.53                     | 0.44              |
| 79:s2:92:A:H61    | 79:s2:444:G:H1'    | 1.82                     | 0.44              |
| 79:s2:478:G:H4'   | 80:cB:409:ARG:NH1  | 2.31                     | 0.44              |
| 79:s2:578:C:H2'   | 79:s2:579:C:H6     | 1.81                     | 0.44              |
| 79:s2:678:U:C4    | 79:s2:679:A:N7     | 2.86                     | 0.44              |
| 79:s2:822:U:O4    | 79:s2:826:A:N7     | 2.50                     | 0.44              |
| 79:s2:909:G:H2'   | 79:s2:910:G:H8     | 1.82                     | 0.44              |
| 79:s2:1207:G:N2   | 79:s2:1837:G:H2'   | 2.32                     | 0.44              |
| 79:s2:1231:C:H2'  | 79:s2:1232:U:O4'   | 2.17                     | 0.44              |
| 79:s2:1255:G:C6   | 79:s2:1257:G:C6    | 3.05                     | 0.44              |
| 79:s2:1683:C:C2   | 79:s2:1684:C:C5    | 3.05                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 79:s2:1752:C:N4    | 79:s2:1754:G:O6    | 2.50                     | 0.44              |
| 80:cB:609:PHE:CD1  | 80:cB:613:LEU:HB2  | 2.51                     | 0.44              |
| 82:pE:29:A:H2'     | 82:pE:30:G:H8      | 1.81                     | 0.44              |
| 83:ls:143:ILE:HG22 | 83:ls:145:THR:HG23 | 1.97                     | 0.44              |
| 85:l5:169:G:N2     | 85:l5:267:G:C4     | 2.85                     | 0.44              |
| 85:l5:185:C:O2     | 85:l5:187:U:O2'    | 2.35                     | 0.44              |
| 85:l5:191:G:N1     | 85:l5:251:C:N3     | 2.65                     | 0.44              |
| 85:l5:675:C:H2'    | 85:l5:676:C:H6     | 1.82                     | 0.44              |
| 85:l5:1328:G:C6    | 85:l5:1329:G:C6    | 3.05                     | 0.44              |
| 85:l5:1519:C:H2'   | 85:l5:1520:C:C6    | 2.52                     | 0.44              |
| 85:l5:1592:G:C2    | 85:l5:1593:A:C8    | 3.06                     | 0.44              |
| 85:l5:1828:C:C2    | 85:l5:1829:G:C8    | 3.05                     | 0.44              |
| 85:l5:1878:G:H2'   | 85:l5:1879:C:H6    | 1.83                     | 0.44              |
| 85:l5:2519:U:O2'   | 85:l5:2530:U:O2    | 2.27                     | 0.44              |
| 85:l5:3611:A:H2    | 85:l5:5016:A:C8    | 2.31                     | 0.44              |
| 85:l5:3872:A:H2'   | 85:l5:3873:G:H8    | 1.83                     | 0.44              |
| 85:l5:4061:G:O2'   | 85:l5:4062:A:OP1   | 2.31                     | 0.44              |
| 85:l5:4192:A:H2'   | 85:l5:4193:C:H6    | 1.81                     | 0.44              |
| 85:l5:4485:C:C2    | 85:l5:4486:C:C5    | 3.05                     | 0.44              |
| 85:l5:4619:U:H2'   | 85:l5:4620:U:H6    | 1.82                     | 0.44              |
| 85:l5:5066:U:H2'   | 85:l5:5067:U:C6    | 2.52                     | 0.44              |
| 80:CB:10:ARG:HH21  | 80:CB:14:ASP:HB3   | 1.82                     | 0.44              |
| 80:CB:309:LYS:O    | 80:CB:312:THR:OG1  | 2.29                     | 0.44              |
| 80:CB:662:LEU:HA   | 80:CB:702:PHE:O    | 2.17                     | 0.44              |
| 2:SE:120:LYS:HD3   | 2:SE:120:LYS:HA    | 1.76                     | 0.44              |
| 7:SJ:33:GLY:HA3    | 86:Se:38:TYR:CD1   | 2.52                     | 0.44              |
| 7:SJ:46:VAL:O      | 7:SJ:49:THR:OG1    | 2.30                     | 0.44              |
| 8:SY:43:LYS:O      | 8:SY:47:MET:HG3    | 2.17                     | 0.44              |
| 10:SA:41:ARG:HB2   | 10:SA:47:TYR:HE1   | 1.81                     | 0.44              |
| 12:SH:163:GLN:CD   | 12:SH:163:GLN:H    | 2.25                     | 0.44              |
| 18:SW:22:LYS:HA    | 19:Sb:3:LEU:HD13   | 1.98                     | 0.44              |
| 85:L5:11:G:H2'     | 85:L5:12:A:C8      | 2.52                     | 0.44              |
| 85:L5:159:C:H3'    | 54:Li:25:ARG:NH2   | 2.32                     | 0.44              |
| 85:L5:221:C:C2     | 85:L5:222:C:C5     | 3.05                     | 0.44              |
| 85:L5:349:A:OP1    | 24:LC:50:GLN:N     | 2.34                     | 0.44              |
| 85:L5:676:C:C2     | 85:L5:677:G:C8     | 3.05                     | 0.44              |
| 85:L5:911:U:H3'    | 85:L5:911:U:OP2    | 2.18                     | 0.44              |
| 85:L5:1823:G:H2'   | 85:L5:1824:G:C8    | 2.52                     | 0.44              |
| 85:L5:2295:C:H2'   | 85:L5:2296:G:H8    | 1.83                     | 0.44              |
| 85:L5:3695:U:H2'   | 85:L5:3696:C:H6    | 1.81                     | 0.44              |
| 85:L5:3949:A:H2'   | 85:L5:3949:A:OP2   | 2.18                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 85:L5:4110:C:O3'   | 85:L5:4112:C:O4'   | 2.35                     | 0.44              |
| 85:L5:4203:A:C4    | 85:L5:4221:C:H5'   | 2.52                     | 0.44              |
| 85:L5:4233:A:OP2   | 60:Lo:99:ARG:NH2   | 2.50                     | 0.44              |
| 85:L5:4321:U:H2'   | 85:L5:4322:G:C8    | 2.52                     | 0.44              |
| 85:L5:4525:C:C2    | 85:L5:4526:U:C5    | 3.06                     | 0.44              |
| 85:L5:4586:G:H2'   | 85:L5:4587:G:C8    | 2.53                     | 0.44              |
| 85:L5:4595:G:H2'   | 85:L5:4596:C:H6    | 1.81                     | 0.44              |
| 20:L7:112:U:H2'    | 20:L7:113:G:H8     | 1.81                     | 0.44              |
| 21:L8:62:A:P       | 53:Lh:51:ARG:HH22  | 2.40                     | 0.44              |
| 21:L8:78:G:H2'     | 21:L8:79:G:C8      | 2.53                     | 0.44              |
| 26:LE:50:LEU:HD22  | 26:LE:56:ARG:HA    | 2.00                     | 0.44              |
| 26:LE:111:LYS:HE2  | 26:LE:111:LYS:HB2  | 1.88                     | 0.44              |
| 39:LS:54:MET:HE3   | 39:LS:55:LYS:H     | 1.82                     | 0.44              |
| 41:LU:21:PHE:CE1   | 41:LU:80:LYS:HB2   | 2.52                     | 0.44              |
| 41:LU:97:ARG:O     | 41:LU:97:ARG:HG3   | 2.17                     | 0.44              |
| 44:LY:112:ASP:OD1  | 44:LY:115:ARG:HB2  | 2.18                     | 0.44              |
| 49:Ld:57:MET:HE3   | 49:Ld:57:MET:HA    | 1.98                     | 0.44              |
| 49:Ld:63:ARG:O     | 49:Ld:105:LEU:HA   | 2.17                     | 0.44              |
| 71:ST:39:LEU:O     | 71:ST:43:LYS:HB3   | 2.17                     | 0.44              |
| 77:SZ:94:LYS:HZ2   | 77:SZ:96:LEU:HB3   | 1.80                     | 0.44              |
| 79:S2:521:A:H2'    | 79:S2:522:A:C8     | 2.53                     | 0.44              |
| 79:S2:696:G:H21    | 79:S2:737:G:N2     | 2.15                     | 0.44              |
| 79:S2:838:G:O2'    | 79:S2:840:C:OP2    | 2.27                     | 0.44              |
| 79:S2:1231:C:H2'   | 79:S2:1232:U:C6    | 2.52                     | 0.44              |
| 79:S2:1458:G:C4    | 79:S2:1459:G:C8    | 3.05                     | 0.44              |
| 79:S2:1722:G:H2'   | 79:S2:1723:G:H8    | 1.82                     | 0.44              |
| 79:S2:1792:G:H2'   | 79:S2:1793:A:C8    | 2.49                     | 0.44              |
| 84:Lt:65:GLN:OE1   | 84:Lt:67:ARG:N     | 2.50                     | 0.44              |
| 84:Lt:127:GLY:CA   | 84:Lt:130:LYS:HG2  | 2.47                     | 0.44              |
| 2:sE:15:PRO:HG3    | 2:sE:39:ARG:HH21   | 1.82                     | 0.44              |
| 3:sI:22:HIS:ND1    | 3:sI:23:LYS:O      | 2.50                     | 0.44              |
| 3:sI:36:THR:HG22   | 3:sI:57:ALA:O      | 2.17                     | 0.44              |
| 3:sI:190:LEU:HD12  | 3:sI:190:LEU:HA    | 1.75                     | 0.44              |
| 9:se:11:LYS:C      | 9:se:15:GLN:HE21   | 2.25                     | 0.44              |
| 9:se:54:GLY:O      | 9:se:57:ALA:HB2    | 2.17                     | 0.44              |
| 10:sA:59:LEU:HD21  | 13:sV:79:VAL:HG11  | 1.99                     | 0.44              |
| 12:sH:143:ARG:HB3  | 12:sH:145:ARG:HH21 | 1.82                     | 0.44              |
| 13:sV:46:PHE:HD1   | 13:sV:48:GLY:H     | 1.64                     | 0.44              |
| 15:sC:204:ILE:HD11 | 15:sC:219:ILE:HG22 | 1.99                     | 0.44              |
| 15:sC:206:SER:OG   | 15:sC:210:PRO:HG2  | 2.17                     | 0.44              |
| 16:sN:20:ARG:NH2   | 79:s2:918:U:H5''   | 2.33                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 16:sN:83:ASP:OD1   | 16:sN:84:LEU:HG    | 2.18                     | 0.44              |
| 16:sN:104:ARG:O    | 16:sN:104:ARG:HG2  | 2.17                     | 0.44              |
| 18:sW:32:LYS:HA    | 18:sW:35:VAL:HG22  | 2.00                     | 0.44              |
| 20:l7:57:C:H2'     | 20:l7:58:A:C8      | 2.53                     | 0.44              |
| 24:lC:146:GLU:N    | 24:lC:146:GLU:CD   | 2.76                     | 0.44              |
| 24:lC:189:MET:SD   | 24:lC:189:MET:N    | 2.91                     | 0.44              |
| 27:lF:190:LEU:H    | 27:lF:190:LEU:HD12 | 1.83                     | 0.44              |
| 29:lH:61:TRP:CE2   | 33:lM:33:GLN:NE2   | 2.85                     | 0.44              |
| 29:lH:172:ILE:HG12 | 58:lm:90:ASN:OD1   | 2.17                     | 0.44              |
| 32:lL:103:ARG:HD3  | 32:lL:103:ARG:H    | 1.82                     | 0.44              |
| 37:lQ:35:LEU:HD23  | 37:lQ:35:LEU:HA    | 1.86                     | 0.44              |
| 38:lR:76:MET:SD    | 38:lR:76:MET:N     | 2.90                     | 0.44              |
| 41:lU:24:ASP:OD1   | 41:lU:25:CYS:N     | 2.50                     | 0.44              |
| 46:la:58:MET:HE1   | 85:l5:4364:G:H1'   | 1.97                     | 0.44              |
| 60:lo:45:GLN:HE22  | 60:lo:51:GLN:CD    | 2.25                     | 0.44              |
| 63:lz:90:LEU:HA    | 63:lz:93:LEU:HG    | 1.99                     | 0.44              |
| 64:sR:17:ILE:CG1   | 64:sR:54:VAL:HG13  | 2.47                     | 0.44              |
| 64:sR:94:GLU:OE1   | 64:sR:94:GLU:HA    | 2.18                     | 0.44              |
| 64:sR:132:ARG:HH11 | 64:sR:133:GLY:HA3  | 1.83                     | 0.44              |
| 65:sD:123:LEU:O    | 65:sD:126:ILE:HG13 | 2.16                     | 0.44              |
| 65:sD:133:GLY:N    | 65:sD:189:MET:SD   | 2.91                     | 0.44              |
| 67:sK:21:MET:CE    | 67:sK:49:MET:HE3   | 2.48                     | 0.44              |
| 69:sQ:41:MET:HE1   | 71:sT:9:VAL:N      | 2.33                     | 0.44              |
| 69:sQ:74:GLY:HA2   | 79:s2:1545:A:H5'   | 2.00                     | 0.44              |
| 70:sS:68:ILE:O     | 70:sS:72:GLN:HG2   | 2.17                     | 0.44              |
| 70:sS:101:ASN:OD1  | 70:sS:102:GLY:N    | 2.50                     | 0.44              |
| 72:sU:66:ARG:HB2   | 79:s2:1256:G:H8    | 1.81                     | 0.44              |
| 75:sg:12:LYS:HD3   | 75:sg:306:LEU:HG   | 1.99                     | 0.44              |
| 75:sg:201:SER:OG   | 75:sg:203:ASP:O    | 2.30                     | 0.44              |
| 79:s2:114:G:C2     | 79:s2:383:G:C5     | 3.06                     | 0.44              |
| 79:s2:342:C:C2     | 79:s2:343:A:C8     | 3.06                     | 0.44              |
| 79:s2:463:C:H4'    | 80:cB:50:ARG:HH22  | 1.82                     | 0.44              |
| 80:cB:110:ASP:OD2  | 80:cB:112:SER:OG   | 2.33                     | 0.44              |
| 81:aP:26:G:C6      | 81:aP:27:U:C4      | 3.06                     | 0.44              |
| 85:l5:104:G:C2     | 85:l5:105:A:N7     | 2.86                     | 0.44              |
| 85:l5:127:G:C6     | 85:l5:142:G:C6     | 3.05                     | 0.44              |
| 85:l5:133:C:H2'    | 85:l5:134:G:H4'    | 1.99                     | 0.44              |
| 85:l5:415:G:C5     | 85:l5:416:U:C5     | 3.06                     | 0.44              |
| 85:l5:726:G:H2'    | 85:l5:727:C:C6     | 2.53                     | 0.44              |
| 85:l5:1097:C:H2'   | 85:l5:1098:G:H8    | 1.81                     | 0.44              |
| 85:l5:1189:G:H2'   | 85:l5:1190:C:C6    | 2.52                     | 0.44              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 85:L5:1568:C:H2'   | 85:L5:1569:U:C6   | 2.52                     | 0.44              |
| 85:L5:1744:U:C2    | 85:L5:1745:G:C8   | 3.05                     | 0.44              |
| 85:L5:2010:A:H2'   | 85:L5:2011:C:O4'  | 2.18                     | 0.44              |
| 85:L5:2370:A:H3'   | 85:L5:2826:U:O2'  | 2.16                     | 0.44              |
| 85:L5:2607:C:H2'   | 85:L5:2608:G:C8   | 2.51                     | 0.44              |
| 85:L5:3748:A:H2'   | 85:L5:3749:C:C6   | 2.53                     | 0.44              |
| 85:L5:3849:A:H2'   | 85:L5:3850:C:C6   | 2.52                     | 0.44              |
| 85:L5:4691:A:N1    | 85:L5:4700:A:C8   | 2.86                     | 0.44              |
| 85:L5:4903:G:N1    | 85:L5:4919:G:C6   | 2.86                     | 0.44              |
| 80:CB:260:LEU:HD12 | 80:CB:260:LEU:HA  | 1.79                     | 0.44              |
| 80:CB:556:ILE:HG13 | 80:CB:557:CYS:N   | 2.32                     | 0.44              |
| 2:SE:173:ILE:HD11  | 2:SE:235:TRP:CE2  | 2.52                     | 0.44              |
| 5:SX:87:ASN:ND2    | 5:SX:134:TYR:CG   | 2.85                     | 0.44              |
| 5:SX:105:PHE:CE1   | 5:SX:112:VAL:HG11 | 2.53                     | 0.44              |
| 6:SG:50:VAL:HG23   | 6:SG:112:VAL:C    | 2.42                     | 0.44              |
| 7:SJ:133:ARG:NH2   | 79:S2:562:U:O2'   | 2.49                     | 0.44              |
| 8:SY:56:PHE:O      | 8:SY:74:MET:N     | 2.48                     | 0.44              |
| 15:SC:82:TYR:CD2   | 15:SC:164:PRO:HD3 | 2.53                     | 0.44              |
| 16:SN:71:ILE:HA    | 16:SN:74:ILE:HD13 | 1.99                     | 0.44              |
| 17:SO:42:VAL:O     | 17:SO:42:VAL:CG1  | 2.65                     | 0.44              |
| 85:L5:119:G:O6     | 28:LG:132:ARG:HG3 | 2.16                     | 0.44              |
| 85:L5:147:A:H2'    | 85:L5:148:C:O4'   | 2.18                     | 0.44              |
| 85:L5:190:G:H2'    | 85:L5:191:G:H8    | 1.83                     | 0.44              |
| 85:L5:243:A:H2'    | 85:L5:244:G:C8    | 2.53                     | 0.44              |
| 85:L5:307:A:O5'    | 85:L5:307:A:H8    | 2.00                     | 0.44              |
| 85:L5:1449:C:H2'   | 85:L5:1450:C:C6   | 2.53                     | 0.44              |
| 85:L5:1487:G:H2'   | 85:L5:1488:G:H8   | 1.81                     | 0.44              |
| 85:L5:1630:A:H5''  | 85:L5:1631:A:N7   | 2.32                     | 0.44              |
| 85:L5:1777:C:H2'   | 85:L5:1778:C:H6   | 1.82                     | 0.44              |
| 85:L5:1802:A:H4'   | 40:LT:105:PHE:CE1 | 2.53                     | 0.44              |
| 85:L5:1833:G:C2    | 85:L5:1835:G:C4   | 3.04                     | 0.44              |
| 85:L5:1912:G:H2'   | 85:L5:1913:C:C6   | 2.52                     | 0.44              |
| 85:L5:1934:A:O2'   | 85:L5:2059:C:OP1  | 2.24                     | 0.44              |
| 85:L5:1961:G:H1'   | 85:L5:2025:A:H61  | 1.83                     | 0.44              |
| 85:L5:2480:G:H2'   | 85:L5:2481:G:C8   | 2.53                     | 0.44              |
| 85:L5:2512:A:C5    | 57:L1:4:HIS:HB3   | 2.52                     | 0.44              |
| 85:L5:2579:G:N1    | 85:L5:2583:C:N3   | 2.66                     | 0.44              |
| 85:L5:2589:C:H2'   | 85:L5:2590:G:O4'  | 2.17                     | 0.44              |
| 85:L5:2656:U:H2'   | 85:L5:2657:G:C8   | 2.53                     | 0.44              |
| 85:L5:3589:G:H8    | 85:L5:3589:G:OP2  | 1.99                     | 0.44              |
| 85:L5:3634:G:N2    | 85:L5:3636:C:H5'' | 2.33                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 85:L5:3661:G:N7    | 22:LA:152:SER:OG   | 2.39                     | 0.44              |
| 85:L5:3855:C:H2'   | 85:L5:3856:A:H8    | 1.82                     | 0.44              |
| 85:L5:4604:G:N2    | 85:L5:4607:A:OP2   | 2.43                     | 0.44              |
| 85:L5:4638:U:H2'   | 85:L5:4639:G:N3    | 2.32                     | 0.44              |
| 85:L5:4754:G:N7    | 26:LE:278:THR:HB   | 2.32                     | 0.44              |
| 85:L5:4877:G:H2'   | 85:L5:4878:C:H6    | 1.82                     | 0.44              |
| 85:L5:4917:C:H2'   | 85:L5:4918:C:C6    | 2.53                     | 0.44              |
| 24:LC:198:ASN:OD1  | 44:LY:10:ASP:HA    | 2.17                     | 0.44              |
| 25:LD:84:PRO:HB3   | 25:LD:89:LYS:HA    | 1.99                     | 0.44              |
| 27:LF:70:ARG:HG3   | 27:LF:71:MET:CE    | 2.47                     | 0.44              |
| 31:LJ:19:LYS:HD3   | 31:LJ:75:ARG:NH2   | 2.32                     | 0.44              |
| 40:LT:93:ILE:O     | 40:LT:96:ILE:HG13  | 2.17                     | 0.44              |
| 48:Lc:37:MET:HE3   | 48:Lc:42:LYS:HZ1   | 1.82                     | 0.44              |
| 53:Lh:22:ASP:O     | 53:Lh:26:VAL:HG12  | 2.17                     | 0.44              |
| 63:Lz:29:LEU:HD11  | 63:Lz:60:ARG:HH21  | 1.82                     | 0.44              |
| 63:Lz:193:LEU:HG   | 63:Lz:194:LEU:H    | 1.82                     | 0.44              |
| 68:SP:28:MET:HE3   | 68:SP:32:GLN:HG2   | 1.99                     | 0.44              |
| 69:SQ:18:THR:OG1   | 79:S2:1672:U:OP1   | 2.34                     | 0.44              |
| 70:SS:70:ILE:HA    | 70:SS:77:TYR:CD2   | 2.52                     | 0.44              |
| 70:SS:110:ASP:O    | 70:SS:113:ARG:HG3  | 2.17                     | 0.44              |
| 79:S2:153:G:N1     | 79:S2:166:A:C6     | 2.86                     | 0.44              |
| 79:S2:1088:U:H4'   | 79:S2:1089:G:OP2   | 2.16                     | 0.44              |
| 79:S2:1230:C:H2'   | 79:S2:1231:C:H6    | 1.82                     | 0.44              |
| 79:S2:1301:A:H2'   | 79:S2:1303:C:C6    | 2.52                     | 0.44              |
| 79:S2:1355:C:H3'   | 79:S2:1356:G:C8    | 2.52                     | 0.44              |
| 79:S2:1720:U:H5''  | 79:S2:1721:U:H5''  | 2.00                     | 0.44              |
| 79:S2:1756:C:N4    | 79:S2:1776:G:O6    | 2.50                     | 0.44              |
| 79:S2:1853:C:H2'   | 79:S2:1854:U:C6    | 2.53                     | 0.44              |
| 83:Ls:138:PHE:CZ   | 83:Ls:152:ILE:HG21 | 2.52                     | 0.44              |
| 87:IW:110:ARG:NH2  | 87:IW:111:ALA:HB2  | 2.33                     | 0.44              |
| 5:sX:131:LEU:HD23  | 5:sX:135:LYS:HG2   | 2.00                     | 0.44              |
| 7:sJ:39:ASN:O      | 7:sJ:42:GLU:HG3    | 2.18                     | 0.44              |
| 7:sJ:169:ARG:HA    | 7:sJ:169:ARG:HD2   | 1.61                     | 0.44              |
| 8:sY:79:LEU:HD23   | 8:sY:79:LEU:H      | 1.81                     | 0.44              |
| 10:sA:5:LEU:H      | 13:sV:79:VAL:HG23  | 1.82                     | 0.44              |
| 10:sA:45:GLY:HA3   | 64:sR:128:PHE:HE2  | 1.82                     | 0.44              |
| 10:sA:121:LEU:HD12 | 10:sA:122:LEU:H    | 1.83                     | 0.44              |
| 11:sB:85:LYS:HG2   | 11:sB:102:GLY:C    | 2.41                     | 0.44              |
| 16:sN:18:TYR:HE1   | 18:sW:56:HIS:CE1   | 2.35                     | 0.44              |
| 16:sN:39:LYS:CA    | 16:sN:42:LYS:HZ2   | 2.31                     | 0.44              |
| 18:sW:28:ARG:HD3   | 79:s2:921:G:C5     | 2.53                     | 0.44              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 18:sW:35:VAL:O     | 18:sW:39:THR:OG1  | 2.25                     | 0.44              |
| 18:sW:106:THR:HG22 | 18:sW:111:MET:SD  | 2.58                     | 0.44              |
| 24:lC:8:ILE:HD11   | 24:lC:24:LEU:HB2  | 1.98                     | 0.44              |
| 25:lD:228:LYS:C    | 25:lD:230:SER:H   | 2.26                     | 0.44              |
| 26:lE:216:TYR:HD2  | 26:lE:217:PHE:CD1 | 2.36                     | 0.44              |
| 26:lE:279:ASN:OD1  | 85:l5:4754:G:N7   | 2.51                     | 0.44              |
| 26:lE:282:TYR:O    | 26:lE:286:LEU:HG  | 2.17                     | 0.44              |
| 27:lF:151:ASN:ND2  | 85:l5:943:A:N7    | 2.66                     | 0.44              |
| 27:lF:185:ILE:HG23 | 27:lF:186:CYS:H   | 1.83                     | 0.44              |
| 29:lH:114:ILE:HG13 | 29:lH:124:ARG:HB2 | 1.99                     | 0.44              |
| 31:lJ:32:ARG:HD3   | 31:lJ:35:ARG:NH2  | 2.33                     | 0.44              |
| 32:lL:77:SER:O     | 32:lL:80:GLU:HG2  | 2.18                     | 0.44              |
| 33:lM:6:PHE:CE1    | 39:lS:152:PHE:C   | 2.96                     | 0.44              |
| 37:lQ:61:LEU:HB3   | 37:lQ:86:ILE:HD13 | 1.98                     | 0.44              |
| 38:lR:24:LEU:HD12  | 85:l5:2386:U:H4'  | 1.99                     | 0.44              |
| 40:lT:41:ASP:C     | 40:lT:42:ILE:HD13 | 2.43                     | 0.44              |
| 43:lX:101:ASP:OD1  | 43:lX:103:LYS:HG3 | 2.17                     | 0.44              |
| 48:lc:13:SER:O     | 48:lc:17:ARG:HG2  | 2.17                     | 0.44              |
| 48:lc:21:VAL:O     | 48:lc:25:GLY:N    | 2.50                     | 0.44              |
| 48:lc:36:LYS:HZ3   | 48:lc:40:GLN:HE21 | 1.62                     | 0.44              |
| 51:lf:79:GLY:O     | 51:lf:81:SER:N    | 2.50                     | 0.44              |
| 53:lh:78:TYR:CE2   | 85:l5:16:G:H5''   | 2.52                     | 0.44              |
| 64:sR:39:ALA:HA    | 65:sD:206:ASP:CA  | 2.47                     | 0.44              |
| 67:sK:1:MET:HE2    | 67:sK:1:MET:HA    | 2.00                     | 0.44              |
| 68:sP:86:LEU:HB3   | 68:sP:88:GLU:OE2  | 2.18                     | 0.44              |
| 69:sQ:80:GLN:O     | 69:sQ:84:ILE:HG12 | 2.17                     | 0.44              |
| 70:sS:88:LYS:HG2   | 79:s2:1612:G:H5'' | 1.99                     | 0.44              |
| 72:sU:56:MET:HG2   | 72:sU:86:LYS:HD2  | 2.00                     | 0.44              |
| 73:sc:54:ASP:C     | 73:sc:54:ASP:OD2  | 2.61                     | 0.44              |
| 75:sg:137:VAL:HG22 | 75:sg:138:CYS:O   | 2.17                     | 0.44              |
| 76:sM:33:ARG:HG3   | 76:sM:91:LEU:HD11 | 2.00                     | 0.44              |
| 76:sM:86:GLY:HA2   | 76:sM:89:VAL:HG12 | 1.99                     | 0.44              |
| 79:s2:140:C:H42    | 79:s2:313:A:H61   | 1.64                     | 0.44              |
| 79:s2:551:U:H2'    | 79:s2:552:G:C8    | 2.52                     | 0.44              |
| 79:s2:751:G:H1'    | 79:s2:793:G:N2    | 2.33                     | 0.44              |
| 79:s2:944:A:H2'    | 79:s2:945:U:H6    | 1.82                     | 0.44              |
| 79:s2:1242:U:C2    | 79:s2:1520:G:C8   | 3.05                     | 0.44              |
| 79:s2:1358:U:H2'   | 79:s2:1359:U:C6   | 2.53                     | 0.44              |
| 79:s2:1359:U:C2    | 79:s2:1360:U:H5   | 2.36                     | 0.44              |
| 79:s2:1548:G:H2'   | 79:s2:1549:U:H6   | 1.82                     | 0.44              |
| 79:s2:1707:U:H2'   | 79:s2:1708:C:O4'  | 2.17                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 80:cB:75:ILE:HA    | 80:cB:454:MET:HA   | 2.00                     | 0.44              |
| 80:cB:857:LYS:HD2  | 80:cB:857:LYS:HA   | 1.77                     | 0.44              |
| 81:aP:38:C:H2'     | 81:aP:39:G:O4'     | 2.18                     | 0.44              |
| 85:l5:100:C:H2'    | 85:l5:101:A:O4'    | 2.18                     | 0.44              |
| 85:l5:1176:C:H42   | 85:l5:1184:A:H61   | 0.62                     | 0.44              |
| 85:l5:1241:C:C4    | 85:l5:1242:G:C8    | 3.06                     | 0.44              |
| 85:l5:1320:U:H2'   | 85:l5:1321:G:O4'   | 2.17                     | 0.44              |
| 85:l5:1973:G:H2'   | 85:l5:1974:U:C5    | 2.52                     | 0.44              |
| 85:l5:2111:G:H2'   | 85:l5:2251:G:C2    | 2.53                     | 0.44              |
| 85:l5:2276:A:H2'   | 85:l5:2277:C:O4'   | 2.18                     | 0.44              |
| 85:l5:2290:C:C2    | 85:l5:2291:G:C8    | 3.05                     | 0.44              |
| 85:l5:2307:A:N6    | 85:l5:2331:G:H1'   | 2.32                     | 0.44              |
| 85:l5:2479:G:H2'   | 85:l5:2480:G:H8    | 1.83                     | 0.44              |
| 85:l5:2487:G:H8    | 85:l5:2487:G:OP2   | 2.00                     | 0.44              |
| 85:l5:4344:U:H2'   | 85:l5:4345:C:H6    | 1.82                     | 0.44              |
| 85:l5:4384:U:O2'   | 85:l5:4386:C:OP1   | 2.35                     | 0.44              |
| 85:l5:4505:C:H2'   | 85:l5:4506:C:H6    | 1.83                     | 0.44              |
| 85:l5:4759:C:H2'   | 85:l5:4760:G:H8    | 1.82                     | 0.44              |
| 85:l5:4774:C:O2'   | 85:l5:4775:C:O5'   | 2.35                     | 0.44              |
| 80:CB:159:LYS:HD3  | 80:CB:159:LYS:HA   | 1.62                     | 0.44              |
| 80:CB:227:GLN:C    | 80:CB:231:MET:SD   | 3.01                     | 0.44              |
| 80:CB:325:SER:HA   | 80:CB:328:LYS:HZ1  | 1.81                     | 0.44              |
| 3:SI:121:LEU:HD12  | 3:SI:121:LEU:HA    | 1.82                     | 0.44              |
| 3:SI:141:ARG:HB2   | 3:SI:146:GLN:OE1   | 2.18                     | 0.44              |
| 6:SG:64:LYS:HE3    | 6:SG:82:SER:HB3    | 1.98                     | 0.44              |
| 10:SA:207:PRO:HA   | 10:SA:210:ILE:CD1  | 2.47                     | 0.44              |
| 12:SH:148:LEU:HD12 | 12:SH:148:LEU:O    | 2.17                     | 0.44              |
| 15:SC:183:LYS:HE2  | 15:SC:196:ILE:HD12 | 1.99                     | 0.44              |
| 17:SO:98:ARG:NH1   | 79:S2:975:G:OP1    | 2.50                     | 0.44              |
| 85:L5:27:C:C2      | 85:L5:56:A:N1      | 2.86                     | 0.44              |
| 85:L5:91:G:O5'     | 85:L5:92:C:H5''    | 2.18                     | 0.44              |
| 85:L5:425:U:H2'    | 85:L5:426:A:C8     | 2.51                     | 0.44              |
| 85:L5:498:C:C2     | 85:L5:499:G:H1'    | 2.53                     | 0.44              |
| 85:L5:1076:C:H2'   | 85:L5:1077:C:C6    | 2.52                     | 0.44              |
| 85:L5:1211:G:H1'   | 27:LF:70:ARG:NH2   | 2.33                     | 0.44              |
| 85:L5:1364:U:H5'   | 85:L5:1365:C:OP1   | 2.17                     | 0.44              |
| 85:L5:1656:U:H2'   | 85:L5:1657:G:H8    | 1.83                     | 0.44              |
| 85:L5:1661:C:OP1   | 50:Le:36:ARG:NE    | 2.39                     | 0.44              |
| 85:L5:1855:G:C6    | 85:L5:1880:G:N2    | 2.86                     | 0.44              |
| 85:L5:1952:G:H2'   | 85:L5:1953:U:C6    | 2.51                     | 0.44              |
| 85:L5:2102:G:H1'   | 85:L5:2103:G:C8    | 2.53                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 85:L5:2109:G:H2'   | 85:L5:2110:C:H6    | 1.83                     | 0.44              |
| 85:L5:2532:C:H2'   | 85:L5:2533:C:C6    | 2.53                     | 0.44              |
| 85:L5:2890:C:H42   | 85:L5:3611:A:H61   | 1.66                     | 0.44              |
| 85:L5:3910:C:C2    | 85:L5:3911:C:C5    | 3.06                     | 0.44              |
| 85:L5:4125:C:H2'   | 85:L5:4126:C:C6    | 2.51                     | 0.44              |
| 85:L5:4645:C:H2'   | 85:L5:4646:U:H6    | 1.82                     | 0.44              |
| 85:L5:4878:C:C2    | 85:L5:4879:C:C5    | 3.05                     | 0.44              |
| 21:L8:5:U:OP2      | 36:LP:62:ARG:NH1   | 2.50                     | 0.44              |
| 21:L8:67:U:H5'     | 55:Lj:86:PRO:HD3   | 2.00                     | 0.44              |
| 22:LA:133:TYR:HB3  | 22:LA:168:VAL:HG22 | 2.00                     | 0.44              |
| 23:LB:309:LEU:HD13 | 23:LB:309:LEU:HA   | 1.86                     | 0.44              |
| 25:LD:182:GLY:HA3  | 25:LD:195:HIS:HB2  | 1.99                     | 0.44              |
| 25:LD:246:ALA:HA   | 25:LD:249:GLU:OE1  | 2.16                     | 0.44              |
| 25:LD:287:PHE:HZ   | 30:LI:214:SER:HB2  | 1.82                     | 0.44              |
| 26:LE:153:LEU:HD11 | 26:LE:195:ILE:HG13 | 1.99                     | 0.44              |
| 26:LE:192:LYS:O    | 51:Lf:107:PRO:HA   | 2.17                     | 0.44              |
| 28:LG:88:ASP:HB3   | 28:LG:91:THR:HG22  | 1.99                     | 0.44              |
| 41:LU:27:HIS:O     | 41:LU:30:GLU:HG3   | 2.17                     | 0.44              |
| 41:LU:63:ILE:HD11  | 41:LU:70:ILE:HG23  | 1.99                     | 0.44              |
| 45:LZ:42:LEU:HD12  | 45:LZ:43:VAL:N     | 2.32                     | 0.44              |
| 45:LZ:89:ILE:HD13  | 45:LZ:121:ARG:CZ   | 2.47                     | 0.44              |
| 46:La:100:ILE:HD11 | 46:La:125:LYS:CG   | 2.40                     | 0.44              |
| 49:Ld:46:LEU:HA    | 49:Ld:49:ILE:HG22  | 1.98                     | 0.44              |
| 63:Lz:55:LEU:HD12  | 63:Lz:55:LEU:HA    | 1.89                     | 0.44              |
| 63:Lz:176:ASP:O    | 63:Lz:180:VAL:HG13 | 2.18                     | 0.44              |
| 65:SD:224:SER:HA   | 75:Sg:188:HIS:HD2  | 1.83                     | 0.44              |
| 66:SF:39:ILE:HD13  | 66:SF:39:ILE:HA    | 1.71                     | 0.44              |
| 66:SF:51:HIS:CD2   | 66:SF:86:LYS:HG2   | 2.53                     | 0.44              |
| 69:SQ:4:LYS:HE3    | 79:S2:1423:C:C5    | 2.53                     | 0.44              |
| 72:SU:29:VAL:HG13  | 72:SU:85:HIS:CD2   | 2.53                     | 0.44              |
| 73:Sc:21:THR:HG21  | 73:Sc:29:GLN:HG2   | 1.99                     | 0.44              |
| 76:SM:45:ARG:HH12  | 76:SM:72:HIS:CA    | 2.29                     | 0.44              |
| 79:S2:89:C:C2      | 79:S2:90:G:C8      | 3.06                     | 0.44              |
| 79:S2:581:U:H3'    | 79:S2:582:U:C6     | 2.53                     | 0.44              |
| 79:S2:1191:C:H2'   | 79:S2:1192:U:C6    | 2.52                     | 0.44              |
| 79:S2:1409:A:C2    | 79:S2:1438:A:C6    | 3.06                     | 0.44              |
| 79:S2:1558:C:H2'   | 79:S2:1559:C:C6    | 2.53                     | 0.44              |
| 84:Lt:123:ARG:HB2  | 84:Lt:129:ILE:CD1  | 2.35                     | 0.44              |
| 1:CH:136:ASP:OD1   | 1:CH:138:GLY:N     | 2.51                     | 0.44              |
| 4:sL:86:ILE:HD12   | 4:sL:86:ILE:HA     | 1.84                     | 0.44              |
| 6:sG:227:GLN:OE1   | 6:sG:230:LYS:NZ    | 2.27                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 12:sH:33:ASN:OD1   | 12:sH:37:LYS:N     | 2.51                     | 0.44              |
| 12:sH:60:ILE:HD11  | 12:sH:90:LYS:HD2   | 2.00                     | 0.44              |
| 15:sC:116:THR:HG23 | 15:sC:120:GLN:HA   | 2.00                     | 0.44              |
| 18:sW:46:TYR:CE2   | 18:sW:130:PHE:HA   | 2.52                     | 0.44              |
| 18:sW:49:GLU:O     | 18:sW:64:ASN:ND2   | 2.51                     | 0.44              |
| 21:l8:2:G:H3'      | 21:l8:3:A:H8       | 1.82                     | 0.44              |
| 21:l8:49:G:H5'     | 53:lh:47:ILE:CD1   | 2.48                     | 0.44              |
| 24:lC:121:ARG:HB3  | 24:lC:277:TYR:CZ   | 2.53                     | 0.44              |
| 24:lC:336:ARG:O    | 24:lC:340:ILE:HG12 | 2.18                     | 0.44              |
| 26:lE:50:LEU:HD13  | 26:lE:56:ARG:HD2   | 2.00                     | 0.44              |
| 34:lN:68:ARG:HD2   | 34:lN:127:TYR:O    | 2.18                     | 0.44              |
| 34:lN:134:LEU:HD23 | 34:lN:134:LEU:HA   | 1.77                     | 0.44              |
| 34:lN:174:LEU:HD23 | 34:lN:183:THR:HB   | 2.00                     | 0.44              |
| 37:lQ:159:PRO:HA   | 37:lQ:160:HIS:HA   | 1.48                     | 0.44              |
| 39:lS:92:ASN:HD21  | 40:lT:156:TYR:H    | 1.65                     | 0.44              |
| 40:lT:84:ILE:HG13  | 47:lb:23:LYS:HA    | 1.99                     | 0.44              |
| 43:lX:105:ASN:OD1  | 43:lX:108:GLN:HG3  | 2.17                     | 0.44              |
| 44:lY:30:MET:CE    | 44:lY:78:TYR:HA    | 2.47                     | 0.44              |
| 45:lZ:64:LYS:HD3   | 45:lZ:64:LYS:HA    | 1.79                     | 0.44              |
| 47:lb:102:PRO:C    | 47:lb:109:ARG:HH22 | 2.25                     | 0.44              |
| 50:le:68:HIS:CD2   | 62:lr:22:LYS:HG3   | 2.53                     | 0.44              |
| 53:lh:27:GLU:CD    | 53:lh:27:GLU:C     | 2.85                     | 0.44              |
| 55:lj:57:ASN:O     | 55:lj:57:ASN:OD1   | 2.36                     | 0.44              |
| 58:lm:81:SER:O     | 58:lm:84:GLN:HG2   | 2.17                     | 0.44              |
| 63:lz:4:LYS:H      | 63:lz:4:LYS:HG2    | 1.60                     | 0.44              |
| 63:lz:24:LYS:HD3   | 63:lz:30:GLU:H     | 1.82                     | 0.44              |
| 65:sD:62:LYS:HE3   | 67:sK:98:ARG:HB2   | 1.99                     | 0.44              |
| 69:sQ:41:MET:CE    | 71:sT:9:VAL:C      | 2.90                     | 0.44              |
| 69:sQ:55:VAL:HG12  | 69:sQ:63:PHE:CE2   | 2.52                     | 0.44              |
| 69:sQ:145:TYR:HB2  | 79:s2:1248:U:O2'   | 2.17                     | 0.44              |
| 71:sT:48:TYR:CE1   | 79:s2:1539:U:H1'   | 2.53                     | 0.44              |
| 74:sd:40:ARG:NH2   | 79:s2:1255:G:O3'   | 2.42                     | 0.44              |
| 77:sZ:66:LYS:O     | 77:sZ:68:ILE:HD12  | 2.17                     | 0.44              |
| 79:s2:91:A:P       | 79:s2:446:G:H22    | 2.41                     | 0.44              |
| 79:s2:208:G:N3     | 79:s2:208:G:H2'    | 2.32                     | 0.44              |
| 79:s2:1466:G:C6    | 79:s2:1467:C:C4    | 3.06                     | 0.44              |
| 79:s2:1781:A:H3'   | 79:s2:1783:C:C2    | 2.53                     | 0.44              |
| 80:cB:17:ALA:HA    | 80:cB:360:SER:OG   | 2.18                     | 0.44              |
| 80:cB:166:GLU:HG2  | 85:l5:4599:A:OP2   | 2.17                     | 0.44              |
| 80:cB:247:ALA:N    | 80:cB:249:ARG:HH21 | 2.15                     | 0.44              |
| 81:aP:14:A:H3'     | 81:aP:15:G:C8      | 2.53                     | 0.44              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 81:aP:68:G:H2'    | 81:aP:69:A:H8      | 1.83                     | 0.44              |
| 84:lt:106:PHE:O   | 84:lt:110:VAL:HG13 | 2.18                     | 0.44              |
| 85:l5:147:A:H2'   | 85:l5:148:C:O4'    | 2.18                     | 0.44              |
| 85:l5:197:A:C5    | 85:l5:225:G:C2     | 3.05                     | 0.44              |
| 85:l5:996:G:H21   | 85:l5:1048:G:P     | 2.39                     | 0.44              |
| 85:l5:1289:C:H2'  | 85:l5:1290:G:H8    | 1.83                     | 0.44              |
| 85:l5:1957:U:H2'  | 85:l5:1958:A:C8    | 2.53                     | 0.44              |
| 85:l5:2270:G:H2'  | 85:l5:2271:C:C6    | 2.53                     | 0.44              |
| 85:l5:2397:G:C8   | 85:l5:2399:G:C8    | 3.05                     | 0.44              |
| 85:l5:3637:U:O4   | 85:l5:3651:A:H2    | 2.01                     | 0.44              |
| 85:l5:3804:G:H2'  | 85:l5:3805:U:C6    | 2.52                     | 0.44              |
| 85:l5:3954:A:HO2' | 85:l5:3955:G:P     | 2.40                     | 0.44              |
| 85:l5:4878:C:H2'  | 85:l5:4879:C:C6    | 2.52                     | 0.44              |
| 2:SE:194:VAL:HG23 | 2:SE:196:THR:HG22  | 2.00                     | 0.44              |
| 3:SI:78:ILE:HG23  | 3:SI:102:VAL:CG1   | 2.48                     | 0.44              |
| 4:SL:130:GLU:HA   | 4:SL:140:PHE:CD1   | 2.53                     | 0.44              |
| 10:SA:69:GLU:CD   | 15:SC:270:THR:HG21 | 2.43                     | 0.44              |
| 10:SA:215:GLN:OE1 | 10:SA:215:GLN:N    | 2.47                     | 0.44              |
| 11:SB:124:HIS:HB2 | 11:SB:138:PHE:CE1  | 2.53                     | 0.44              |
| 12:SH:76:GLN:O    | 12:SH:79:LEU:HG    | 2.18                     | 0.44              |
| 15:SC:148:ALA:O   | 15:SC:152:ARG:HD3  | 2.18                     | 0.44              |
| 18:SW:10:ALA:O    | 18:SW:14:ILE:HG12  | 2.17                     | 0.44              |
| 85:L5:25:A:C4     | 85:L5:341:G:C8     | 3.05                     | 0.44              |
| 85:L5:35:U:O2'    | 85:L5:1651:G:N3    | 2.46                     | 0.44              |
| 85:L5:54:G:OP1    | 55:Lj:43:ARG:NE    | 2.50                     | 0.44              |
| 85:L5:342:G:H2'   | 85:L5:343:C:H6     | 1.82                     | 0.44              |
| 85:L5:498:C:N4    | 85:L5:657:C:H42    | 2.15                     | 0.44              |
| 85:L5:724:C:OP1   | 24:LC:350:ARG:NE   | 2.51                     | 0.44              |
| 85:L5:739:G:N2    | 85:L5:926:G:H1'    | 2.33                     | 0.44              |
| 85:L5:1384:C:C2   | 85:L5:1385:G:C8    | 3.06                     | 0.44              |
| 85:L5:1397:A:C8   | 46:La:114:LYS:HD2  | 2.53                     | 0.44              |
| 85:L5:1784:U:H5'  | 30:LI:90:ARG:HG3   | 2.00                     | 0.44              |
| 85:L5:2520:C:H2'  | 85:L5:2521:G:C8    | 2.52                     | 0.44              |
| 85:L5:4122:G:O3'  | 52:Lg:90:ARG:NH2   | 2.50                     | 0.44              |
| 85:L5:4631:G:H2'  | 85:L5:4632:U:C6    | 2.52                     | 0.44              |
| 85:L5:4689:U:O4   | 85:L5:4698:C:H4'   | 2.18                     | 0.44              |
| 85:L5:4862:G:H2'  | 85:L5:4863:G:C8    | 2.53                     | 0.44              |
| 85:L5:4911:A:OP2  | 23:LB:100:ARG:NE   | 2.47                     | 0.44              |
| 85:L5:4924:C:H2'  | 85:L5:4925:U:C6    | 2.53                     | 0.44              |
| 21:L8:71:A:H2'    | 44:LY:50:ARG:NH1   | 2.33                     | 0.44              |
| 21:L8:119:C:H2'   | 21:L8:120:G:C8     | 2.53                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:LB:122:TRP:O    | 23:LB:127:LYS:NZ   | 2.51                     | 0.44              |
| 25:LD:239:MET:HE2  | 25:LD:239:MET:C    | 2.43                     | 0.44              |
| 36:LP:139:TYR:N    | 36:LP:140:MET:HE2  | 2.33                     | 0.44              |
| 37:LQ:61:LEU:HD11  | 37:LQ:65:ARG:HB3   | 1.99                     | 0.44              |
| 40:LT:66:ASN:ND2   | 47:Lb:35:VAL:HA    | 2.33                     | 0.44              |
| 41:LU:26:THR:HG22  | 41:LU:68:SER:HB3   | 2.00                     | 0.44              |
| 43:LX:122:ALA:HB2  | 43:LX:141:ALA:HA   | 2.00                     | 0.44              |
| 44:LY:10:ASP:OD1   | 44:LY:12:SER:N     | 2.51                     | 0.44              |
| 44:LY:26:ARG:NH1   | 44:LY:75:ARG:O     | 2.45                     | 0.44              |
| 44:LY:56:GLN:NE2   | 44:LY:65:GLN:HA    | 2.33                     | 0.44              |
| 44:LY:62:TYR:HE2   | 44:LY:97:VAL:HG11  | 1.83                     | 0.44              |
| 45:LZ:89:ILE:HD11  | 45:LZ:121:ARG:HG2  | 1.99                     | 0.44              |
| 46:La:74:ASN:ND2   | 46:La:114:LYS:HB3  | 2.32                     | 0.44              |
| 50:Le:37:LYS:HD3   | 50:Le:39:ARG:HE    | 1.83                     | 0.44              |
| 62:Lr:81:THR:O     | 62:Lr:82:ILE:HD13  | 2.17                     | 0.44              |
| 64:SR:81:ARG:NH2   | 64:SR:82:ASP:HA    | 2.33                     | 0.44              |
| 65:SD:1:MET:HE3    | 65:SD:1:MET:O      | 2.18                     | 0.44              |
| 70:SS:78:LYS:HZ3   | 71:ST:32:GLU:HB2   | 1.82                     | 0.44              |
| 70:SS:105:ASN:OD1  | 70:SS:106:LYS:N    | 2.50                     | 0.44              |
| 73:Sc:11:LEU:HD23  | 73:Sc:11:LEU:HA    | 1.74                     | 0.44              |
| 75:Sg:248:LEU:HD12 | 75:Sg:259:TRP:HE1  | 1.82                     | 0.44              |
| 77:SZ:47:LEU:HD23  | 77:SZ:80:ARG:HD2   | 2.00                     | 0.44              |
| 77:SZ:91:LEU:HA    | 77:SZ:94:LYS:HG2   | 1.98                     | 0.44              |
| 79:S2:746:C:H2'    | 79:S2:747:U:H6     | 1.81                     | 0.44              |
| 79:S2:929:G:H21    | 79:S2:1104:G:H4'   | 1.82                     | 0.44              |
| 79:S2:930:C:H42    | 79:S2:1011:A:H62   | 1.64                     | 0.44              |
| 79:S2:1177:U:H2'   | 79:S2:1178:U:H6    | 1.83                     | 0.44              |
| 79:S2:1266:C:H2'   | 79:S2:1267:C:C6    | 2.53                     | 0.44              |
| 3:sI:144:LYS:H     | 3:sI:144:LYS:HG2   | 1.52                     | 0.44              |
| 5:sX:108:LYS:HD2   | 79:s2:650:A:OP2    | 2.17                     | 0.44              |
| 7:sJ:79:ARG:HG3    | 7:sJ:80:ARG:N      | 2.33                     | 0.44              |
| 8:sY:129:LYS:HA    | 8:sY:129:LYS:HD3   | 1.83                     | 0.44              |
| 12:sH:106:ARG:HH21 | 79:s2:861:A:H2'    | 1.82                     | 0.44              |
| 15:sC:148:ALA:O    | 15:sC:151:ILE:HG12 | 2.17                     | 0.44              |
| 17:sO:56:VAL:HG12  | 17:sO:77:ALA:HB1   | 1.98                     | 0.44              |
| 17:sO:103:ASN:HB2  | 17:sO:142:ARG:HB2  | 2.00                     | 0.44              |
| 17:sO:149:ARG:NH1  | 79:s2:1064:C:O3'   | 2.50                     | 0.44              |
| 19:sb:14:GLU:HA    | 19:sb:14:GLU:OE1   | 2.17                     | 0.44              |
| 21:l8:60:G:N1      | 53:lh:59:THR:HG22  | 2.33                     | 0.44              |
| 21:l8:131:G:H5''   | 43:lX:108:GLN:HE21 | 1.81                     | 0.44              |
| 22:lA:179:ILE:HG21 | 22:lA:185:ALA:HB2  | 1.99                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:lC:18:SER:HB2   | 24:lC:20:LYS:NZ    | 2.33                     | 0.44              |
| 25:lD:215:ASP:OD1  | 25:lD:216:GLU:N    | 2.50                     | 0.44              |
| 27:lF:147:LEU:HD23 | 27:lF:148:LYS:N    | 2.33                     | 0.44              |
| 28:lG:174:CYS:HA   | 28:lG:177:MET:SD   | 2.58                     | 0.44              |
| 31:lJ:17:ILE:HD11  | 31:lJ:165:TRP:HZ2  | 1.83                     | 0.44              |
| 34:lN:99:GLN:O     | 34:lN:103:GLU:HG2  | 2.17                     | 0.44              |
| 34:lN:125:SER:OG   | 85:l5:3937:C:O2    | 2.28                     | 0.44              |
| 38:lR:136:ARG:HH12 | 85:l5:2896:G:P     | 2.40                     | 0.44              |
| 40:lT:7:LYS:H      | 40:lT:7:LYS:HG2    | 1.53                     | 0.44              |
| 46:la:9:ARG:HH22   | 85:l5:2344:U:H2'   | 1.83                     | 0.44              |
| 46:la:72:THR:CG2   | 46:la:112:LEU:HG   | 2.48                     | 0.44              |
| 52:lg:61:PRO:HB3   | 85:l5:2598:A:N3    | 2.33                     | 0.44              |
| 53:lh:85:PRO:HA    | 55:lj:80:GLU:OE1   | 2.18                     | 0.44              |
| 57:ll:28:ARG:HH11  | 57:ll:33:ASN:HD21  | 1.64                     | 0.44              |
| 63:lz:63:PHE:HE1   | 63:lz:155:ILE:HG23 | 1.83                     | 0.44              |
| 65:sD:16:ILE:HD13  | 74:sd:22:ARG:HH11  | 1.82                     | 0.44              |
| 66:sF:32:ASP:OD1   | 66:sF:33:ILE:N     | 2.51                     | 0.44              |
| 69:sQ:10:VAL:HG21  | 69:sQ:94:ALA:HB1   | 1.98                     | 0.44              |
| 69:sQ:78:VAL:HG22  | 79:s2:1673:U:H5''  | 2.00                     | 0.44              |
| 70:sS:5:ILE:HG23   | 70:sS:9:PHE:HD2    | 1.82                     | 0.44              |
| 72:sU:28:ASN:O     | 72:sU:32:LEU:HD23  | 2.17                     | 0.44              |
| 75:sg:21:ILE:N     | 75:sg:288:SER:OG   | 2.51                     | 0.44              |
| 79:s2:153:G:N1     | 79:s2:166:A:C6     | 2.86                     | 0.44              |
| 79:s2:390:C:H2'    | 79:s2:391:C:C6     | 2.53                     | 0.44              |
| 79:s2:799:U:C4     | 79:s2:867:G:N1     | 2.86                     | 0.44              |
| 79:s2:960:U:H2'    | 79:s2:962:A:OP2    | 2.17                     | 0.44              |
| 79:s2:1172:U:C2    | 79:s2:1188:A:N7    | 2.86                     | 0.44              |
| 79:s2:1390:U:H2'   | 79:s2:1391:C:C6    | 2.53                     | 0.44              |
| 79:s2:1576:G:H2'   | 79:s2:1577:G:O4'   | 2.17                     | 0.44              |
| 79:s2:1781:A:H5''  | 79:s2:1783:C:C4    | 2.53                     | 0.44              |
| 80:cB:337:LYS:CA   | 80:cB:341:ARG:HH12 | 2.31                     | 0.44              |
| 80:cB:671:TYR:O    | 80:cB:675:ILE:HG12 | 2.18                     | 0.44              |
| 82:pE:30:G:H3'     | 82:pE:31:A:H8      | 1.83                     | 0.44              |
| 85:l5:470:A:C4     | 85:l5:471:A:C8     | 3.06                     | 0.44              |
| 85:l5:646:G:H2'    | 85:l5:647:G:O4'    | 2.18                     | 0.44              |
| 85:l5:930:G:H2'    | 85:l5:931:C:C6     | 2.52                     | 0.44              |
| 85:l5:984:C:C2     | 85:l5:1070:G:N2    | 2.86                     | 0.44              |
| 85:l5:1569:U:H2'   | 85:l5:1570:G:H8    | 1.83                     | 0.44              |
| 85:l5:1737:A:C4    | 85:l5:1738:A:C8    | 3.06                     | 0.44              |
| 85:l5:1739:G:N3    | 85:l5:1742:A:N6    | 2.66                     | 0.44              |
| 85:l5:2657:G:H2'   | 85:l5:2658:G:C8    | 2.53                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 85:L5:2659:A:N6    | 85:L5:2673:G:N3    | 2.65                     | 0.44              |
| 85:L5:2743:A:H2'   | 85:L5:2744:A:H8    | 1.83                     | 0.44              |
| 85:L5:3835:C:H2'   | 85:L5:3836:A:H8    | 1.82                     | 0.44              |
| 85:L5:4122:G:C6    | 85:L5:4123:C:C4    | 3.06                     | 0.44              |
| 85:L5:4259:C:H2'   | 85:L5:4260:U:H6    | 1.83                     | 0.44              |
| 85:L5:4389:C:H2'   | 85:L5:4390:A:C8    | 2.52                     | 0.44              |
| 85:L5:4711:C:H2'   | 85:L5:4712:C:O4'   | 2.18                     | 0.44              |
| 85:L5:4878:C:C2    | 85:L5:4879:C:C5    | 3.06                     | 0.44              |
| 85:L5:5045:G:H2'   | 85:L5:5046:U:O4'   | 2.18                     | 0.44              |
| 80:CB:157:MET:O    | 80:CB:160:MET:HE3  | 2.18                     | 0.44              |
| 80:CB:788:LEU:HD12 | 80:CB:789:PRO:HD2  | 2.00                     | 0.44              |
| 2:SE:30:ARG:HD2    | 2:SE:30:ARG:HA     | 1.73                     | 0.44              |
| 2:SE:222:LEU:HD12  | 2:SE:225:ILE:HD12  | 1.99                     | 0.44              |
| 6:SG:116:LYS:NZ    | 6:SG:120:ASP:HA    | 2.32                     | 0.44              |
| 6:SG:198:ARG:HD2   | 79:S2:126:G:P      | 2.58                     | 0.44              |
| 6:SG:234:LEU:HD23  | 79:S2:787:G:H3'    | 1.99                     | 0.44              |
| 86:Se:41:ARG:HH12  | 79:S2:639:C:H5''   | 1.82                     | 0.44              |
| 10:SA:220:LYS:HA   | 10:SA:220:LYS:HD3  | 1.69                     | 0.44              |
| 15:SC:172:ASN:O    | 15:SC:172:ASN:OD1  | 2.36                     | 0.44              |
| 15:SC:172:ASN:OD1  | 15:SC:174:ILE:HG12 | 2.17                     | 0.44              |
| 15:SC:274:VAL:HA   | 15:SC:278:THR:OG1  | 2.17                     | 0.44              |
| 85:L5:423:G:H2'    | 85:L5:424:U:H6     | 1.82                     | 0.44              |
| 85:L5:746:A:H2'    | 85:L5:747:A:H8     | 1.80                     | 0.44              |
| 85:L5:909:A:N6     | 85:L5:910:G:O6     | 2.51                     | 0.44              |
| 85:L5:1559:G:H2'   | 85:L5:1560:A:H8    | 1.82                     | 0.44              |
| 85:L5:1568:C:H2'   | 85:L5:1569:U:C6    | 2.52                     | 0.44              |
| 85:L5:1749:A:O3'   | 30:LI:39:LYS:HD2   | 2.18                     | 0.44              |
| 85:L5:1831:G:H2'   | 85:L5:1832:C:O4'   | 2.18                     | 0.44              |
| 85:L5:2032:U:H2'   | 85:L5:2033:A:C8    | 2.53                     | 0.44              |
| 85:L5:2286:G:H2'   | 85:L5:2287:G:C8    | 2.52                     | 0.44              |
| 85:L5:2296:G:C6    | 85:L5:2297:G:C5    | 3.06                     | 0.44              |
| 85:L5:2413:U:C2    | 85:L5:2414:G:C8    | 3.06                     | 0.44              |
| 85:L5:2676:A:H2'   | 85:L5:2677:G:O4'   | 2.18                     | 0.44              |
| 85:L5:2890:C:H2'   | 85:L5:2891:U:C6    | 2.53                     | 0.44              |
| 85:L5:3688:U:H2'   | 85:L5:3689:G:H8    | 1.82                     | 0.44              |
| 85:L5:3949:A:N6    | 85:L5:4064:C:H42   | 2.16                     | 0.44              |
| 85:L5:4096:C:P     | 85:L5:4109:G:O2'   | 2.76                     | 0.44              |
| 85:L5:4122:G:C5    | 52:Lg:97:ILE:HD11  | 2.52                     | 0.44              |
| 85:L5:4461:C:H1'   | 85:L5:4516:G:N2    | 2.33                     | 0.44              |
| 85:L5:4700:A:C2    | 85:L5:4701:A:C8    | 3.06                     | 0.44              |
| 85:L5:4771:C:H2'   | 85:L5:4772:C:H6    | 1.83                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 85:L5:4973:U:H3    | 85:L5:4985:U:H3    | 1.64                     | 0.44              |
| 23:LB:56:ILE:HG22  | 23:LB:368:ILE:HG23 | 2.00                     | 0.44              |
| 25:LD:8:LYS:HB3    | 25:LD:13:PHE:CZ    | 2.53                     | 0.44              |
| 26:LE:141:ARG:HH21 | 51:Lf:110:ILE:C    | 2.26                     | 0.44              |
| 33:LM:48:GLN:HG3   | 33:LM:50:MET:CE    | 2.48                     | 0.44              |
| 35:LO:12:ARG:HD3   | 35:LO:37:ARG:CZ    | 2.47                     | 0.44              |
| 35:LO:118:MET:HE1  | 39:LS:169:THR:N    | 2.33                     | 0.44              |
| 35:LO:193:THR:O    | 35:LO:197:LYS:N    | 2.44                     | 0.44              |
| 37:LQ:35:LEU:HD23  | 37:LQ:35:LEU:HA    | 1.83                     | 0.44              |
| 37:LQ:70:MET:HE1   | 37:LQ:137:VAL:CG1  | 2.48                     | 0.44              |
| 40:LT:20:ARG:C     | 40:LT:21:LYS:HD2   | 2.42                     | 0.44              |
| 43:LX:93:ASN:OD1   | 43:LX:93:ASN:N     | 2.51                     | 0.44              |
| 44:LY:51:LYS:O     | 44:LY:70:VAL:HG13  | 2.18                     | 0.44              |
| 46:La:75:LEU:CB    | 46:La:117:LEU:HD21 | 2.43                     | 0.44              |
| 46:La:83:SER:OG    | 46:La:85:GLN:HB3   | 2.18                     | 0.44              |
| 52:Lg:108:LYS:HE3  | 52:Lg:108:LYS:HB3  | 1.82                     | 0.44              |
| 65:SD:68:GLU:O     | 65:SD:72:VAL:HG22  | 2.17                     | 0.44              |
| 66:SF:124:ASP:HA   | 66:SF:200:ALA:HB2  | 2.00                     | 0.44              |
| 66:SF:195:GLU:O    | 66:SF:198:ARG:HG3  | 2.18                     | 0.44              |
| 67:SK:51:SER:HA    | 79:S2:1276:A:O2'   | 2.18                     | 0.44              |
| 67:SK:51:SER:O     | 67:SK:55:ARG:HG2   | 2.18                     | 0.44              |
| 69:SQ:78:VAL:HA    | 69:SQ:81:ILE:HG22  | 2.00                     | 0.44              |
| 72:SU:43:ALA:HB1   | 72:SU:48:LEU:HD21  | 2.00                     | 0.44              |
| 76:SM:18:LEU:HA    | 76:SM:21:VAL:HG22  | 2.00                     | 0.44              |
| 76:SM:40:LYS:HA    | 76:SM:40:LYS:HD3   | 1.81                     | 0.44              |
| 79:S2:482:G:N2     | 79:S2:485:A:OP2    | 2.51                     | 0.44              |
| 79:S2:830:A:C5     | 79:S2:831:G:H1'    | 2.52                     | 0.44              |
| 79:S2:1208:A:H4'   | 79:S2:1835:A:N7    | 2.32                     | 0.44              |
| 82:PE:1:G:C6       | 82:PE:73:G:C6      | 3.06                     | 0.44              |
| 1:CH:57:ASN:OD1    | 1:CH:59:ALA:HB3    | 2.17                     | 0.44              |
| 1:CH:122:GLY:O     | 1:CH:125:GLU:HB3   | 2.17                     | 0.44              |
| 6:sG:216:ARG:HD3   | 6:sG:216:ARG:HA    | 1.64                     | 0.44              |
| 8:sY:86:GLU:OE2    | 8:sY:90:ARG:NH1    | 2.48                     | 0.44              |
| 11:sB:104:ASP:HA   | 11:sB:213:ARG:O    | 2.18                     | 0.44              |
| 11:sB:126:ASP:HA   | 11:sB:136:ARG:HA   | 1.99                     | 0.44              |
| 12:sH:64:VAL:O     | 12:sH:96:ALA:HA    | 2.18                     | 0.44              |
| 12:sH:141:GLY:C    | 12:sH:157:HIS:HD1  | 2.23                     | 0.44              |
| 16:sN:40:LEU:HB3   | 16:sN:50:ILE:HD12  | 2.00                     | 0.44              |
| 19:sb:18:LYS:HE2   | 19:sb:18:LYS:HB2   | 1.83                     | 0.44              |
| 21:l8:108:A:C6     | 21:l8:109:C:C4     | 3.06                     | 0.44              |
| 21:l8:141:C:H2'    | 21:l8:142:U:H6     | 1.82                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:1A:9:ARG:NH1    | 85:l5:1628:C:O5'   | 2.51                     | 0.44              |
| 23:1B:194:LEU:O    | 23:1B:198:ARG:HG3  | 2.18                     | 0.44              |
| 23:1B:223:THR:HA   | 23:1B:338:VAL:HG22 | 2.00                     | 0.44              |
| 29:1H:44:GLU:OE2   | 33:1M:2:VAL:HG13   | 2.17                     | 0.44              |
| 32:1L:188:ASN:HA   | 32:1L:195:ARG:HH12 | 1.83                     | 0.44              |
| 33:1M:69:HIS:HB2   | 33:1M:72:TYR:HE2   | 1.83                     | 0.44              |
| 33:1M:72:TYR:CE1   | 85:l5:918:G:H5'    | 2.53                     | 0.44              |
| 34:1N:115:VAL:HG12 | 34:1N:134:LEU:HD21 | 1.99                     | 0.44              |
| 36:1P:23:ARG:NH2   | 85:l5:2419:C:OP1   | 2.50                     | 0.44              |
| 36:1P:107:LEU:HD12 | 36:1P:108:ASP:N    | 2.32                     | 0.44              |
| 37:1Q:50:ARG:HA    | 37:1Q:53:MET:SD    | 2.57                     | 0.44              |
| 37:1Q:80:ALA:HB3   | 37:1Q:100:VAL:HG23 | 2.00                     | 0.44              |
| 38:1R:152:LYS:HE3  | 38:1R:152:LYS:HB2  | 1.75                     | 0.44              |
| 39:1S:170:LYS:NZ   | 85:l5:4875:G:H5''  | 2.33                     | 0.44              |
| 40:1T:146:LYS:HE3  | 40:1T:146:LYS:HB2  | 1.62                     | 0.44              |
| 43:1X:76:ILE:HD13  | 43:1X:108:GLN:HB3  | 1.99                     | 0.44              |
| 45:1Z:100:VAL:HG13 | 45:1Z:106:LEU:CD2  | 2.47                     | 0.44              |
| 46:1a:75:LEU:HB2   | 46:1a:117:LEU:HD21 | 2.00                     | 0.44              |
| 49:1d:64:ILE:CD1   | 85:l5:2373:C:H4'   | 2.36                     | 0.44              |
| 50:1e:8:VAL:HG23   | 85:l5:703:G:OP1    | 2.17                     | 0.44              |
| 64:sR:49:LYS:O     | 79:s2:1466:G:H5'   | 2.18                     | 0.44              |
| 67:sK:1:MET:HE2    | 67:sK:1:MET:CA     | 2.48                     | 0.44              |
| 68:sP:71:GLU:OE2   | 68:sP:73:PRO:HA    | 2.17                     | 0.44              |
| 69:sQ:145:TYR:HB3  | 79:s2:1249:C:H5'   | 1.99                     | 0.44              |
| 70:sS:55:ARG:N     | 70:sS:58:GLU:OE2   | 2.36                     | 0.44              |
| 75:sg:208:ALA:CB   | 75:sg:248:LEU:HD21 | 2.48                     | 0.44              |
| 79:s2:441:C:H2'    | 79:s2:442:C:C6     | 2.52                     | 0.44              |
| 79:s2:476:A:H2'    | 79:s2:477:G:O4'    | 2.18                     | 0.44              |
| 79:s2:681:U:H2'    | 79:s2:682:U:C6     | 2.53                     | 0.44              |
| 79:s2:1067:C:H3'   | 79:s2:1068:G:H8    | 1.83                     | 0.44              |
| 79:s2:1348:G:C8    | 79:s2:1349:G:C8    | 3.06                     | 0.44              |
| 79:s2:1633:A:H2'   | 79:s2:1634:A:H8    | 1.81                     | 0.44              |
| 79:s2:1753:C:H4'   | 79:s2:1780:G:H1    | 1.82                     | 0.44              |
| 79:s2:1784:G:C6    | 79:s2:1785:C:C4    | 3.06                     | 0.44              |
| 80:cB:22:MET:CE    | 80:cB:354:ILE:HB   | 2.48                     | 0.44              |
| 80:cB:385:ILE:HD13 | 80:cB:417:PHE:HB3  | 1.99                     | 0.44              |
| 80:cB:750:GLN:HE22 | 80:cB:811:GLN:HG3  | 1.82                     | 0.44              |
| 80:cB:772:GLU:HG2  | 80:cB:785:LYS:HD2  | 1.99                     | 0.44              |
| 83:ls:20:LEU:HD11  | 83:ls:52:VAL:HG21  | 1.99                     | 0.44              |
| 83:ls:58:ASN:ND2   | 83:ls:84:GLY:O     | 2.45                     | 0.44              |
| 85:l5:269:G:H2'    | 85:l5:270:U:H6     | 1.83                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 85:L5:1328:G:H2'   | 85:L5:1329:G:C8    | 2.53                     | 0.44              |
| 85:L5:1912:G:C6    | 85:L5:2057:A:C2    | 3.06                     | 0.44              |
| 85:L5:1984:A:H2'   | 85:L5:2011:C:OP1   | 2.17                     | 0.44              |
| 85:L5:2328:G:H2'   | 85:L5:2329:U:C6    | 2.53                     | 0.44              |
| 85:L5:2483:G:C6    | 85:L5:2496:G:C6    | 3.06                     | 0.44              |
| 85:L5:2737:C:H2'   | 85:L5:2738:C:C6    | 2.53                     | 0.44              |
| 85:L5:3659:G:H2'   | 85:L5:3660:C:C6    | 2.52                     | 0.44              |
| 85:L5:4156:G:C8    | 85:L5:4157:A:C8    | 3.05                     | 0.44              |
| 85:L5:4174:U:H2'   | 85:L5:4175:G:C8    | 2.43                     | 0.44              |
| 85:L5:4192:A:H2'   | 85:L5:4193:C:C6    | 2.53                     | 0.44              |
| 85:L5:4396:A:OP1   | 85:L5:4443:C:O2'   | 2.29                     | 0.44              |
| 85:L5:4494:G:C6    | 85:L5:4507:A:N1    | 2.86                     | 0.44              |
| 85:L5:4907:G:N1    | 85:L5:4914:C:N3    | 2.41                     | 0.44              |
| 80:CB:297:ILE:HD13 | 80:CB:343:TRP:CH2  | 2.53                     | 0.44              |
| 80:CB:373:TYR:HA   | 80:CB:494:MET:HE1  | 1.99                     | 0.44              |
| 2:SE:54:TYR:HB3    | 8:SY:17:LEU:CD2    | 2.47                     | 0.44              |
| 3:SI:98:LYS:O      | 3:SI:175:ILE:HG23  | 2.18                     | 0.44              |
| 3:SI:110:ARG:NH2   | 3:SI:122:GLY:HA3   | 2.32                     | 0.44              |
| 4:SL:20:LYS:HA     | 4:SL:20:LYS:HD3    | 1.79                     | 0.44              |
| 7:SJ:33:GLY:HA3    | 86:Se:38:TYR:CG    | 2.53                     | 0.44              |
| 8:SY:41:ARG:HD2    | 8:SY:55:ILE:HG23   | 1.98                     | 0.44              |
| 10:SA:192:GLU:OE2  | 10:SA:192:GLU:N    | 2.51                     | 0.44              |
| 11:SB:185:VAL:O    | 11:SB:189:ILE:HD12 | 2.18                     | 0.44              |
| 12:SH:141:GLY:O    | 12:SH:156:VAL:HG23 | 2.18                     | 0.44              |
| 14:Sa:98:PRO:HG2   | 79:S2:1867:U:C2    | 2.52                     | 0.44              |
| 15:SC:176:LYS:HG3  | 15:SC:177:PRO:HD2  | 1.99                     | 0.44              |
| 16:SN:64:ARG:HH22  | 79:S2:918:U:C5'    | 2.31                     | 0.44              |
| 85:L5:6:C:H5''     | 28:LG:197:LYS:HG3  | 2.00                     | 0.44              |
| 85:L5:120:A:H2'    | 85:L5:149:A:H61    | 1.82                     | 0.44              |
| 85:L5:1275:G:H2'   | 85:L5:1276:C:C6    | 2.52                     | 0.44              |
| 85:L5:1461:C:C2    | 85:L5:1462:A:C8    | 3.06                     | 0.44              |
| 85:L5:1559:G:H2'   | 85:L5:1560:A:C8    | 2.53                     | 0.44              |
| 85:L5:1644:C:C2    | 85:L5:1645:C:C5    | 3.06                     | 0.44              |
| 85:L5:1664:U:H2'   | 85:L5:1665:C:C6    | 2.52                     | 0.44              |
| 85:L5:2458:C:OP1   | 34:LN:67:ARG:NH2   | 2.46                     | 0.44              |
| 85:L5:2557:G:H2'   | 85:L5:2558:C:C6    | 2.52                     | 0.44              |
| 85:L5:2891:U:P     | 38:LR:74:ARG:HH21  | 2.41                     | 0.44              |
| 85:L5:3598:C:H2'   | 85:L5:3599:A:H8    | 1.83                     | 0.44              |
| 85:L5:3644:U:O2'   | 85:L5:4555:U:H5'   | 2.18                     | 0.44              |
| 85:L5:4155:C:H2'   | 85:L5:4156:G:O4'   | 2.17                     | 0.44              |
| 85:L5:4486:C:H2'   | 85:L5:4487:A:O4'   | 2.18                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 85:L5:4941:G:P     | 26:LE:188:ARG:HH12 | 2.41                     | 0.44              |
| 85:L5:5040:U:H4'   | 85:L5:5041:G:H5'   | 1.99                     | 0.44              |
| 20:L7:71:G:H2'     | 20:L7:72:U:C6      | 2.52                     | 0.44              |
| 23:LB:21:ARG:HB3   | 23:LB:274:TYR:CD2  | 2.52                     | 0.44              |
| 23:LB:291:TYR:HB3  | 23:LB:297:LYS:HE2  | 2.00                     | 0.44              |
| 23:LB:322:HIS:O    | 23:LB:342:LYS:NZ   | 2.33                     | 0.44              |
| 24:LC:44:LEU:CB    | 24:LC:238:LEU:HD21 | 2.48                     | 0.44              |
| 24:LC:228:THR:HG22 | 24:LC:248:ARG:NH2  | 2.33                     | 0.44              |
| 28:LG:39:PHE:CE1   | 28:LG:47:PRO:HD3   | 2.53                     | 0.44              |
| 29:LH:165:THR:O    | 29:LH:165:THR:OG1  | 2.36                     | 0.44              |
| 31:LJ:46:GLN:HE21  | 31:LJ:74:VAL:HG12  | 1.83                     | 0.44              |
| 35:LO:194:GLU:O    | 35:LO:198:THR:HG22 | 2.18                     | 0.44              |
| 36:LP:139:TYR:H    | 36:LP:140:MET:CE   | 2.31                     | 0.44              |
| 38:LR:159:ALA:O    | 38:LR:162:ARG:HG2  | 2.18                     | 0.44              |
| 39:LS:27:LEU:HD23  | 39:LS:27:LEU:N     | 2.28                     | 0.44              |
| 45:LZ:13:VAL:HG22  | 45:LZ:75:TYR:HE2   | 1.83                     | 0.44              |
| 48:Lc:20:LEU:O     | 48:Lc:20:LEU:HD12  | 2.18                     | 0.44              |
| 48:Lc:64:ALA:O     | 48:Lc:68:LYS:N     | 2.51                     | 0.44              |
| 50:Le:87:VAL:HG13  | 50:Le:88:LEU:HD13  | 1.99                     | 0.44              |
| 56:Lk:32:VAL:HG21  | 56:Lk:53:ALA:HB2   | 1.99                     | 0.44              |
| 65:SD:12:VAL:O     | 65:SD:16:ILE:HG12  | 2.17                     | 0.44              |
| 75:Sg:17:TRP:CG    | 75:Sg:36:ARG:HG3   | 2.53                     | 0.44              |
| 78:Sf:118:ARG:HB3  | 78:Sf:132:MET:O    | 2.17                     | 0.44              |
| 79:S2:2:A:OP2      | 79:S2:418:A:H5'    | 2.18                     | 0.44              |
| 79:S2:480:G:C5     | 79:S2:481:C:C4     | 3.05                     | 0.44              |
| 79:S2:558:G:HO2'   | 79:S2:559:G:P      | 2.40                     | 0.44              |
| 79:S2:695:C:H5''   | 79:S2:696:G:C8     | 2.52                     | 0.44              |
| 79:S2:893:U:H3'    | 79:S2:894:G:H8     | 1.81                     | 0.44              |
| 79:S2:1058:A:H2'   | 79:S2:1059:G:C8    | 2.53                     | 0.44              |
| 79:S2:1353:A:H2'   | 79:S2:1354:G:C8    | 2.52                     | 0.44              |
| 79:S2:1391:C:H2'   | 79:S2:1392:U:C6    | 2.53                     | 0.44              |
| 79:S2:1476:A:H4'   | 79:S2:1477:U:H5''  | 2.00                     | 0.44              |
| 79:S2:1859:A:H2'   | 79:S2:1860:A:C8    | 2.53                     | 0.44              |
| 83:Ls:17:ILE:HD12  | 83:Ls:17:ILE:HA    | 1.85                     | 0.44              |
| 84:Lt:70:GLN:N     | 84:Lt:70:GLN:OE1   | 2.51                     | 0.44              |
| 1:CH:66:GLU:OE2    | 1:CH:66:GLU:N      | 2.43                     | 0.43              |
| 2:sE:49:ARG:O      | 2:sE:53:LYS:HA     | 2.17                     | 0.43              |
| 4:sL:82:MET:HG3    | 4:sL:85:THR:OG1    | 2.18                     | 0.43              |
| 6:sG:68:LEU:HD21   | 79:s2:1745:A:O4'   | 2.18                     | 0.43              |
| 6:sG:132:ARG:CZ    | 79:s2:167:G:N2     | 2.81                     | 0.43              |
| 7:sJ:63:LEU:HD23   | 7:sJ:70:ARG:HB2    | 1.99                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:sA:149:ASN:ND2  | 10:sA:164:ASN:OD1  | 2.51                     | 0.43              |
| 11:sB:84:PHE:C     | 11:sB:85:LYS:HD2   | 2.43                     | 0.43              |
| 11:sB:139:CYS:SG   | 11:sB:168:MET:HE1  | 2.58                     | 0.43              |
| 13:sV:43:THR:HG23  | 13:sV:45:ARG:HB2   | 1.99                     | 0.43              |
| 16:sN:118:ILE:O    | 16:sN:122:ILE:HG12 | 2.18                     | 0.43              |
| 18:sW:5:ASN:ND2    | 18:sW:8:ALA:HB2    | 2.33                     | 0.43              |
| 20:l7:26:C:H2'     | 20:l7:27:G:O4'     | 2.18                     | 0.43              |
| 21:l8:57:C:H2'     | 21:l8:58:G:H8      | 1.83                     | 0.43              |
| 22:lA:57:PRO:HB2   | 22:lA:78:ALA:HB3   | 1.99                     | 0.43              |
| 23:lB:58:ARG:NH2   | 23:lB:60:VAL:HG22  | 2.33                     | 0.43              |
| 23:lB:300:LYS:HZ2  | 23:lB:310:SER:C    | 2.26                     | 0.43              |
| 25:lD:63:GLN:C     | 25:lD:64:ILE:HD13  | 2.43                     | 0.43              |
| 26:lE:244:GLU:O    | 26:lE:248:ILE:HG22 | 2.17                     | 0.43              |
| 29:lH:142:ASP:OD1  | 29:lH:142:ASP:N    | 2.49                     | 0.43              |
| 29:lH:168:LYS:NZ   | 85:l5:4471:U:OP1   | 2.36                     | 0.43              |
| 30:lI:16:PRO:HA    | 30:lI:95:HIS:CE1   | 2.53                     | 0.43              |
| 30:lI:91:LEU:HD23  | 30:lI:135:ILE:HA   | 1.99                     | 0.43              |
| 33:lM:114:LYS:NZ   | 85:l5:4929:C:OP1   | 2.39                     | 0.43              |
| 34:lN:189:ARG:C    | 34:lN:193:ARG:HH21 | 2.26                     | 0.43              |
| 34:lN:190:ALA:N    | 34:lN:193:ARG:HH21 | 2.16                     | 0.43              |
| 34:lN:195:ARG:NH2  | 85:l5:98:A:O3'     | 2.48                     | 0.43              |
| 35:lO:103:LYS:HE3  | 35:lO:103:LYS:HB2  | 1.75                     | 0.43              |
| 38:lR:155:LEU:O    | 38:lR:158:GLN:NE2  | 2.51                     | 0.43              |
| 39:lS:174:THR:HG23 | 85:l5:4764:A:OP2   | 2.18                     | 0.43              |
| 45:lZ:56:ALA:C     | 45:lZ:57:MET:SD    | 3.00                     | 0.43              |
| 49:ld:24:GLU:CD    | 49:ld:24:GLU:C     | 2.85                     | 0.43              |
| 49:ld:67:ARG:H     | 49:ld:67:ARG:HG2   | 1.65                     | 0.43              |
| 50:le:48:ARG:O     | 85:l5:1883:G:O2'   | 2.22                     | 0.43              |
| 57:ll:24:PRO:O     | 57:ll:27:ILE:HG12  | 2.18                     | 0.43              |
| 62:lr:2:SER:C      | 62:lr:6:GLN:HE21   | 2.26                     | 0.43              |
| 64:sR:93:GLN:HG2   | 64:sR:95:ILE:H     | 1.82                     | 0.43              |
| 68:sP:86:LEU:HB2   | 68:sP:89:MET:HE1   | 1.99                     | 0.43              |
| 77:sZ:47:LEU:CB    | 77:sZ:80:ARG:H     | 2.30                     | 0.43              |
| 77:sZ:53:ALA:O     | 77:sZ:57:LYS:NZ    | 2.41                     | 0.43              |
| 78:sf:108:VAL:HB   | 78:sf:112:GLY:HA2  | 1.99                     | 0.43              |
| 79:s2:220:U:C4     | 79:s2:302:A:N6     | 2.85                     | 0.43              |
| 79:s2:224:A:H2'    | 79:s2:225:G:C8     | 2.53                     | 0.43              |
| 79:s2:322:C:H2'    | 79:s2:323:C:C1'    | 2.48                     | 0.43              |
| 79:s2:431:G:H2'    | 79:s2:432:G:H8     | 1.82                     | 0.43              |
| 79:s2:520:A:O2'    | 79:s2:825:A:N3     | 2.35                     | 0.43              |
| 79:s2:637:U:H2'    | 79:s2:638:C:H6     | 1.81                     | 0.43              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 79:s2:644:G:H2'    | 79:s2:645:C:H6    | 1.83                     | 0.43              |
| 79:s2:1035:A:H2'   | 79:s2:1036:A:O4'  | 2.18                     | 0.43              |
| 79:s2:1411:G:H2'   | 79:s2:1412:C:O4'  | 2.17                     | 0.43              |
| 79:s2:1749:G:H2'   | 79:s2:1750:C:C6   | 2.52                     | 0.43              |
| 80:cB:226:LYS:HG2  | 80:cB:227:GLN:NE2 | 2.32                     | 0.43              |
| 85:l5:5:A:H2'      | 85:l5:6:C:O4'     | 2.18                     | 0.43              |
| 85:l5:84:A:N1      | 85:l5:98:A:H5''   | 2.33                     | 0.43              |
| 85:l5:1360:G:H2'   | 85:l5:1361:G:H8   | 1.82                     | 0.43              |
| 85:l5:1427:A:OP2   | 85:l5:1457:G:N1   | 2.48                     | 0.43              |
| 85:l5:1462:A:H2'   | 85:l5:1463:C:C6   | 2.53                     | 0.43              |
| 85:l5:1618:G:C4    | 85:l5:1619:G:C8   | 3.06                     | 0.43              |
| 85:l5:1855:G:H2'   | 85:l5:1856:C:H6   | 1.83                     | 0.43              |
| 85:l5:2500:U:H2'   | 85:l5:2501:C:H6   | 1.82                     | 0.43              |
| 85:l5:2675:G:H1'   | 85:l5:2676:A:OP2  | 2.17                     | 0.43              |
| 85:l5:2821:U:C4    | 85:l5:2822:G:C5   | 3.06                     | 0.43              |
| 85:l5:3831:U:H2'   | 85:l5:3832:U:H6   | 1.83                     | 0.43              |
| 85:l5:3969:G:O4'   | 85:l5:3970:G:N2   | 2.50                     | 0.43              |
| 85:l5:3970:G:HO2'  | 85:l5:4052:C:H41  | 1.59                     | 0.43              |
| 85:l5:4653:C:H2'   | 85:l5:4654:C:H6   | 1.83                     | 0.43              |
| 80:CB:8:GLN:HG2    | 8:SY:130:LYS:HE3  | 1.99                     | 0.43              |
| 80:CB:170:GLU:HB3  | 80:CB:173:GLU:OE2 | 2.18                     | 0.43              |
| 3:SI:28:GLU:N      | 3:SI:28:GLU:OE1   | 2.51                     | 0.43              |
| 3:SI:73:THR:OG1    | 79:S2:301:A:N3    | 2.45                     | 0.43              |
| 3:SI:101:ILE:HD13  | 3:SI:198:TYR:CD1  | 2.53                     | 0.43              |
| 4:SL:84:ARG:HB3    | 79:S2:374:G:H5'   | 2.00                     | 0.43              |
| 11:SB:105:LEU:HD12 | 11:SB:109:LYS:HG2 | 2.00                     | 0.43              |
| 12:SH:148:LEU:HA   | 18:SW:42:MET:CE   | 2.48                     | 0.43              |
| 14:Sa:82:LYS:HZ2   | 79:S2:1209:A:H5'' | 1.83                     | 0.43              |
| 17:SO:27:VAL:HG23  | 17:SO:90:ILE:HD13 | 1.99                     | 0.43              |
| 17:SO:32:HIS:N     | 17:SO:43:HIS:O    | 2.51                     | 0.43              |
| 85:L5:132:G:H2'    | 85:L5:133:C:H4'   | 1.99                     | 0.43              |
| 85:L5:160:G:C4     | 54:Li:26:HIS:CE1  | 3.06                     | 0.43              |
| 85:L5:227:A:N3     | 44:LY:2:LYS:HD2   | 2.32                     | 0.43              |
| 85:L5:393:U:H2'    | 85:L5:394:G:C8    | 2.53                     | 0.43              |
| 85:L5:930:G:H2'    | 85:L5:931:C:C6    | 2.52                     | 0.43              |
| 85:L5:1281:G:C5    | 26:LE:128:HIS:CD2 | 3.06                     | 0.43              |
| 85:L5:1380:G:H1'   | 85:L5:1382:G:O6   | 2.18                     | 0.43              |
| 85:L5:1384:C:H2'   | 85:L5:1385:G:C8   | 2.53                     | 0.43              |
| 85:L5:1618:G:H2'   | 85:L5:1619:G:H8   | 1.82                     | 0.43              |
| 85:L5:1708:G:N2    | 85:L5:1709:C:O2'  | 2.50                     | 0.43              |
| 85:L5:1778:C:H4'   | 25:LD:4:VAL:C     | 2.43                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 85:L5:2552:G:OP2   | 85:L5:2553:A:O2'   | 2.34                     | 0.43              |
| 85:L5:2576:G:C6    | 85:L5:2588:C:C4    | 3.06                     | 0.43              |
| 85:L5:2625:U:H1'   | 85:L5:4647:G:N7    | 2.32                     | 0.43              |
| 85:L5:2865:U:H2'   | 85:L5:2866:C:C6    | 2.53                     | 0.43              |
| 85:L5:3707:U:H2'   | 85:L5:3708:C:H6    | 1.82                     | 0.43              |
| 85:L5:3844:U:OP2   | 23:LB:239:LYS:HB2  | 2.17                     | 0.43              |
| 85:L5:3867:A:H2'   | 85:L5:3868:G:C8    | 2.53                     | 0.43              |
| 85:L5:4159:C:H2'   | 85:L5:4160:C:H6    | 1.82                     | 0.43              |
| 85:L5:4395:U:O2'   | 85:L5:4447:C:N4    | 2.50                     | 0.43              |
| 85:L5:4625:C:H2'   | 85:L5:4626:A:N3    | 2.33                     | 0.43              |
| 85:L5:4685:U:H2'   | 85:L5:4686:G:H8    | 1.83                     | 0.43              |
| 85:L5:5018:C:H2'   | 85:L5:5019:A:C8    | 2.53                     | 0.43              |
| 20:L7:114:U:H2'    | 20:L7:115:A:H8     | 1.81                     | 0.43              |
| 22:LA:176:ASP:OD1  | 22:LA:176:ASP:N    | 2.51                     | 0.43              |
| 23:LB:58:ARG:NH2   | 23:LB:60:VAL:HG22  | 2.32                     | 0.43              |
| 23:LB:317:LEU:HB2  | 23:LB:372:SER:HB2  | 2.00                     | 0.43              |
| 24:LC:33:ARG:CZ    | 37:LQ:22:ASP:OD1   | 2.66                     | 0.43              |
| 25:LD:208:MET:HE2  | 25:LD:208:MET:C    | 2.43                     | 0.43              |
| 25:LD:270:LYS:HD3  | 25:LD:270:LYS:HA   | 1.83                     | 0.43              |
| 26:LE:138:ARG:HH21 | 26:LE:170:SER:HA   | 1.83                     | 0.43              |
| 29:LH:158:ALA:O    | 29:LH:161:ILE:HG13 | 2.18                     | 0.43              |
| 31:LJ:9:GLU:C      | 31:LJ:11:PRO:HD2   | 2.43                     | 0.43              |
| 33:LM:6:PHE:H      | 33:LM:11:ARG:NH2   | 2.16                     | 0.43              |
| 34:LN:10:LEU:O     | 34:LN:19:MET:HE1   | 2.17                     | 0.43              |
| 34:LN:131:GLU:OE2  | 34:LN:131:GLU:HA   | 2.17                     | 0.43              |
| 35:LO:10:ASP:OD2   | 35:LO:37:ARG:NH2   | 2.51                     | 0.43              |
| 35:LO:77:SER:HB2   | 35:LO:104:VAL:HG22 | 2.00                     | 0.43              |
| 35:LO:120:VAL:HG22 | 39:LS:167:PHE:CD2  | 2.53                     | 0.43              |
| 40:LT:149:GLU:OE1  | 40:LT:149:GLU:N    | 2.48                     | 0.43              |
| 44:LY:10:ASP:OD1   | 44:LY:13:LYS:HG3   | 2.17                     | 0.43              |
| 45:LZ:11:VAL:HG21  | 45:LZ:80:LEU:HB2   | 1.99                     | 0.43              |
| 45:LZ:64:LYS:O     | 45:LZ:67:LYS:HG2   | 2.18                     | 0.43              |
| 51:Lf:88:PHE:CD2   | 51:Lf:92:LEU:HD21  | 2.52                     | 0.43              |
| 54:Li:60:LEU:HD23  | 54:Li:60:LEU:C     | 2.42                     | 0.43              |
| 65:SD:20:GLU:HG3   | 67:SK:64:TRP:CD2   | 2.53                     | 0.43              |
| 65:SD:24:PHE:HE2   | 67:SK:68:TYR:CE1   | 2.36                     | 0.43              |
| 67:SK:1:MET:HE3    | 67:SK:47:LYS:HE2   | 1.99                     | 0.43              |
| 71:ST:62:ARG:HE    | 71:ST:62:ARG:HB3   | 1.44                     | 0.43              |
| 71:ST:104:LEU:HG   | 71:ST:121:ARG:CZ   | 2.48                     | 0.43              |
| 72:SU:67:LYS:HG3   | 72:SU:78:ASP:HB2   | 2.00                     | 0.43              |
| 75:Sg:167:SER:OG   | 75:Sg:175:LYS:HB2  | 2.18                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 75:Sg:248:LEU:HB3  | 75:Sg:259:TRP:HE1  | 1.82                     | 0.43              |
| 78:Sf:87:THR:H     | 79:S2:1507:G:H1    | 1.66                     | 0.43              |
| 79:S2:452:G:H2'    | 79:S2:453:C:C6     | 2.53                     | 0.43              |
| 79:S2:641:A:H2'    | 79:S2:642:U:C6     | 2.53                     | 0.43              |
| 79:S2:1402:A:H8    | 79:S2:1402:A:OP2   | 2.01                     | 0.43              |
| 79:S2:1418:C:H4'   | 79:S2:1420:G:N2    | 2.19                     | 0.43              |
| 79:S2:1485:U:H2'   | 79:S2:1486:A:O4'   | 2.18                     | 0.43              |
| 79:S2:1550:G:O2'   | 79:S2:1558:C:O2    | 2.31                     | 0.43              |
| 79:S2:1764:G:H5'   | 79:S2:1765:C:H5''  | 1.99                     | 0.43              |
| 79:S2:1839:U:H2'   | 79:S2:1840:U:C6    | 2.53                     | 0.43              |
| 81:AP:19:G:C2      | 81:AP:57:G:C2      | 3.05                     | 0.43              |
| 1:CH:39:GLU:OE2    | 86:Se:47:PRO:HG3   | 2.18                     | 0.43              |
| 1:cH:85:ARG:HE     | 1:cH:85:ARG:HB3    | 1.15                     | 0.43              |
| 2:sE:92:ILE:HG12   | 2:sE:97:GLU:HB2    | 2.00                     | 0.43              |
| 4:sL:129:GLY:CA    | 4:sL:140:PHE:CE1   | 3.01                     | 0.43              |
| 5:sX:85:VAL:CG1    | 5:sX:122:VAL:HB    | 2.47                     | 0.43              |
| 5:sX:125:VAL:O     | 5:sX:126:ALA:C     | 2.61                     | 0.43              |
| 7:sJ:91:LYS:HB2    | 7:sJ:91:LYS:HE3    | 1.86                     | 0.43              |
| 8:sY:39:GLU:HA     | 8:sY:42:GLU:HG2    | 2.00                     | 0.43              |
| 11:sB:89:GLU:N     | 11:sB:89:GLU:OE1   | 2.51                     | 0.43              |
| 17:sO:61:LYS:HG3   | 17:sO:76:LEU:HG    | 2.00                     | 0.43              |
| 18:sW:91:ASN:OD1   | 18:sW:91:ASN:C     | 2.61                     | 0.43              |
| 18:sW:107:SER:HA   | 79:s2:862:A:N7     | 2.32                     | 0.43              |
| 19:sb:49:HIS:HD2   | 79:s2:1015:U:H5'   | 1.82                     | 0.43              |
| 20:l7:60:G:C2'     | 20:l7:61:G:H5'     | 2.49                     | 0.43              |
| 21:l8:154:G:C6     | 85:l5:4:G:N1       | 2.86                     | 0.43              |
| 27:lF:144:TYR:CE2  | 27:lF:237:GLU:HG3  | 2.50                     | 0.43              |
| 28:lG:214:ALA:HA   | 28:lG:217:LYS:HD3  | 1.99                     | 0.43              |
| 29:lH:111:LEU:HB2  | 29:lH:127:ARG:NH1  | 2.33                     | 0.43              |
| 33:lM:104:MET:HE3  | 33:lM:104:MET:CA   | 2.48                     | 0.43              |
| 34:lN:83:LYS:O     | 34:lN:85:VAL:N     | 2.51                     | 0.43              |
| 38:lR:49:LEU:HD23  | 38:lR:49:LEU:HA    | 1.74                     | 0.43              |
| 38:lR:79:GLY:O     | 85:l5:3619:G:H4'   | 2.18                     | 0.43              |
| 39:lS:43:ARG:HD2   | 39:lS:43:ARG:HA    | 1.56                     | 0.43              |
| 40:lT:34:TYR:HE2   | 40:lT:93:ILE:HG23  | 1.83                     | 0.43              |
| 41:lU:24:ASP:OD1   | 41:lU:24:ASP:C     | 2.61                     | 0.43              |
| 43:lX:109:ILE:O    | 43:lX:113:VAL:HG12 | 2.18                     | 0.43              |
| 55:lJ:59:THR:HG22  | 85:l5:23:C:H4'     | 2.00                     | 0.43              |
| 64:sR:67:ARG:HB2   | 79:s2:1375:G:P     | 2.58                     | 0.43              |
| 65:sD:172:VAL:HG22 | 65:sD:185:LYS:HD3  | 1.99                     | 0.43              |
| 68:sP:34:MET:HB2   | 68:sP:35:GLN:NE2   | 2.33                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 70:sS:47:LYS:O     | 70:sS:77:TYR:OH    | 2.35                     | 0.43              |
| 71:sT:40:ALA:O     | 71:sT:42:HIS:N     | 2.51                     | 0.43              |
| 71:sT:64:LEU:HD12  | 71:sT:68:GLY:HA2   | 2.00                     | 0.43              |
| 79:s2:80:G:H2'     | 79:s2:81:U:H6      | 1.82                     | 0.43              |
| 79:s2:573:U:O2     | 79:s2:576:A:H8     | 2.00                     | 0.43              |
| 79:s2:1037:G:H4'   | 79:s2:1845:A:H4'   | 2.00                     | 0.43              |
| 79:s2:1177:U:H2'   | 79:s2:1178:U:C6    | 2.53                     | 0.43              |
| 79:s2:1406:G:H2'   | 79:s2:1407:U:C6    | 2.52                     | 0.43              |
| 79:s2:1413:G:H2'   | 79:s2:1414:A:H8    | 1.83                     | 0.43              |
| 79:s2:1617:G:N1    | 79:s2:1620:A:OP2   | 2.52                     | 0.43              |
| 79:s2:1779:G:H2'   | 79:s2:1780:G:H8    | 1.81                     | 0.43              |
| 80:cB:45:ILE:HB    | 80:cB:78:PHE:HB2   | 2.01                     | 0.43              |
| 80:cB:68:ILE:HG23  | 80:cB:108:HIS:NE2  | 2.32                     | 0.43              |
| 80:cB:337:LYS:O    | 80:cB:341:ARG:NH1  | 2.51                     | 0.43              |
| 80:cB:453:MET:SD   | 80:cB:454:MET:N    | 2.91                     | 0.43              |
| 80:cB:558:LEU:HD13 | 80:cB:572:LYS:NZ   | 2.20                     | 0.43              |
| 81:aP:34:A:H2'     | 81:aP:35:A:H8      | 1.83                     | 0.43              |
| 82:pE:50:A:C6      | 82:pE:65:G:N1      | 2.86                     | 0.43              |
| 85:l5:86:U:OP2     | 85:l5:97:G:N1      | 2.36                     | 0.43              |
| 85:l5:1274:A:C4    | 85:l5:1275:G:C8    | 3.06                     | 0.43              |
| 85:l5:1474:C:H2'   | 85:l5:1475:G:C8    | 2.53                     | 0.43              |
| 85:l5:1773:U:H2'   | 85:l5:1774:C:C6    | 2.52                     | 0.43              |
| 85:l5:1797:G:H2'   | 85:l5:1798:G:C8    | 2.54                     | 0.43              |
| 85:l5:2904:U:H5''  | 85:l5:2905:C:OP1   | 2.18                     | 0.43              |
| 85:l5:4141:G:H5'   | 85:l5:4142:C:C5    | 2.53                     | 0.43              |
| 85:l5:4523:A:H2'   | 85:l5:4559:A:N7    | 2.33                     | 0.43              |
| 85:l5:4974:C:H1'   | 85:l5:4985:U:O2    | 2.18                     | 0.43              |
| 85:l5:5010:U:H2'   | 85:l5:5011:A:H8    | 1.83                     | 0.43              |
| 80:CB:264:ARG:HG3  | 80:CB:288:THR:HG21 | 1.99                     | 0.43              |
| 80:CB:343:TRP:CE3  | 80:CB:344:LEU:HG   | 2.54                     | 0.43              |
| 80:CB:395:MET:SD   | 80:CB:395:MET:O    | 2.76                     | 0.43              |
| 80:CB:480:VAL:HA   | 80:CB:529:LYS:CE   | 2.48                     | 0.43              |
| 2:SE:52:LEU:HD11   | 2:SE:111:VAL:HG11  | 2.00                     | 0.43              |
| 6:SG:20:ASP:O      | 6:SG:24:LEU:HG     | 2.18                     | 0.43              |
| 6:SG:136:LYS:HE3   | 6:SG:174:PRO:HB2   | 2.00                     | 0.43              |
| 6:SG:201:LYS:HE3   | 6:SG:201:LYS:HB3   | 1.76                     | 0.43              |
| 11:SB:25:PHE:HZ    | 17:SO:53:ILE:O     | 2.00                     | 0.43              |
| 11:SB:89:GLU:OE1   | 11:SB:99:ASN:ND2   | 2.52                     | 0.43              |
| 11:SB:97:LEU:HD22  | 11:SB:232:HIS:CD2  | 2.53                     | 0.43              |
| 11:SB:187:LYS:C    | 11:SB:190:PRO:HD2  | 2.43                     | 0.43              |
| 14:Sa:10:ARG:HD3   | 14:Sa:33:ASP:OD2   | 2.17                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 16:SN:56:ASP:OD2   | 19:Sb:51:GLN:N     | 2.47                     | 0.43              |
| 18:SW:24:GLN:HB2   | 18:SW:63:VAL:O     | 2.18                     | 0.43              |
| 18:SW:103:VAL:HA   | 18:SW:112:ASP:HA   | 2.00                     | 0.43              |
| 85:L5:221:C:H2'    | 85:L5:222:C:H6     | 1.81                     | 0.43              |
| 85:L5:482:G:N1     | 85:L5:673:C:N3     | 2.66                     | 0.43              |
| 85:L5:727:C:H5''   | 27:LF:73:ARG:HH12  | 1.82                     | 0.43              |
| 85:L5:920:C:H5''   | 39:LS:74:ARG:NH2   | 2.32                     | 0.43              |
| 85:L5:1444:G:H2'   | 85:L5:1445:U:C6    | 2.54                     | 0.43              |
| 85:L5:1552:G:O2'   | 85:L5:1553:A:OP2   | 2.35                     | 0.43              |
| 85:L5:1664:U:H2'   | 85:L5:1665:C:H6    | 1.84                     | 0.43              |
| 85:L5:1922:G:C2    | 85:L5:2063:G:C5    | 3.05                     | 0.43              |
| 85:L5:1967:A:C6    | 85:L5:2021:G:C6    | 3.06                     | 0.43              |
| 85:L5:2111:G:H2'   | 85:L5:2251:G:C2    | 2.53                     | 0.43              |
| 85:L5:2448:G:H2'   | 85:L5:2449:A:C8    | 2.53                     | 0.43              |
| 85:L5:2485:U:H1'   | 85:L5:2486:G:C6    | 2.53                     | 0.43              |
| 85:L5:2503:G:O6    | 22:LA:72:ARG:NH1   | 2.51                     | 0.43              |
| 85:L5:2891:U:H2'   | 85:L5:2892:C:O4'   | 2.18                     | 0.43              |
| 85:L5:3936:A:H2'   | 85:L5:3937:C:C6    | 2.52                     | 0.43              |
| 85:L5:4103:C:P     | 85:L5:4108:G:N2    | 2.91                     | 0.43              |
| 85:L5:4647:G:C2    | 85:L5:4648:A:C8    | 3.06                     | 0.43              |
| 85:L5:4768:G:C6    | 85:L5:4867:G:C6    | 3.07                     | 0.43              |
| 20:L7:18:C:H2'     | 20:L7:19:C:H6      | 1.83                     | 0.43              |
| 24:LC:167:ALA:HB1  | 24:LC:221:PHE:HE2  | 1.84                     | 0.43              |
| 26:LE:223:ARG:NH1  | 26:LE:237:LYS:HB3  | 2.33                     | 0.43              |
| 26:LE:283:PRO:HB2  | 51:Lf:41:PHE:CE2   | 2.51                     | 0.43              |
| 27:LF:40:LYS:HG2   | 27:LF:41:MET:SD    | 2.59                     | 0.43              |
| 29:LH:188:GLN:O    | 29:LH:190:ALA:N    | 2.51                     | 0.43              |
| 30:LI:70:ILE:HG22  | 30:LI:74:LYS:NZ    | 2.26                     | 0.43              |
| 35:LO:198:THR:HG23 | 35:LO:199:HIS:ND1  | 2.34                     | 0.43              |
| 37:LQ:27:LEU:HD21  | 62:Lr:5:LEU:HD13   | 2.00                     | 0.43              |
| 41:LU:105:ASN:ND2  | 41:LU:111:GLU:OE1  | 2.51                     | 0.43              |
| 42:LV:85:ARG:H     | 42:LV:101:ASN:HD21 | 1.66                     | 0.43              |
| 44:LY:47:MET:CE    | 44:LY:48:PRO:HD2   | 2.48                     | 0.43              |
| 44:LY:69:LYS:O     | 44:LY:69:LYS:HG3   | 2.18                     | 0.43              |
| 48:Lc:26:LYS:HG3   | 48:Lc:98:ASP:OD1   | 2.18                     | 0.43              |
| 48:Lc:62:TYR:CD2   | 48:Lc:66:LEU:HD23  | 2.53                     | 0.43              |
| 49:Ld:96:GLU:OE2   | 49:Ld:98:SER:OG    | 2.35                     | 0.43              |
| 60:Lo:61:LYS:HD3   | 60:Lo:61:LYS:HA    | 1.68                     | 0.43              |
| 61:Lp:59:SER:OG    | 61:Lp:60:CYS:N     | 2.52                     | 0.43              |
| 62:Lr:97:ILE:HD13  | 62:Lr:107:ARG:CA   | 2.48                     | 0.43              |
| 67:SK:95:ARG:HH11  | 67:SK:96:ARG:H     | 1.66                     | 0.43              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 74:Sd:13:LYS:HG3   | 74:Sd:14:PHE:H    | 1.83                     | 0.43              |
| 75:Sg:42:MET:SD    | 75:Sg:42:MET:C    | 3.00                     | 0.43              |
| 77:SZ:66:LYS:O     | 77:SZ:68:ILE:HG12 | 2.18                     | 0.43              |
| 78:Sf:103:LEU:HD23 | 78:Sf:103:LEU:H   | 1.84                     | 0.43              |
| 79:S2:389:A:H2'    | 79:S2:390:C:H6    | 1.81                     | 0.43              |
| 79:S2:570:C:H2'    | 79:S2:571:U:O4'   | 2.18                     | 0.43              |
| 79:S2:672:A:N6     | 79:S2:1027:A:OP1  | 2.38                     | 0.43              |
| 79:S2:884:C:H2'    | 79:S2:885:U:O4'   | 2.18                     | 0.43              |
| 79:S2:929:G:N2     | 79:S2:1104:G:H4'  | 2.32                     | 0.43              |
| 79:S2:1308:U:H2'   | 79:S2:1309:C:H6   | 1.83                     | 0.43              |
| 79:S2:1415:C:H5'   | 79:S2:1416:C:OP2  | 2.19                     | 0.43              |
| 83:Ls:40:MET:HA    | 83:Ls:43:ILE:HG22 | 2.00                     | 0.43              |
| 83:Ls:192:VAL:O    | 83:Ls:198:ILE:HA  | 2.19                     | 0.43              |
| 87:IW:54:LEU:HD12  | 87:IW:55:TYR:N    | 2.33                     | 0.43              |
| 87:IW:90:ILE:HG13  | 87:IW:91:MET:N    | 2.32                     | 0.43              |
| 1:CH:46:ALA:O      | 1:CH:48:GLN:NE2   | 2.51                     | 0.43              |
| 1:cH:75:LEU:HD23   | 1:cH:76:GLU:N     | 2.34                     | 0.43              |
| 2:sE:10:LYS:NZ     | 79:s2:95:G:OP1    | 2.51                     | 0.43              |
| 2:sE:101:LEU:HD21  | 2:sE:109:PHE:CZ   | 2.53                     | 0.43              |
| 2:sE:114:ILE:HD12  | 2:sE:118:GLU:HB3  | 1.99                     | 0.43              |
| 3:sI:143:LYS:HD2   | 3:sI:147:LYS:NZ   | 2.33                     | 0.43              |
| 3:sI:150:ASP:O     | 3:sI:154:LYS:HG3  | 2.18                     | 0.43              |
| 3:sI:184:ARG:NH2   | 79:s2:218:U:O2    | 2.51                     | 0.43              |
| 6:sG:32:MET:H      | 6:sG:32:MET:HG3   | 1.57                     | 0.43              |
| 6:sG:131:ARG:CZ    | 79:s2:168:C:H4'   | 2.48                     | 0.43              |
| 6:sG:143:LYS:HE3   | 6:sG:143:LYS:HB3  | 1.59                     | 0.43              |
| 7:sJ:103:GLU:OE2   | 7:sJ:103:GLU:N    | 2.39                     | 0.43              |
| 7:sJ:163:SER:C     | 7:sJ:165:TYR:H    | 2.26                     | 0.43              |
| 8:sY:18:LEU:O      | 8:sY:19:GLN:HG2   | 2.19                     | 0.43              |
| 11:sB:39:PHE:CE1   | 11:sB:74:LEU:HD21 | 2.53                     | 0.43              |
| 12:sH:33:ASN:HD21  | 12:sH:37:LYS:HE2  | 1.84                     | 0.43              |
| 13:sV:35:ASN:HB3   | 13:sV:50:PHE:CD2  | 2.52                     | 0.43              |
| 14:sa:21:ILE:O     | 14:sa:30:VAL:N    | 2.40                     | 0.43              |
| 15:sC:99:GLY:C     | 15:sC:101:SER:H   | 2.26                     | 0.43              |
| 16:sN:38:TYR:CE1   | 16:sN:78:LYS:HG2  | 2.51                     | 0.43              |
| 21:l8:26:C:H2'     | 21:l8:27:U:H6     | 1.83                     | 0.43              |
| 23:lB:297:LYS:HA   | 23:lB:297:LYS:HD2 | 1.73                     | 0.43              |
| 23:lB:305:THR:OG1  | 23:lB:365:LEU:O   | 2.36                     | 0.43              |
| 23:lB:378:ARG:HH21 | 87:IW:11:TYR:HE2  | 1.64                     | 0.43              |
| 24:lC:63:SER:O     | 24:lC:63:SER:OG   | 2.34                     | 0.43              |
| 25:lD:177:THR:HA   | 25:lD:180:PHE:HE2 | 1.81                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:ID:238:GLU:O    | 25:ID:242:LYS:HG3  | 2.19                     | 0.43              |
| 26:IE:179:LEU:HD11 | 85:l5:4938:A:C6    | 2.54                     | 0.43              |
| 28:IG:51:LEU:O     | 28:IG:55:VAL:HG23  | 2.18                     | 0.43              |
| 29:IH:99:PHE:CD2   | 29:IH:118:LEU:HA   | 2.53                     | 0.43              |
| 30:II:36:LEU:HD21  | 30:II:69:ARG:HH11  | 1.83                     | 0.43              |
| 33:IM:9:VAL:HG11   | 33:IM:66:HIS:HA    | 2.00                     | 0.43              |
| 34:IN:41:ARG:NE    | 85:l5:8:U:OP1      | 2.38                     | 0.43              |
| 34:IN:68:ARG:HH12  | 85:l5:303:C:P      | 2.41                     | 0.43              |
| 35:IO:49:ARG:HH22  | 85:l5:1932:A:P     | 2.41                     | 0.43              |
| 36:IP:25:HIS:HD2   | 85:l5:2361:G:C5    | 2.36                     | 0.43              |
| 37:IQ:101:CYS:CB   | 37:IQ:126:LEU:HD13 | 2.49                     | 0.43              |
| 38:IR:10:LEU:HD23  | 38:IR:10:LEU:HA    | 1.85                     | 0.43              |
| 63:lz:29:LEU:HB3   | 63:lz:171:HIS:CE1  | 2.53                     | 0.43              |
| 63:lz:39:LYS:H     | 63:lz:198:TRP:HB3  | 1.83                     | 0.43              |
| 64:sR:10:LYS:CE    | 79:s2:1367:U:H1'   | 2.48                     | 0.43              |
| 65:sD:47:GLU:C     | 65:sD:48:ILE:HD12  | 2.43                     | 0.43              |
| 66:sF:23:TRP:CH2   | 66:sF:97:PHE:HB3   | 2.53                     | 0.43              |
| 70:sS:130:ARG:NH2  | 79:s2:1230:C:OP1   | 2.35                     | 0.43              |
| 75:sg:10:THR:HG23  | 75:sg:308:ARG:HB3  | 2.00                     | 0.43              |
| 75:sg:113:PHE:CZ   | 75:sg:117:ASN:HA   | 2.53                     | 0.43              |
| 76:sM:49:LEU:HB2   | 76:sM:127:TYR:HE1  | 1.82                     | 0.43              |
| 77:sZ:88:LEU:HD23  | 77:sZ:88:LEU:HA    | 1.75                     | 0.43              |
| 79:s2:44:U:O2      | 79:s2:482:G:H1'    | 2.18                     | 0.43              |
| 79:s2:72:C:O2'     | 79:s2:73:C:O4'     | 2.34                     | 0.43              |
| 79:s2:317:C:H2'    | 79:s2:318:A:H5''   | 1.99                     | 0.43              |
| 79:s2:529:A:H2'    | 79:s2:530:U:C6     | 2.53                     | 0.43              |
| 79:s2:1017:U:H2'   | 79:s2:1018:U:C6    | 2.53                     | 0.43              |
| 79:s2:1305:C:H2'   | 79:s2:1306:U:C6    | 2.54                     | 0.43              |
| 79:s2:1355:C:C2    | 79:s2:1356:G:C2    | 3.06                     | 0.43              |
| 79:s2:1562:C:H2'   | 79:s2:1563:G:C8    | 2.52                     | 0.43              |
| 80:cB:37:ASP:CG    | 80:cB:55:ARG:HB2   | 2.42                     | 0.43              |
| 80:cB:256:MET:SD   | 80:cB:256:MET:C    | 3.01                     | 0.43              |
| 80:cB:400:LYS:HD3  | 80:cB:401:MET:H    | 1.84                     | 0.43              |
| 80:cB:570:ILE:HD12 | 80:cB:570:ILE:HA   | 1.80                     | 0.43              |
| 83:ls:26:LYS:NZ    | 83:ls:93:GLU:O     | 2.49                     | 0.43              |
| 83:ls:84:GLY:C     | 85:l5:2021:G:H4'   | 2.43                     | 0.43              |
| 84:lt:22:VAL:HA    | 84:lt:48:LYS:HG2   | 2.00                     | 0.43              |
| 85:l5:144:G:H2'    | 85:l5:145:G:H8     | 1.83                     | 0.43              |
| 85:l5:273:U:H2'    | 85:l5:274:C:H6     | 1.82                     | 0.43              |
| 85:l5:731:G:C6     | 85:l5:932:A:C4     | 3.06                     | 0.43              |
| 85:l5:1306:C:H2'   | 85:l5:1307:A:H8    | 1.83                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 85:L5:1622:U:O2    | 85:L5:1627:G:O2'   | 2.36                     | 0.43              |
| 85:L5:1821:G:H2'   | 85:L5:1821:G:N3    | 2.33                     | 0.43              |
| 85:L5:2465:C:H2'   | 85:L5:2466:G:O4'   | 2.18                     | 0.43              |
| 85:L5:3890:A:N6    | 85:L5:4571:A:O4'   | 2.51                     | 0.43              |
| 85:L5:4356:G:C2    | 85:L5:4357:G:C8    | 3.07                     | 0.43              |
| 85:L5:4439:U:H2'   | 85:L5:4440:G:O4'   | 2.17                     | 0.43              |
| 85:L5:4525:C:C2    | 85:L5:4526:U:C5    | 3.06                     | 0.43              |
| 85:L5:4538:G:C6    | 85:L5:4539:U:C4    | 3.06                     | 0.43              |
| 85:L5:4889:G:H2'   | 85:L5:4890:G:H8    | 1.82                     | 0.43              |
| 85:L5:4989:U:C6    | 85:L5:4991:U:H1'   | 2.53                     | 0.43              |
| 80:CB:295:ASP:O    | 80:CB:299:LYS:HG3  | 2.18                     | 0.43              |
| 80:CB:626:GLN:HE21 | 80:CB:630:GLN:HG3  | 1.83                     | 0.43              |
| 80:CB:769:HIS:ND1  | 85:L5:1981:G:H1'   | 2.32                     | 0.43              |
| 4:SL:32:LYS:HE2    | 4:SL:32:LYS:HA     | 1.99                     | 0.43              |
| 6:SG:69:THR:O      | 6:SG:99:GLY:HA3    | 2.17                     | 0.43              |
| 8:SY:27:VAL:O      | 8:SY:68:LYS:HA     | 2.18                     | 0.43              |
| 10:SA:179:ALA:O    | 10:SA:183:LEU:HD23 | 2.18                     | 0.43              |
| 12:SH:122:LEU:HD21 | 79:S2:688:U:H5'    | 2.00                     | 0.43              |
| 13:SV:61:ARG:NH1   | 79:S2:1138:C:N3    | 2.66                     | 0.43              |
| 14:Sa:20:PRO:HA    | 14:Sa:31:PRO:HA    | 2.00                     | 0.43              |
| 16:SN:23:PRO:O     | 16:SN:26:LEU:HD23  | 2.18                     | 0.43              |
| 85:L5:324:A:C6     | 85:L5:325:U:C4     | 3.06                     | 0.43              |
| 85:L5:724:C:H1'    | 24:LC:343:GLN:NE2  | 2.33                     | 0.43              |
| 85:L5:981:C:C4     | 26:LE:73:TYR:CE2   | 3.04                     | 0.43              |
| 85:L5:1748:U:C4    | 85:L5:1783:C:C4    | 3.06                     | 0.43              |
| 85:L5:2078:C:H2'   | 85:L5:2079:G:H8    | 1.82                     | 0.43              |
| 85:L5:2086:G:C2    | 85:L5:2272:C:C2    | 3.07                     | 0.43              |
| 85:L5:2329:U:C4    | 85:L5:2330:G:C6    | 3.06                     | 0.43              |
| 85:L5:2558:C:H2'   | 85:L5:2559:G:H8    | 1.83                     | 0.43              |
| 85:L5:2793:G:C2    | 85:L5:2797:C:C2    | 3.06                     | 0.43              |
| 85:L5:3794:C:H2'   | 85:L5:3795:A:C8    | 2.53                     | 0.43              |
| 85:L5:3871:A:H2'   | 85:L5:3872:A:C8    | 2.52                     | 0.43              |
| 85:L5:3884:U:C2    | 85:L5:3885:G:C8    | 3.07                     | 0.43              |
| 85:L5:4313:A:H4'   | 40:LT:71:ALA:HB3   | 1.99                     | 0.43              |
| 85:L5:4361:U:H2'   | 85:L5:4362:A:H8    | 1.83                     | 0.43              |
| 85:L5:4879:C:H2'   | 85:L5:4880:C:C6    | 2.53                     | 0.43              |
| 21:L8:4:C:C2       | 21:L8:5:U:C5       | 3.06                     | 0.43              |
| 21:L8:89:U:H2'     | 21:L8:90:C:C6      | 2.53                     | 0.43              |
| 22:LA:227:ARG:HB2  | 22:LA:239:ALA:HB2  | 2.00                     | 0.43              |
| 23:LB:216:MET:CE   | 23:LB:281:ASN:H    | 2.17                     | 0.43              |
| 27:LF:126:ASN:ND2  | 27:LF:129:SER:OG   | 2.51                     | 0.43              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 27:LF:142:TRP:CE2  | 27:LF:235:ASN:HB2 | 2.53                     | 0.43              |
| 28:LG:255:LYS:HD2  | 28:LG:258:ALA:HB3 | 1.99                     | 0.43              |
| 30:LI:179:ASP:OD2  | 30:LI:180:GLU:N   | 2.52                     | 0.43              |
| 36:LP:138:PRO:HB2  | 36:LP:140:MET:HE3 | 1.96                     | 0.43              |
| 38:LR:165:LYS:HE3  | 38:LR:165:LYS:HB3 | 1.78                     | 0.43              |
| 39:LS:32:ILE:HD12  | 39:LS:43:ARG:HB2  | 1.99                     | 0.43              |
| 42:LV:49:LEU:HD12  | 42:LV:50:ASN:N    | 2.33                     | 0.43              |
| 44:LY:52:ASP:CG    | 44:LY:69:LYS:HZ2  | 2.26                     | 0.43              |
| 46:La:58:MET:N     | 46:La:58:MET:SD   | 2.91                     | 0.43              |
| 47:Lb:39:PHE:CE2   | 47:Lb:43:MET:HE2  | 2.54                     | 0.43              |
| 53:Lh:108:GLN:OE1  | 53:Lh:109:ARG:N   | 2.51                     | 0.43              |
| 60:Lo:81:ARG:NH1   | 60:Lo:83:LEU:HD21 | 2.33                     | 0.43              |
| 62:Lr:103:ARG:O    | 62:Lr:105:ASP:N   | 2.47                     | 0.43              |
| 63:Lz:4:LYS:H      | 63:Lz:4:LYS:HG2   | 1.63                     | 0.43              |
| 63:Lz:58:THR:N     | 63:Lz:59:PRO:HD3  | 2.34                     | 0.43              |
| 66:SF:100:ILE:HD12 | 66:SF:100:ILE:HA  | 1.85                     | 0.43              |
| 67:SK:3:MET:C      | 67:SK:3:MET:HE3   | 2.43                     | 0.43              |
| 67:SK:84:HIS:HB2   | 76:SM:27:ILE:HG23 | 2.00                     | 0.43              |
| 68:SP:30:TYR:O     | 68:SP:33:LEU:N    | 2.51                     | 0.43              |
| 68:SP:88:GLU:CD    | 68:SP:88:GLU:H    | 2.26                     | 0.43              |
| 68:SP:94:VAL:O     | 68:SP:105:VAL:N   | 2.41                     | 0.43              |
| 69:SQ:125:ARG:NH2  | 79:S2:1648:G:C4   | 2.86                     | 0.43              |
| 74:Sd:14:PHE:HB2   | 79:S2:1661:A:H8   | 1.83                     | 0.43              |
| 74:Sd:33:LYS:HB3   | 74:Sd:34:TYR:CD2  | 2.54                     | 0.43              |
| 75:Sg:45:LEU:HA    | 75:Sg:52:TYR:O    | 2.17                     | 0.43              |
| 75:Sg:109:LEU:HD12 | 75:Sg:151:VAL:O   | 2.18                     | 0.43              |
| 75:Sg:140:TYR:CZ   | 75:Sg:142:VAL:HA  | 2.53                     | 0.43              |
| 79:S2:291:G:OP1    | 79:S2:291:G:H8    | 2.01                     | 0.43              |
| 79:S2:293:C:O2'    | 79:S2:294:U:H3'   | 2.18                     | 0.43              |
| 79:S2:314:U:H2'    | 79:S2:315:C:C6    | 2.52                     | 0.43              |
| 79:S2:367:U:O4'    | 79:S2:371:A:H1'   | 2.18                     | 0.43              |
| 79:S2:698:G:N7     | 79:S2:731:G:H3'   | 2.33                     | 0.43              |
| 79:S2:746:C:O2'    | 79:S2:798:G:N2    | 2.49                     | 0.43              |
| 79:S2:1222:G:H2'   | 79:S2:1223:A:H8   | 1.84                     | 0.43              |
| 79:S2:1673:U:H2'   | 79:S2:1674:G:O4'  | 2.18                     | 0.43              |
| 79:S2:1748:G:H2'   | 79:S2:1749:G:C8   | 2.53                     | 0.43              |
| 79:S2:1823:A:H5'   | 79:S2:1824:A:P    | 2.59                     | 0.43              |
| 79:S2:1844:U:H2'   | 79:S2:1845:A:C8   | 2.54                     | 0.43              |
| 82:PE:61:C:H2'     | 82:PE:62:C:H6     | 1.83                     | 0.43              |
| 87:LW:93:LYS:O     | 87:LW:96:GLN:NE2  | 2.48                     | 0.43              |
| 1:cH:45:ALA:HB1    | 9:se:55:PRO:CB    | 2.48                     | 0.43              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 4:sL:106:HIS:N     | 79:s2:399:C:O2    | 2.46                     | 0.43              |
| 4:sL:107:LYS:HB2   | 4:sL:107:LYS:HE2  | 1.80                     | 0.43              |
| 10:sA:12:GLU:HA    | 10:sA:15:VAL:CG2  | 2.48                     | 0.43              |
| 10:sA:39:TYR:CE1   | 64:sR:105:MET:HG2 | 2.52                     | 0.43              |
| 10:sA:141:ASN:O    | 10:sA:141:ASN:CG  | 2.62                     | 0.43              |
| 10:sA:166:LYS:HB3  | 10:sA:166:LYS:HE3 | 1.77                     | 0.43              |
| 11:sB:171:ILE:O    | 11:sB:174:ARG:HG3 | 2.17                     | 0.43              |
| 11:sB:209:ASP:OD1  | 11:sB:211:PHE:HE1 | 2.01                     | 0.43              |
| 16:sN:18:TYR:CD1   | 18:sW:56:HIS:NE2  | 2.86                     | 0.43              |
| 16:sN:71:ILE:HD11  | 79:s2:1018:U:H4'  | 2.00                     | 0.43              |
| 17:sO:33:ILE:HD12  | 17:sO:33:ILE:HA   | 1.77                     | 0.43              |
| 19:sb:22:LYS:HA    | 79:s2:921:G:C5    | 2.53                     | 0.43              |
| 22:lA:224:THR:HG21 | 85:l5:3705:G:H21  | 1.82                     | 0.43              |
| 23:lB:357:ARG:HE   | 23:lB:357:ARG:HB2 | 1.59                     | 0.43              |
| 28:lG:111:LYS:HE3  | 28:lG:111:LYS:HB3 | 1.73                     | 0.43              |
| 30:lI:149:ILE:HD13 | 30:lI:149:ILE:HA  | 1.87                     | 0.43              |
| 37:lQ:88:ASP:HB3   | 85:l5:1354:A:OP1  | 2.18                     | 0.43              |
| 37:lQ:148:VAL:HG12 | 85:l5:1346:C:OP1  | 2.19                     | 0.43              |
| 38:lR:19:LYS:H     | 85:l5:2823:G:P    | 2.41                     | 0.43              |
| 38:lR:180:LYS:HA   | 38:lR:180:LYS:CE  | 2.48                     | 0.43              |
| 42:lV:57:VAL:HG13  | 42:lV:84:GLN:OE1  | 2.18                     | 0.43              |
| 44:lY:74:TYR:HB3   | 44:lY:77:LYS:HB2  | 2.01                     | 0.43              |
| 45:lZ:57:MET:HE2   | 45:lZ:57:MET:HB2  | 1.68                     | 0.43              |
| 48:lc:12:GLU:O     | 48:lc:16:SER:HB3  | 2.19                     | 0.43              |
| 53:lh:91:MET:HA    | 53:lh:94:ARG:HG3  | 2.00                     | 0.43              |
| 55:lj:28:HIS:HD2   | 85:l5:1532:G:H5'  | 1.84                     | 0.43              |
| 56:lk:13:LEU:HD12  | 56:lk:14:THR:N    | 2.33                     | 0.43              |
| 60:lo:17:LYS:HA    | 85:l5:4318:C:H4'  | 2.00                     | 0.43              |
| 60:lo:44:LYS:NZ    | 85:l5:91:G:OP1    | 2.32                     | 0.43              |
| 64:sR:6:THR:OG1    | 64:sR:9:VAL:HG22  | 2.18                     | 0.43              |
| 64:sR:16:ILE:HG23  | 64:sR:20:TYR:CE2  | 2.53                     | 0.43              |
| 64:sR:68:GLY:HA3   | 64:sR:69:ILE:HA   | 1.56                     | 0.43              |
| 68:sP:49:LEU:HD23  | 68:sP:54:HIS:CE1  | 2.53                     | 0.43              |
| 70:sS:18:THR:OG1   | 70:sS:19:ASN:N    | 2.52                     | 0.43              |
| 70:sS:39:ARG:HD3   | 79:s2:1629:C:OP1  | 2.18                     | 0.43              |
| 75:sg:121:VAL:HG13 | 75:sg:156:PHE:CE1 | 2.53                     | 0.43              |
| 76:sM:19:GLN:O     | 76:sM:23:LYS:HG2  | 2.18                     | 0.43              |
| 78:sf:94:LYS:HA    | 78:sf:94:LYS:HD3  | 1.83                     | 0.43              |
| 78:sf:118:ARG:HD3  | 78:sf:131:PHE:CE1 | 2.47                     | 0.43              |
| 79:s2:14:C:H2'     | 79:s2:15:U:C6     | 2.54                     | 0.43              |
| 79:s2:26:U:H2'     | 79:s2:27:A:H8     | 1.83                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 79:s2:187:G:C6     | 79:s2:188:C:C4     | 3.06                     | 0.43              |
| 79:s2:805:U:H2'    | 79:s2:806:U:H6     | 1.83                     | 0.43              |
| 79:s2:1258:A:C2    | 79:s2:1663:A:H2'   | 2.52                     | 0.43              |
| 79:s2:1351:G:C2    | 79:s2:1379:A:C6    | 3.07                     | 0.43              |
| 79:s2:1358:U:H6    | 79:s2:1358:U:OP2   | 2.01                     | 0.43              |
| 79:s2:1625:U:H2'   | 79:s2:1626:C:H6    | 1.84                     | 0.43              |
| 79:s2:1677:U:O4    | 79:s2:1678:A:N6    | 2.50                     | 0.43              |
| 79:s2:1826:G:H2'   | 79:s2:1827:U:H6    | 1.83                     | 0.43              |
| 80:cB:53:GLU:N     | 80:cB:55:ARG:HH21  | 2.16                     | 0.43              |
| 80:cB:421:VAL:HG12 | 80:cB:464:VAL:O    | 2.18                     | 0.43              |
| 81:aP:63:G:C6      | 81:aP:64:G:N7      | 2.86                     | 0.43              |
| 82:pE:9:A:H4'      | 82:pE:47:U:OP2     | 2.19                     | 0.43              |
| 82:pE:72:C:O2      | 82:pE:72:C:H2'     | 2.17                     | 0.43              |
| 83:ls:38:LYS:HA    | 83:ls:38:LYS:HD3   | 1.92                     | 0.43              |
| 84:lt:109:ILE:HD12 | 84:lt:109:ILE:H    | 1.84                     | 0.43              |
| 84:lt:134:GLY:C    | 84:lt:137:GLN:HE22 | 2.22                     | 0.43              |
| 85:l5:39:A:N7      | 85:l5:1654:G:C5    | 2.86                     | 0.43              |
| 85:l5:256:G:H2'    | 85:l5:257:C:H6     | 1.81                     | 0.43              |
| 85:l5:427:A:H2'    | 85:l5:428:G:C8     | 2.53                     | 0.43              |
| 85:l5:1320:U:O2'   | 85:l5:1891:A:N1    | 2.48                     | 0.43              |
| 85:l5:1350:C:H2'   | 85:l5:1351:G:C8    | 2.53                     | 0.43              |
| 85:l5:1804:A:C4    | 85:l5:1833:G:C6    | 3.06                     | 0.43              |
| 85:l5:1846:G:H2'   | 85:l5:1847:C:C6    | 2.53                     | 0.43              |
| 85:l5:1907:A:H2'   | 85:l5:1908:A:C8    | 2.53                     | 0.43              |
| 85:l5:1972:G:C6    | 85:l5:1995:G:C6    | 3.06                     | 0.43              |
| 85:l5:2075:G:H2'   | 85:l5:2076:G:H8    | 1.82                     | 0.43              |
| 85:l5:2381:A:H1'   | 85:l5:2383:C:OP2   | 2.19                     | 0.43              |
| 85:l5:2422:C:N3    | 85:l5:2829:U:O2'   | 2.51                     | 0.43              |
| 85:l5:2751:G:H2'   | 85:l5:2752:G:C8    | 2.51                     | 0.43              |
| 85:l5:4040:C:OP1   | 85:l5:4045:G:N2    | 2.50                     | 0.43              |
| 85:l5:4068:U:H2'   | 85:l5:4069:U:C6    | 2.53                     | 0.43              |
| 85:l5:4412:C:C2    | 85:l5:4413:C:C5    | 3.06                     | 0.43              |
| 85:l5:4749:C:H2'   | 85:l5:4750:G:O4'   | 2.19                     | 0.43              |
| 85:l5:4751:G:C5    | 85:l5:4752:U:C5    | 3.06                     | 0.43              |
| 85:l5:4981:G:OP2   | 85:l5:4981:G:N2    | 2.41                     | 0.43              |
| 80:CB:45:ILE:HD13  | 80:CB:45:ILE:N     | 2.32                     | 0.43              |
| 80:CB:420:LEU:HD12 | 80:CB:465:PRO:HB3  | 2.01                     | 0.43              |
| 80:CB:747:VAL:HA   | 80:CB:812:CYS:HA   | 1.99                     | 0.43              |
| 2:SE:69:PHE:CE1    | 8:SY:17:LEU:HD12   | 2.42                     | 0.43              |
| 2:SE:122:LYS:C     | 2:SE:161:GLN:HE22  | 2.25                     | 0.43              |
| 3:SI:98:LYS:HB2    | 79:S2:378:U:OP1    | 2.18                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:SI:125:LYS:H     | 3:SI:128:LYS:HZ1   | 1.65                     | 0.43              |
| 4:SL:128:VAL:HA    | 4:SL:142:VAL:HA    | 2.00                     | 0.43              |
| 5:SX:50:ILE:O      | 5:SX:50:ILE:HG13   | 2.17                     | 0.43              |
| 5:SX:131:LEU:HD23  | 5:SX:131:LEU:H     | 1.83                     | 0.43              |
| 11:SB:85:LYS:N     | 11:SB:85:LYS:HD3   | 2.33                     | 0.43              |
| 11:SB:144:LYS:HB3  | 11:SB:208:HIS:HB3  | 1.99                     | 0.43              |
| 12:SH:158:LEU:HD13 | 12:SH:158:LEU:HA   | 1.87                     | 0.43              |
| 12:SH:166:VAL:HA   | 12:SH:169:LYS:NZ   | 2.33                     | 0.43              |
| 13:SV:38:GLU:HB2   | 13:SV:47:ASN:ND2   | 2.30                     | 0.43              |
| 14:Sa:22:ARG:NH1   | 17:SO:142:ARG:H    | 2.16                     | 0.43              |
| 14:Sa:77:CYS:O     | 14:Sa:81:SER:OG    | 2.24                     | 0.43              |
| 85:L5:71:C:N3      | 85:L5:73:A:C4      | 2.86                     | 0.43              |
| 85:L5:169:G:N2     | 85:L5:267:G:C4     | 2.86                     | 0.43              |
| 85:L5:661:C:H2'    | 85:L5:662:C:C6     | 2.53                     | 0.43              |
| 85:L5:1326:A:OP2   | 85:L5:4445:U:O2'   | 2.33                     | 0.43              |
| 85:L5:1460:C:C2    | 85:L5:1461:C:C5    | 3.06                     | 0.43              |
| 85:L5:1558:A:O3'   | 38:LR:126:LYS:NZ   | 2.48                     | 0.43              |
| 85:L5:1604:G:H2'   | 85:L5:1605:G:H8    | 1.80                     | 0.43              |
| 85:L5:1614:C:H2'   | 85:L5:1615:C:H6    | 1.83                     | 0.43              |
| 85:L5:1887:G:N1    | 85:L5:1893:C:C4    | 2.86                     | 0.43              |
| 85:L5:1932:A:H2'   | 85:L5:1933:G:C8    | 2.53                     | 0.43              |
| 85:L5:2340:C:H4'   | 24:LC:42:THR:OG1   | 2.18                     | 0.43              |
| 85:L5:2624:G:OP2   | 41:LU:97:ARG:NH2   | 2.51                     | 0.43              |
| 85:L5:2800:G:H2'   | 85:L5:2801:U:C6    | 2.53                     | 0.43              |
| 85:L5:3650:C:H2'   | 85:L5:3651:A:H8    | 1.82                     | 0.43              |
| 85:L5:4116:C:C3'   | 85:L5:4117:U:H5'   | 2.49                     | 0.43              |
| 85:L5:4123:C:H2'   | 85:L5:4124:G:C8    | 2.53                     | 0.43              |
| 85:L5:4343:U:H2'   | 85:L5:4344:U:C6    | 2.53                     | 0.43              |
| 85:L5:4454:G:H1    | 85:L5:4526:U:H3    | 1.67                     | 0.43              |
| 85:L5:4454:G:H2'   | 85:L5:4455:G:H8    | 1.82                     | 0.43              |
| 21:L8:10:G:H2'     | 21:L8:11:C:C6      | 2.53                     | 0.43              |
| 22:LA:80:GLU:OE1   | 22:LA:80:GLU:HA    | 2.18                     | 0.43              |
| 24:LC:109:ARG:HD2  | 24:LC:111:TRP:CZ3  | 2.53                     | 0.43              |
| 24:LC:208:CYS:HG   | 24:LC:248:ARG:HE   | 1.67                     | 0.43              |
| 26:LE:63:TYR:CD1   | 26:LE:68:MET:HB3   | 2.53                     | 0.43              |
| 27:LF:229:GLU:OE1  | 27:LF:229:GLU:N    | 2.51                     | 0.43              |
| 28:LG:162:ASP:C    | 28:LG:162:ASP:OD2  | 2.61                     | 0.43              |
| 28:LG:180:PRO:HA   | 28:LG:227:ASN:OD1  | 2.19                     | 0.43              |
| 29:LH:93:ARG:O     | 29:LH:179:ILE:HD12 | 2.18                     | 0.43              |
| 34:LN:33:LEU:HD13  | 34:LN:37:HIS:CD2   | 2.53                     | 0.43              |
| 35:LO:54:TYR:OH    | 35:LO:73:PHE:O     | 2.36                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 43:LX:73:HIS:ND1   | 43:LX:115:LYS:HD2  | 2.34                     | 0.43              |
| 64:SR:59:LYS:O     | 64:SR:63:ARG:NH2   | 2.51                     | 0.43              |
| 65:SD:40:ARG:HG3   | 72:SU:108:PRO:HG3  | 2.00                     | 0.43              |
| 65:SD:217:ILE:HG13 | 65:SD:218:LEU:H    | 1.82                     | 0.43              |
| 66:SF:47:LYS:HA    | 69:SQ:115:TYR:OH   | 2.17                     | 0.43              |
| 67:SK:15:LEU:HA    | 67:SK:15:LEU:HD13  | 1.76                     | 0.43              |
| 68:SP:50:ARG:HD2   | 68:SP:50:ARG:HA    | 1.82                     | 0.43              |
| 71:ST:14:PHE:CE1   | 71:ST:62:ARG:HD2   | 2.53                     | 0.43              |
| 72:SU:54:VAL:HG22  | 72:SU:88:LEU:O     | 2.18                     | 0.43              |
| 73:Sc:20:ARG:HG3   | 79:S2:1680:G:H4'   | 1.99                     | 0.43              |
| 75:Sg:10:THR:HA    | 75:Sg:308:ARG:HA   | 1.99                     | 0.43              |
| 75:Sg:59:LEU:HG    | 75:Sg:90:TRP:CE2   | 2.53                     | 0.43              |
| 79:S2:314:U:H2'    | 79:S2:315:C:H6     | 1.83                     | 0.43              |
| 79:S2:903:A:H1'    | 79:S2:904:A:C2     | 2.54                     | 0.43              |
| 79:S2:936:G:H2'    | 79:S2:937:C:C6     | 2.53                     | 0.43              |
| 79:S2:1034:A:H2'   | 79:S2:1035:A:O4'   | 2.18                     | 0.43              |
| 79:S2:1383:A:H2'   | 79:S2:1384:C:H6    | 1.83                     | 0.43              |
| 84:Lt:54:LYS:HA    | 84:Lt:55:GLY:HA2   | 1.83                     | 0.43              |
| 84:Lt:142:ASN:CG   | 84:Lt:146:ARG:HH22 | 2.26                     | 0.43              |
| 1:CH:142:GLU:H     | 1:CH:142:GLU:HG2   | 1.56                     | 0.43              |
| 2:sE:199:GLU:CD    | 2:sE:199:GLU:C     | 2.87                     | 0.43              |
| 3:sI:154:LYS:HE2   | 3:sI:154:LYS:HB2   | 1.72                     | 0.43              |
| 4:sL:21:LYS:HD2    | 4:sL:21:LYS:HA     | 1.82                     | 0.43              |
| 4:sL:82:MET:SD     | 4:sL:82:MET:C      | 2.98                     | 0.43              |
| 10:sA:141:ASN:HB2  | 13:sV:31:SER:O     | 2.19                     | 0.43              |
| 11:sB:41:ILE:HB    | 11:sB:74:LEU:O     | 2.18                     | 0.43              |
| 12:sH:158:LEU:CD2  | 12:sH:187:PHE:HB3  | 2.48                     | 0.43              |
| 15:sC:113:GLN:CB   | 15:sC:122:THR:HA   | 2.48                     | 0.43              |
| 15:sC:268:GLU:HG3  | 15:sC:269:PHE:CD2  | 2.53                     | 0.43              |
| 18:sW:57:ARG:NH1   | 19:sb:26:GLN:OE1   | 2.51                     | 0.43              |
| 21:l8:45:C:H2'     | 21:l8:46:G:H8      | 1.83                     | 0.43              |
| 23:lB:223:THR:HG23 | 23:lB:275:HIS:O    | 2.19                     | 0.43              |
| 24:lC:326:LEU:HD13 | 24:lC:333:LYS:HB2  | 1.99                     | 0.43              |
| 25:lD:63:GLN:HB2   | 25:lD:74:ILE:HD13  | 2.00                     | 0.43              |
| 25:lD:175:HIS:HA   | 85:l5:4323:A:O2'   | 2.19                     | 0.43              |
| 27:lF:131:ASN:O    | 27:lF:135:ILE:HG13 | 2.19                     | 0.43              |
| 27:lF:235:ASN:OD1  | 27:lF:236:ARG:N    | 2.52                     | 0.43              |
| 28:lG:117:ARG:HE   | 28:lG:121:LYS:HE3  | 1.84                     | 0.43              |
| 28:lG:132:ARG:HA   | 28:lG:133:PRO:HD3  | 1.92                     | 0.43              |
| 29:lH:129:ARG:HA   | 29:lH:129:ARG:HD3  | 1.79                     | 0.43              |
| 34:lN:104:GLU:HA   | 34:lN:160:GLU:CG   | 2.49                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 34:IN:146:PRO:HA   | 34:IN:149:GLN:HE22 | 1.82                     | 0.43              |
| 35:IO:113:ASP:OD1  | 35:IO:114:LYS:N    | 2.50                     | 0.43              |
| 42:IV:48:ARG:HB3   | 42:IV:51:ARG:HB3   | 2.00                     | 0.43              |
| 42:IV:97:TYR:HE1   | 87:IW:19:ARG:NE    | 2.13                     | 0.43              |
| 43:IX:83:THR:HG22  | 43:IX:86:ALA:HB2   | 1.99                     | 0.43              |
| 44:IY:77:LYS:HB3   | 44:IY:79:VAL:HG22  | 2.01                     | 0.43              |
| 45:IZ:135:ARG:HD2  | 45:IZ:135:ARG:HA   | 1.74                     | 0.43              |
| 46:la:109:TYR:O    | 46:la:126:ALA:HB1  | 2.19                     | 0.43              |
| 47:lb:53:GLY:O     | 47:lb:56:LYS:HE2   | 2.18                     | 0.43              |
| 47:lb:67:ALA:O     | 47:lb:70:GLU:HG3   | 2.18                     | 0.43              |
| 47:lb:111:ARG:HG3  | 47:lb:112:ILE:N    | 2.32                     | 0.43              |
| 48:lc:73:HIS:O     | 48:lc:74:TYR:C     | 2.61                     | 0.43              |
| 48:lc:91:VAL:HG12  | 85:l5:2673:G:O2'   | 2.18                     | 0.43              |
| 49:ld:57:MET:SD    | 49:ld:57:MET:N     | 2.92                     | 0.43              |
| 60:lo:56:PHE:CE1   | 60:lo:58:LYS:HB2   | 2.54                     | 0.43              |
| 61:lp:39:CYS:HB3   | 61:lp:42:CYS:SG    | 2.57                     | 0.43              |
| 61:lp:85:ARG:NH1   | 79:s2:940:U:OP1    | 2.52                     | 0.43              |
| 64:sR:24:LEU:HD22  | 64:sR:55:THR:HG22  | 2.00                     | 0.43              |
| 64:sR:43:SER:HA    | 79:s2:1389:C:N4    | 2.34                     | 0.43              |
| 65:sD:173:ARG:HG3  | 65:sD:174:HIS:N    | 2.32                     | 0.43              |
| 66:sF:110:GLN:NE2  | 66:sF:114:ASN:OD1  | 2.40                     | 0.43              |
| 68:sP:86:LEU:HD13  | 68:sP:87:PRO:HD2   | 2.00                     | 0.43              |
| 68:sP:115:TYR:HB2  | 68:sP:118:GLU:HG2  | 2.01                     | 0.43              |
| 69:sQ:25:CYS:SG    | 69:sQ:91:ALA:HB1   | 2.59                     | 0.43              |
| 70:sS:43:VAL:HG21  | 70:sS:83:PHE:CE1   | 2.54                     | 0.43              |
| 71:sT:26:GLY:O     | 71:sT:27:LYS:HD3   | 2.19                     | 0.43              |
| 75:sg:143:GLN:C    | 75:sg:145:GLU:H    | 2.25                     | 0.43              |
| 75:sg:257:LYS:HG2  | 75:sg:269:GLU:HB2  | 1.99                     | 0.43              |
| 75:sg:270:LEU:HD22 | 75:sg:310:TRP:CE3  | 2.54                     | 0.43              |
| 77:sZ:79:ILE:CG2   | 77:sZ:84:ALA:HB2   | 2.47                     | 0.43              |
| 79:s2:1040:G:C6    | 79:s2:1076:G:C6    | 3.07                     | 0.43              |
| 79:s2:1354:G:C5    | 79:s2:1356:G:P     | 3.11                     | 0.43              |
| 80:cB:31:GLY:HA2   | 80:cB:34:THR:HG23  | 1.99                     | 0.43              |
| 80:cB:155:LEU:HD11 | 80:cB:157:MET:HB3  | 2.01                     | 0.43              |
| 81:aP:5:C:H2'      | 81:aP:6:C:H6       | 1.82                     | 0.43              |
| 82:pE:37:A:H3'     | 82:pE:38:A:C8      | 2.33                     | 0.43              |
| 83:ls:40:MET:HE3   | 83:ls:41:GLN:HG3   | 2.00                     | 0.43              |
| 85:l5:199:G:C4     | 85:l5:201:C:C5     | 3.07                     | 0.43              |
| 85:l5:216:C:P      | 85:l5:219:G:HO2'   | 2.41                     | 0.43              |
| 85:l5:678:C:C2     | 85:l5:679:C:C5     | 3.06                     | 0.43              |
| 85:l5:1217:G:H3'   | 85:l5:1218:G:H8    | 1.83                     | 0.43              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 85:L5:1323:A:H2'  | 85:L5:1324:A:O4'   | 2.19                     | 0.43              |
| 85:L5:3807:A:C4   | 85:L5:3808:C:C5    | 3.06                     | 0.43              |
| 85:L5:3814:U:H2'  | 85:L5:3815:G:H8    | 1.82                     | 0.43              |
| 85:L5:4571:A:H2'  | 85:L5:4572:U:C6    | 2.53                     | 0.43              |
| 85:L5:4622:A:H2'  | 85:L5:4623:G:H8    | 1.83                     | 0.43              |
| 80:CB:19:ILE:HD12 | 80:CB:99:LEU:HB3   | 2.01                     | 0.43              |
| 80:CB:71:LYS:HB2  | 80:CB:71:LYS:HE2   | 1.83                     | 0.43              |
| 80:CB:453:MET:SD  | 80:CB:453:MET:O    | 2.76                     | 0.43              |
| 80:CB:571:LYS:HE2 | 80:CB:571:LYS:HB2  | 1.88                     | 0.43              |
| 80:CB:665:ILE:N   | 80:CB:704:VAL:O    | 2.50                     | 0.43              |
| 80:CB:665:ILE:HB  | 80:CB:705:HIS:HA   | 2.00                     | 0.43              |
| 3:SI:117:TYR:HB3  | 3:SI:119:LEU:HD12  | 2.00                     | 0.43              |
| 5:SX:61:GLN:NE2   | 79:S2:1824:A:P     | 2.92                     | 0.43              |
| 6:SG:32:MET:HE2   | 6:SG:32:MET:HB2    | 1.69                     | 0.43              |
| 7:SJ:40:LYS:H     | 86:Se:34:ARG:HH21  | 1.66                     | 0.43              |
| 7:SJ:55:LYS:O     | 7:SJ:59:GLU:HG3    | 2.17                     | 0.43              |
| 8:SY:18:LEU:HD13  | 8:SY:20:ARG:NE     | 2.34                     | 0.43              |
| 86:Se:15:GLN:CD   | 79:S2:612:U:H5'    | 2.43                     | 0.43              |
| 11:SB:103:MET:O   | 11:SB:214:LYS:HA   | 2.19                     | 0.43              |
| 12:SH:186:ASN:OD1 | 12:SH:186:ASN:N    | 2.50                     | 0.43              |
| 16:SN:115:LEU:O   | 16:SN:118:ILE:HG22 | 2.18                     | 0.43              |
| 85:L5:2:G:H2'     | 85:L5:3:C:H6       | 1.82                     | 0.43              |
| 85:L5:247:G:H2'   | 85:L5:248:C:C6     | 2.53                     | 0.43              |
| 85:L5:431:G:N2    | 85:L5:3889:G:OP2   | 2.51                     | 0.43              |
| 85:L5:485:C:H2'   | 85:L5:485:C:O2     | 2.19                     | 0.43              |
| 85:L5:745:G:H2'   | 85:L5:746:A:C8     | 2.53                     | 0.43              |
| 85:L5:1564:A:H8   | 85:L5:1564:A:OP2   | 2.01                     | 0.43              |
| 85:L5:1917:A:H5'  | 51:Lf:78:HIS:HE1   | 1.82                     | 0.43              |
| 85:L5:2007:G:C2   | 85:L5:2013:A:N6    | 2.86                     | 0.43              |
| 85:L5:2033:A:H5'' | 39:LS:91:HIS:NE2   | 2.33                     | 0.43              |
| 85:L5:2326:G:C4   | 85:L5:2327:G:C8    | 3.06                     | 0.43              |
| 85:L5:2385:U:H2'  | 85:L5:2386:U:C6    | 2.53                     | 0.43              |
| 85:L5:2484:A:H3'  | 85:L5:2486:G:H22   | 1.83                     | 0.43              |
| 85:L5:2635:U:H2'  | 85:L5:2636:U:C6    | 2.53                     | 0.43              |
| 85:L5:2706:G:N2   | 85:L5:2709:C:H5''  | 2.33                     | 0.43              |
| 85:L5:3662:A:C8   | 85:L5:3664:G:C4    | 3.06                     | 0.43              |
| 85:L5:3688:U:H2'  | 85:L5:3689:G:C8    | 2.54                     | 0.43              |
| 85:L5:3690:U:H2'  | 85:L5:3691:G:O4'   | 2.18                     | 0.43              |
| 85:L5:3730:U:H2'  | 85:L5:3731:C:C6    | 2.52                     | 0.43              |
| 85:L5:4093:G:O6   | 85:L5:4114:C:H2'   | 2.18                     | 0.43              |
| 85:L5:4102:C:C5'  | 85:L5:4106:G:N3    | 2.82                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 85:L5:4216:G:C6    | 85:L5:4217:G:C5    | 3.07                     | 0.43              |
| 85:L5:4279:A:OP1   | 40:LT:23:GLY:HA2   | 2.18                     | 0.43              |
| 85:L5:4308:C:H2'   | 85:L5:4309:G:O4'   | 2.18                     | 0.43              |
| 85:L5:4344:U:H3    | 85:L5:4368:G:H1    | 1.65                     | 0.43              |
| 85:L5:4679:G:H2'   | 85:L5:4680:G:H8    | 1.83                     | 0.43              |
| 85:L5:4891:G:H3'   | 85:L5:4892:A:C2    | 2.51                     | 0.43              |
| 20:L7:29:C:H1'     | 20:L7:51:G:N1      | 2.34                     | 0.43              |
| 23:LB:370:THR:O    | 23:LB:370:THR:OG1  | 2.36                     | 0.43              |
| 25:LD:94:ASN:OD1   | 25:LD:96:ALA:N     | 2.49                     | 0.43              |
| 27:LF:91:PHE:HB2   | 27:LF:122:PHE:CE2  | 2.53                     | 0.43              |
| 30:LI:85:PHE:HA    | 30:LI:140:THR:HG22 | 2.01                     | 0.43              |
| 31:LJ:19:LYS:HB3   | 31:LJ:75:ARG:NH1   | 2.34                     | 0.43              |
| 36:LP:30:ARG:NH1   | 36:LP:31:GLU:OE2   | 2.42                     | 0.43              |
| 37:LQ:167:VAL:HG23 | 37:LQ:175:GLU:HG3  | 2.00                     | 0.43              |
| 39:LS:27:LEU:CD2   | 40:LT:146:LYS:NZ   | 2.81                     | 0.43              |
| 50:Le:85:LEU:CD2   | 50:Le:111:ILE:HD12 | 2.48                     | 0.43              |
| 52:Lg:9:ARG:N      | 52:Lg:34:TYR:OH    | 2.49                     | 0.43              |
| 54:Li:99:LYS:HE3   | 54:Li:99:LYS:HB2   | 1.66                     | 0.43              |
| 58:Lm:110:CYS:O    | 58:Lm:117:HIS:HA   | 2.19                     | 0.43              |
| 63:Lz:16:GLU:HG2   | 63:Lz:18:LEU:HD13  | 1.99                     | 0.43              |
| 63:Lz:141:ASN:ND2  | 63:Lz:149:ASP:O    | 2.51                     | 0.43              |
| 67:SK:31:LYS:HZ2   | 67:SK:39:ASN:HA    | 1.82                     | 0.43              |
| 68:SP:74:GLU:OE2   | 68:SP:74:GLU:N     | 2.51                     | 0.43              |
| 70:SS:88:LYS:HE2   | 79:S2:1612:G:H5''  | 2.01                     | 0.43              |
| 71:ST:11:GLN:O     | 71:ST:15:VAL:HG22  | 2.18                     | 0.43              |
| 71:ST:40:ALA:O     | 71:ST:42:HIS:N     | 2.52                     | 0.43              |
| 71:ST:101:ARG:NH2  | 79:S2:1566:G:OP2   | 2.48                     | 0.43              |
| 71:ST:112:MET:O    | 71:ST:124:THR:HG22 | 2.16                     | 0.43              |
| 71:ST:134:ILE:O    | 71:ST:138:VAL:HG13 | 2.18                     | 0.43              |
| 72:SU:100:GLN:HG2  | 72:SU:101:ILE:N    | 2.34                     | 0.43              |
| 78:Sf:95:ARG:HH12  | 79:S2:1305:C:H3'   | 1.83                     | 0.43              |
| 79:S2:454:U:H2'    | 79:S2:455:A:C8     | 2.49                     | 0.43              |
| 79:S2:497:C:H2'    | 79:S2:498:C:H6     | 1.83                     | 0.43              |
| 79:S2:554:A:H2     | 79:S2:555:A:H62    | 1.67                     | 0.43              |
| 79:S2:937:C:H2'    | 79:S2:938:A:H8     | 1.84                     | 0.43              |
| 79:S2:1196:A:C2    | 79:S2:1197:G:H1'   | 2.53                     | 0.43              |
| 79:S2:1620:A:C4    | 79:S2:1624:U:C6    | 3.06                     | 0.43              |
| 79:S2:1661:A:C6    | 79:S2:1662:U:C4    | 3.06                     | 0.43              |
| 84:Lt:126:SER:C    | 84:Lt:130:LYS:HG2  | 2.43                     | 0.43              |
| 1:cH:120:VAL:O     | 1:cH:124:ILE:HG13  | 2.19                     | 0.43              |
| 5:sX:75:ILE:HD13   | 5:sX:75:ILE:HA     | 1.84                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 6:sG:205:GLU:HA    | 6:sG:208:GLU:HG3   | 2.01                     | 0.43              |
| 10:sA:60:LEU:HD12  | 10:sA:63:ARG:HE    | 1.84                     | 0.43              |
| 12:sH:99:ARG:NH2   | 79:s2:913:A:OP2    | 2.51                     | 0.43              |
| 17:sO:143:LYS:HE3  | 79:s2:1066:U:OP2   | 2.18                     | 0.43              |
| 18:sW:40:VAL:HG11  | 18:sW:103:VAL:HG21 | 2.00                     | 0.43              |
| 18:sW:86:LEU:O     | 18:sW:90:GLN:HG2   | 2.19                     | 0.43              |
| 21:l8:19:C:H2'     | 21:l8:20:A:H8      | 1.84                     | 0.43              |
| 21:l8:145:C:H2'    | 21:l8:146:U:H6     | 1.83                     | 0.43              |
| 23:lB:5:LYS:HE3    | 23:lB:5:LYS:HB2    | 1.80                     | 0.43              |
| 23:lB:117:ARG:HA   | 23:lB:177:LYS:HD2  | 2.00                     | 0.43              |
| 23:lB:252:ALA:HB1  | 85:l5:4524:G:N3    | 2.34                     | 0.43              |
| 24:lC:207:PRO:HB3  | 24:lC:249:PHE:CD2  | 2.53                     | 0.43              |
| 25:lD:236:MET:O    | 25:lD:236:MET:HG2  | 2.18                     | 0.43              |
| 26:lE:73:TYR:N     | 26:lE:73:TYR:CD2   | 2.85                     | 0.43              |
| 26:lE:124:LYS:HE3  | 85:l5:958:G:C4     | 2.53                     | 0.43              |
| 26:lE:150:LEU:O    | 26:lE:161:ARG:HA   | 2.18                     | 0.43              |
| 26:lE:270:TYR:CE1  | 33:lM:110:PHE:CB   | 2.99                     | 0.43              |
| 27:lF:187:MET:HA   | 27:lF:190:LEU:CD1  | 2.47                     | 0.43              |
| 28:lG:166:LEU:HD23 | 28:lG:166:LEU:H    | 1.84                     | 0.43              |
| 29:lH:140:GLN:CD   | 29:lH:141:LYS:N    | 2.77                     | 0.43              |
| 32:lL:104:ASN:OD1  | 32:lL:104:ASN:N    | 2.50                     | 0.43              |
| 32:lL:162:LYS:HB2  | 32:lL:162:LYS:HE2  | 1.83                     | 0.43              |
| 33:lM:71:LYS:HG3   | 33:lM:72:TYR:N     | 2.34                     | 0.43              |
| 34:lN:44:ARG:HH12  | 34:lN:47:LYS:HD3   | 1.84                     | 0.43              |
| 37:lQ:27:LEU:HA    | 37:lQ:27:LEU:HD23  | 1.73                     | 0.43              |
| 42:lV:83:ARG:NH2   | 42:lV:120:PRO:O    | 2.41                     | 0.43              |
| 42:lV:97:TYR:CE2   | 87:lW:21:TYR:CD2   | 3.06                     | 0.43              |
| 46:la:23:GLY:N     | 85:l5:1852:U:OP1   | 2.51                     | 0.43              |
| 48:lc:78:ASN:OD1   | 48:lc:78:ASN:N     | 2.51                     | 0.43              |
| 49:ld:37:GLY:O     | 49:ld:41:ARG:HG3   | 2.18                     | 0.43              |
| 55:lj:49:TRP:CE3   | 55:lj:50:SER:HB3   | 2.54                     | 0.43              |
| 64:sR:7:LYS:O      | 64:sR:10:LYS:HB3   | 2.19                     | 0.43              |
| 69:sQ:134:GLY:HA2  | 69:sQ:141:TYR:CD2  | 2.53                     | 0.43              |
| 70:sS:9:PHE:CD1    | 70:sS:57:GLY:HA3   | 2.54                     | 0.43              |
| 77:sZ:56:ASP:O     | 77:sZ:60:LYS:HG2   | 2.18                     | 0.43              |
| 77:sZ:68:ILE:O     | 77:sZ:108:ILE:HD12 | 2.18                     | 0.43              |
| 79:s2:210:U:H2'    | 79:s2:211:G:H8     | 1.84                     | 0.43              |
| 79:s2:420:G:N2     | 79:s2:662:G:H1     | 2.17                     | 0.43              |
| 79:s2:675:U:H2'    | 79:s2:676:C:H6     | 1.84                     | 0.43              |
| 79:s2:1039:C:H2'   | 79:s2:1040:G:H8    | 1.82                     | 0.43              |
| 79:s2:1199:A:H2'   | 79:s2:1200:A:H8    | 1.81                     | 0.43              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 79:s2:1349:G:H2'  | 79:s2:1350:U:H6    | 1.82                     | 0.43              |
| 79:s2:1495:G:H2'  | 79:s2:1496:U:C6    | 2.53                     | 0.43              |
| 80:cB:56:PHE:HB3  | 80:cB:455:GLY:HA3  | 2.00                     | 0.43              |
| 80:cB:59:THR:OG1  | 80:cB:73:THR:HG21  | 2.18                     | 0.43              |
| 80:cB:439:LYS:HA  | 80:cB:442:LEU:HD13 | 2.01                     | 0.43              |
| 82:pE:35:U:H2'    | 82:pE:36:U:C6      | 2.52                     | 0.43              |
| 83:ls:28:PHE:HB2  | 83:ls:192:VAL:HG23 | 2.01                     | 0.43              |
| 83:ls:98:ILE:O    | 83:ls:101:MET:SD   | 2.77                     | 0.43              |
| 84:lt:22:VAL:HA   | 84:lt:48:LYS:CG    | 2.49                     | 0.43              |
| 85:l5:59:A:C8     | 85:l5:338:A:C6     | 3.06                     | 0.43              |
| 85:l5:665:C:H1'   | 85:l5:668:C:H41    | 1.84                     | 0.43              |
| 85:l5:716:C:H2'   | 85:l5:717:U:O4'    | 2.18                     | 0.43              |
| 85:l5:750:U:C2    | 85:l5:751:G:C8     | 3.06                     | 0.43              |
| 85:l5:752:G:C5    | 85:l5:753:C:C2     | 3.06                     | 0.43              |
| 85:l5:1373:A:H2'  | 85:l5:1374:G:C8    | 2.53                     | 0.43              |
| 85:l5:1609:U:H2'  | 85:l5:1610:C:O4'   | 2.19                     | 0.43              |
| 85:l5:1941:A:C6   | 85:l5:2040:A:C4    | 3.06                     | 0.43              |
| 85:l5:1951:G:O6   | 85:l5:2033:A:N6    | 2.52                     | 0.43              |
| 85:l5:3752:C:O2'  | 85:l5:3776:G:H1'   | 2.18                     | 0.43              |
| 85:l5:3933:G:H2'  | 85:l5:3934:G:H8    | 1.83                     | 0.43              |
| 85:l5:4039:G:N3   | 85:l5:4050:A:H1'   | 2.34                     | 0.43              |
| 80:CB:255:ASP:HA  | 80:CB:258:LYS:HG2  | 2.00                     | 0.43              |
| 80:CB:406:ASP:OD1 | 80:CB:407:LYS:N    | 2.42                     | 0.43              |
| 80:CB:548:GLY:HA3 | 80:CB:554:LEU:HD21 | 2.01                     | 0.43              |
| 2:SE:118:GLU:OE1  | 2:SE:236:ILE:HD11  | 2.18                     | 0.43              |
| 3:SI:80:ASP:O     | 3:SI:103:LEU:N     | 2.50                     | 0.43              |
| 10:SA:27:GLY:HA3  | 10:SA:28:THR:HA    | 1.86                     | 0.43              |
| 10:SA:126:ASP:HB2 | 10:SA:165:ASN:ND2  | 2.27                     | 0.43              |
| 11:SB:110:MET:CE  | 11:SB:113:MET:HE1  | 2.48                     | 0.43              |
| 14:Sa:13:LYS:CE   | 79:S2:1133:A:H4'   | 2.38                     | 0.43              |
| 14:Sa:90:GLU:H    | 14:Sa:90:GLU:CD    | 2.24                     | 0.43              |
| 15:SC:65:LYS:O    | 15:SC:69:LEU:HG    | 2.18                     | 0.43              |
| 18:SW:52:ILE:HD13 | 18:SW:61:ILE:HG12  | 2.01                     | 0.43              |
| 85:L5:261:G:N1    | 85:L5:262:G:C6     | 2.87                     | 0.43              |
| 85:L5:294:G:H2'   | 46:La:61:TYR:OH    | 2.18                     | 0.43              |
| 85:L5:679:C:C2    | 85:L5:680:G:C8     | 3.07                     | 0.43              |
| 85:L5:956:A:N7    | 85:L5:1283:G:O2'   | 2.37                     | 0.43              |
| 85:L5:1176:C:C2   | 85:L5:1185:G:N2    | 2.86                     | 0.43              |
| 85:L5:1186:U:H4'  | 25:LD:278:ASP:OD2  | 2.18                     | 0.43              |
| 85:L5:1194:G:H2'  | 85:L5:1195:G:C8    | 2.53                     | 0.43              |
| 85:L5:1617:G:H1'  | 85:L5:2513:A:H61   | 1.84                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 85:L5:1633:G:O6    | 22:LA:207:VAL:HG11 | 2.19                     | 0.43              |
| 85:L5:1650:A:H5'   | 24:LC:92:PHE:CE2   | 2.54                     | 0.43              |
| 85:L5:1721:G:H2'   | 85:L5:1722:C:H6    | 1.82                     | 0.43              |
| 85:L5:1961:G:O2'   | 85:L5:2025:A:N6    | 2.51                     | 0.43              |
| 85:L5:2072:C:H2'   | 85:L5:2073:C:H6    | 1.83                     | 0.43              |
| 85:L5:2436:U:C4    | 43:LX:130:PRO:HG3  | 2.54                     | 0.43              |
| 85:L5:2468:U:C2    | 85:L5:2506:G:C2    | 3.06                     | 0.43              |
| 85:L5:2485:U:H1'   | 85:L5:2486:G:N1    | 2.33                     | 0.43              |
| 85:L5:2635:U:H2'   | 85:L5:2636:U:H6    | 1.83                     | 0.43              |
| 85:L5:2811:G:H22   | 85:L5:2813:A:H3'   | 1.83                     | 0.43              |
| 85:L5:2823:G:H2'   | 85:L5:2824:C:C6    | 2.53                     | 0.43              |
| 85:L5:3711:A:O2'   | 85:L5:3712:A:H8    | 2.01                     | 0.43              |
| 85:L5:3819:G:H2'   | 85:L5:3820:G:H8    | 1.84                     | 0.43              |
| 85:L5:4101:C:C5    | 85:L5:4106:G:H4'   | 2.51                     | 0.43              |
| 85:L5:4131:G:C6    | 85:L5:4154:G:C6    | 3.07                     | 0.43              |
| 85:L5:4177:C:C2    | 85:L5:4178:A:C8    | 3.06                     | 0.43              |
| 85:L5:4318:C:H2'   | 85:L5:4319:C:O4'   | 2.18                     | 0.43              |
| 85:L5:4650:G:H2'   | 85:L5:4651:A:O4'   | 2.18                     | 0.43              |
| 85:L5:4675:U:O3'   | 23:LB:281:ASN:HB2  | 2.19                     | 0.43              |
| 85:L5:4886:C:H2'   | 85:L5:4887:C:H6    | 1.84                     | 0.43              |
| 20:L7:45:U:H2'     | 20:L7:46:C:C6      | 2.53                     | 0.43              |
| 21:L8:24:G:H2'     | 21:L8:25:G:O4'     | 2.18                     | 0.43              |
| 24:LC:318:PRO:C    | 24:LC:320:LYS:H    | 2.27                     | 0.43              |
| 26:LE:164:PHE:CE1  | 26:LE:173:LEU:HB3  | 2.53                     | 0.43              |
| 29:LH:68:ALA:O     | 29:LH:72:THR:HG23  | 2.18                     | 0.43              |
| 29:LH:181:VAL:HG13 | 58:Lm:89:TYR:OH    | 2.19                     | 0.43              |
| 33:LM:9:VAL:HG12   | 33:LM:28:VAL:O     | 2.19                     | 0.43              |
| 36:LP:60:PHE:O     | 36:LP:78:TRP:NE1   | 2.52                     | 0.43              |
| 39:LS:27:LEU:CD2   | 40:LT:146:LYS:HZ2  | 2.32                     | 0.43              |
| 39:LS:82:LEU:HD21  | 39:LS:95:ARG:HG3   | 1.99                     | 0.43              |
| 42:LV:26:ILE:HG12  | 42:LV:37:LEU:HB2   | 2.00                     | 0.43              |
| 60:Lo:22:LYS:HG2   | 60:Lo:71:GLU:HB3   | 2.00                     | 0.43              |
| 65:SD:214:LYS:HG3  | 65:SD:215:ASP:H    | 1.84                     | 0.43              |
| 69:SQ:11:GLN:CD    | 79:S2:1442:U:H1'   | 2.44                     | 0.43              |
| 71:ST:120:GLY:N    | 79:S2:1562:C:H4'   | 2.30                     | 0.43              |
| 75:Sg:178:ASN:HD21 | 75:Sg:181:ASN:H    | 1.67                     | 0.43              |
| 76:SM:33:ARG:H     | 76:SM:33:ARG:HG2   | 1.61                     | 0.43              |
| 76:SM:36:ARG:HA    | 76:SM:36:ARG:HD3   | 1.88                     | 0.43              |
| 78:Sf:137:ASP:OD1  | 78:Sf:138:ARG:N    | 2.52                     | 0.43              |
| 79:S2:113:G:O6     | 79:S2:290:U:H1'    | 2.18                     | 0.43              |
| 79:S2:193:C:H2'    | 79:S2:194:C:H6     | 1.83                     | 0.43              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 79:S2:751:G:H1'   | 79:S2:793:G:N2     | 2.33                     | 0.43              |
| 79:S2:920:A:O2'   | 79:S2:922:A:O5'    | 2.36                     | 0.43              |
| 79:S2:1204:A:H2'  | 79:S2:1205:C:C6    | 2.53                     | 0.43              |
| 79:S2:1260:A:C5   | 79:S2:1619:A:C6    | 3.07                     | 0.43              |
| 79:S2:1290:G:N2   | 79:S2:1310:U:H1'   | 2.33                     | 0.43              |
| 79:S2:1310:U:H2'  | 79:S2:1311:C:H6    | 1.83                     | 0.43              |
| 79:S2:1397:U:OP1  | 79:S2:1398:G:H8    | 2.01                     | 0.43              |
| 81:AP:14:A:C6     | 81:AP:22:U:C4      | 3.06                     | 0.43              |
| 82:PE:42:G:C2     | 82:PE:43:A:C5      | 3.06                     | 0.43              |
| 1:cH:50:LYS:HG2   | 9:se:59:SER:HA     | 1.99                     | 0.43              |
| 2:sE:248:ILE:O    | 2:sE:251:GLU:HG3   | 2.19                     | 0.43              |
| 4:sL:150:GLY:HA2  | 4:sL:153:LYS:HZ3   | 1.82                     | 0.43              |
| 6:sG:163:ASN:OD1  | 6:sG:169:PRO:HB3   | 2.18                     | 0.43              |
| 7:sJ:101:LYS:HB3  | 7:sJ:103:GLU:OE2   | 2.18                     | 0.43              |
| 10:sA:71:PRO:C    | 10:sA:73:ASP:H     | 2.27                     | 0.43              |
| 12:sH:91:HIS:CD2  | 12:sH:172:THR:HG21 | 2.54                     | 0.43              |
| 12:sH:122:LEU:HG  | 79:s2:688:U:OP1    | 2.19                     | 0.43              |
| 13:sV:7:GLU:CD    | 13:sV:7:GLU:C      | 2.87                     | 0.43              |
| 15:sC:68:ARG:O    | 15:sC:72:ASP:OD1   | 2.37                     | 0.43              |
| 16:sN:85:PRO:HG2  | 16:sN:129:TYR:CE2  | 2.53                     | 0.43              |
| 18:sW:93:LEU:HD13 | 18:sW:128:PHE:CD2  | 2.54                     | 0.43              |
| 20:l7:18:C:H2'    | 20:l7:19:C:C6      | 2.53                     | 0.43              |
| 21:l8:4:C:H2'     | 21:l8:5:U:H6       | 1.84                     | 0.43              |
| 21:l8:110:U:N3    | 85:l5:2510:G:OP1   | 2.52                     | 0.43              |
| 22:lA:34:PHE:O    | 22:lA:37:ARG:N     | 2.42                     | 0.43              |
| 24:lC:71:ARG:O    | 24:lC:73:VAL:N     | 2.47                     | 0.43              |
| 24:lC:308:LYS:HD2 | 85:l5:1702:C:H4'   | 2.00                     | 0.43              |
| 30:lI:15:LYS:O    | 30:lI:16:PRO:C     | 2.61                     | 0.43              |
| 30:lI:144:ASN:N   | 30:lI:144:ASN:HD22 | 2.16                     | 0.43              |
| 35:lO:178:ARG:O   | 35:lO:182:GLU:HG3  | 2.18                     | 0.43              |
| 39:lS:85:ASP:OD1  | 39:lS:90:THR:HB    | 2.18                     | 0.43              |
| 42:lV:37:LEU:HD23 | 42:lV:37:LEU:HA    | 1.83                     | 0.43              |
| 42:lV:109:LYS:HD2 | 42:lV:109:LYS:HA   | 1.71                     | 0.43              |
| 44:lY:69:LYS:N    | 44:lY:83:GLU:OE2   | 2.50                     | 0.43              |
| 44:lY:101:PRO:O   | 44:lY:104:VAL:HG22 | 2.18                     | 0.43              |
| 47:lb:57:MET:CE   | 85:l5:1811:G:H21   | 2.31                     | 0.43              |
| 48:lc:17:ARG:O    | 48:lc:21:VAL:HG12  | 2.19                     | 0.43              |
| 54:li:51:ALA:O    | 54:li:55:ARG:HG2   | 2.18                     | 0.43              |
| 57:ll:48:LYS:NZ   | 85:l5:2791:C:OP1   | 2.52                     | 0.43              |
| 62:lr:118:LEU:O   | 62:lr:121:GLN:HB3  | 2.18                     | 0.43              |
| 64:sR:67:ARG:HA   | 64:sR:68:GLY:HA3   | 1.56                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 66:sF:165:ASN:OD1 | 66:sF:167:LYS:HG3 | 2.19                     | 0.43              |
| 73:sc:13:ARG:NH2  | 73:sc:53:GLY:O    | 2.51                     | 0.43              |
| 73:sc:34:PHE:O    | 73:sc:36:ASP:N    | 2.52                     | 0.43              |
| 75:sg:172:LYS:HE3 | 75:sg:193:GLY:H   | 1.83                     | 0.43              |
| 79:s2:57:U:H5''   | 79:s2:504:G:H1'   | 2.01                     | 0.43              |
| 79:s2:344:U:H2'   | 79:s2:345:U:H6    | 1.83                     | 0.43              |
| 79:s2:480:G:H2'   | 79:s2:481:C:C6    | 2.53                     | 0.43              |
| 79:s2:849:A:H2'   | 79:s2:850:C:C6    | 2.54                     | 0.43              |
| 79:s2:962:A:H2'   | 79:s2:963:A:O4'   | 2.19                     | 0.43              |
| 79:s2:1006:C:H2'  | 79:s2:1007:C:C6   | 2.53                     | 0.43              |
| 79:s2:1205:C:H2'  | 79:s2:1206:G:C8   | 2.52                     | 0.43              |
| 79:s2:1279:C:H2'  | 79:s2:1280:G:C8   | 2.52                     | 0.43              |
| 79:s2:1284:A:H5'' | 79:s2:1286:G:O4'  | 2.19                     | 0.43              |
| 79:s2:1461:G:H3'  | 79:s2:1463:U:N3   | 2.33                     | 0.43              |
| 79:s2:1501:C:H2'  | 79:s2:1502:C:C6   | 2.54                     | 0.43              |
| 79:s2:1689:C:H2'  | 79:s2:1690:U:C6   | 2.53                     | 0.43              |
| 79:s2:1716:C:C2   | 79:s2:1717:C:C5   | 3.07                     | 0.43              |
| 79:s2:1754:G:C5   | 79:s2:1779:G:N2   | 2.86                     | 0.43              |
| 80:cB:592:LEU:HA  | 80:cB:602:LEU:O   | 2.19                     | 0.43              |
| 81:aP:49:C:C2     | 81:aP:50:U:C5     | 3.05                     | 0.43              |
| 83:ls:108:PRO:O   | 83:ls:109:ALA:C   | 2.61                     | 0.43              |
| 85:l5:253:G:H2'   | 85:l5:254:G:N7    | 2.34                     | 0.43              |
| 85:l5:440:U:H2'   | 85:l5:441:G:H8    | 1.84                     | 0.43              |
| 85:l5:493:G:C6    | 85:l5:494:U:C4    | 3.07                     | 0.43              |
| 85:l5:511:C:H2'   | 85:l5:512:U:O4'   | 2.18                     | 0.43              |
| 85:l5:1341:U:H2'  | 85:l5:1342:A:H8   | 1.84                     | 0.43              |
| 85:l5:1980:U:H1'  | 85:l5:1982:G:OP2  | 2.18                     | 0.43              |
| 85:l5:2000:G:H5'' | 85:l5:2001:G:H5'  | 2.00                     | 0.43              |
| 85:l5:2407:G:N2   | 85:l5:2407:G:OP2  | 2.51                     | 0.43              |
| 85:l5:2496:G:H2'  | 85:l5:2497:C:H6   | 1.84                     | 0.43              |
| 85:l5:2615:C:H2'  | 85:l5:2616:C:C6   | 2.53                     | 0.43              |
| 85:l5:2654:C:C2   | 85:l5:2655:C:C5   | 3.07                     | 0.43              |
| 85:l5:2846:G:H2'  | 85:l5:2847:G:C8   | 2.54                     | 0.43              |
| 85:l5:3792:G:C6   | 85:l5:3793:U:C4   | 3.07                     | 0.43              |
| 85:l5:3806:G:C4   | 85:l5:3807:A:C8   | 3.07                     | 0.43              |
| 85:l5:3816:A:O2'  | 85:l5:3819:G:N3   | 2.37                     | 0.43              |
| 85:l5:3819:G:H2'  | 85:l5:3820:G:H8   | 1.84                     | 0.43              |
| 85:l5:4108:G:H2'  | 85:l5:4109:G:H8   | 1.81                     | 0.43              |
| 85:l5:4209:G:C6   | 85:l5:4210:U:C4   | 3.07                     | 0.43              |
| 85:l5:4453:C:H2'  | 85:l5:4454:G:O4'  | 2.19                     | 0.43              |
| 85:l5:4683:U:H2'  | 85:l5:4684:A:C8   | 2.54                     | 0.43              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 85:L5:4685:U:H2'  | 85:L5:4686:G:C8    | 2.54                     | 0.43              |
| 85:L5:4768:G:H2'  | 85:L5:4769:G:H8    | 1.84                     | 0.43              |
| 80:CB:638:LYS:HE2 | 80:CB:639:TYR:CZ   | 2.54                     | 0.43              |
| 80:CB:645:GLU:HA  | 80:CB:648:LYS:HE2  | 2.01                     | 0.43              |
| 4:SL:23:VAL:HG13  | 4:SL:25:LEU:HB2    | 1.99                     | 0.43              |
| 8:SY:20:ARG:HD2   | 8:SY:74:MET:HE2    | 2.01                     | 0.43              |
| 8:SY:48:TYR:OH    | 79:S2:838:G:N2     | 2.52                     | 0.43              |
| 12:SH:95:ILE:HD11 | 12:SH:133:LEU:HB2  | 2.01                     | 0.43              |
| 13:SV:3:ASN:OD1   | 15:SC:173:LYS:HB2  | 2.19                     | 0.43              |
| 13:SV:34:MET:HB3  | 13:SV:53:TYR:HB2   | 2.01                     | 0.43              |
| 14:Sa:13:LYS:CE   | 79:S2:1133:A:C4'   | 2.94                     | 0.43              |
| 15:SC:62:PRO:HD3  | 15:SC:71:LYS:HD3   | 1.99                     | 0.43              |
| 15:SC:194:ARG:CZ  | 79:S2:1154:U:H1'   | 2.48                     | 0.43              |
| 16:SN:5:HIS:HB3   | 16:SN:117:LEU:HD13 | 2.00                     | 0.43              |
| 17:SO:121:ARG:NH1 | 73:Sc:62:GLU:HG2   | 2.34                     | 0.43              |
| 85:L5:371:A:H2    | 85:L5:1532:G:H1'   | 1.82                     | 0.43              |
| 85:L5:1281:G:N1   | 26:LE:128:HIS:HB2  | 2.33                     | 0.43              |
| 85:L5:1305:C:H2'  | 85:L5:1306:C:C6    | 2.53                     | 0.43              |
| 85:L5:1701:A:N6   | 85:L5:2096:G:H22   | 2.16                     | 0.43              |
| 85:L5:2021:G:H2'  | 85:L5:2022:C:C6    | 2.54                     | 0.43              |
| 85:L5:2033:A:H5'' | 39:LS:91:HIS:CE1   | 2.54                     | 0.43              |
| 85:L5:2061:U:H2'  | 85:L5:2062:C:O4'   | 2.18                     | 0.43              |
| 85:L5:2273:G:H2'  | 85:L5:2274:C:H6    | 1.84                     | 0.43              |
| 85:L5:2367:A:C8   | 85:L5:2798:A:C5    | 3.07                     | 0.43              |
| 85:L5:2634:C:C2   | 85:L5:2635:U:C5    | 3.07                     | 0.43              |
| 85:L5:2697:A:C4   | 85:L5:2698:G:C8    | 3.06                     | 0.43              |
| 85:L5:2844:A:O2'  | 85:L5:4631:G:H4'   | 2.18                     | 0.43              |
| 85:L5:3928:A:H2'  | 85:L5:3929:G:O4'   | 2.18                     | 0.43              |
| 85:L5:3967:G:N3   | 85:L5:3967:G:H2'   | 2.34                     | 0.43              |
| 85:L5:3969:G:N7   | 85:L5:4051:C:N4    | 2.67                     | 0.43              |
| 85:L5:4051:C:O2   | 85:L5:4052:C:N4    | 2.52                     | 0.43              |
| 85:L5:4108:G:O2'  | 85:L5:4109:G:P     | 2.77                     | 0.43              |
| 85:L5:4179:G:C2   | 85:L5:4180:G:C8    | 3.06                     | 0.43              |
| 85:L5:4493:U:C2   | 85:L5:4512:U:C4    | 3.07                     | 0.43              |
| 85:L5:4960:G:H2'  | 85:L5:4961:G:C8    | 2.54                     | 0.43              |
| 21:L8:75:G:OP1    | 57:L1:31:THR:HG23  | 2.18                     | 0.43              |
| 21:L8:82:A:N7     | 21:L8:84:A:H3'     | 2.34                     | 0.43              |
| 24:LC:46:LYS:HE3  | 24:LC:113:ARG:NH1  | 2.34                     | 0.43              |
| 31:LJ:19:LYS:HD3  | 31:LJ:75:ARG:HH22  | 1.83                     | 0.43              |
| 31:LJ:40:LEU:HA   | 31:LJ:43:LEU:CD2   | 2.49                     | 0.43              |
| 33:LM:118:MET:HB3 | 35:LO:192:TYR:CE2  | 2.54                     | 0.43              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 35:LO:46:ASN:HD21  | 35:LO:49:ARG:HB3  | 1.82                     | 0.43              |
| 43:LX:119:ILE:HD12 | 43:LX:144:TYR:CD1 | 2.54                     | 0.43              |
| 43:LX:149:VAL:HA   | 43:LX:152:LYS:HG2 | 1.99                     | 0.43              |
| 45:LZ:91:LEU:HD23  | 45:LZ:91:LEU:HA   | 1.86                     | 0.43              |
| 45:LZ:124:THR:HG1  | 45:LZ:126:LYS:NZ  | 2.14                     | 0.43              |
| 46:La:85:GLN:HA    | 46:La:88:VAL:HG22 | 2.00                     | 0.43              |
| 52:Lg:19:LYS:HD2   | 52:Lg:19:LYS:HA   | 1.64                     | 0.43              |
| 53:Lh:33:VAL:O     | 53:Lh:37:THR:HG23 | 2.18                     | 0.43              |
| 63:Lz:156:LYS:HD2  | 63:Lz:156:LYS:H   | 1.84                     | 0.43              |
| 66:SF:74:ASN:OD1   | 79:S2:1675:A:O2'  | 2.16                     | 0.43              |
| 66:SF:76:MET:HB2   | 66:SF:89:THR:HG23 | 2.01                     | 0.43              |
| 69:SQ:100:VAL:HG22 | 69:SQ:101:ASP:OD1 | 2.19                     | 0.43              |
| 73:Sc:31:ARG:HE    | 73:Sc:43:ILE:HB   | 1.83                     | 0.43              |
| 79:S2:536:A:H3'    | 79:S2:537:C:C5'   | 2.49                     | 0.43              |
| 79:S2:1073:U:H2'   | 79:S2:1074:C:C6   | 2.54                     | 0.43              |
| 83:Ls:136:SER:HA   | 83:Ls:139:GLN:HG3 | 2.01                     | 0.43              |
| 1:cH:43:LYS:HG3    | 1:cH:45:ALA:HB3   | 2.01                     | 0.43              |
| 1:cH:45:ALA:HB1    | 9:se:55:PRO:CA    | 2.49                     | 0.43              |
| 1:cH:109:TYR:CD2   | 1:cH:114:ALA:HB1  | 2.53                     | 0.43              |
| 2:sE:87:MET:CE     | 2:sE:122:LYS:HE2  | 2.44                     | 0.43              |
| 3:sI:41:ARG:HA     | 3:sI:59:ARG:O     | 2.18                     | 0.43              |
| 3:sI:87:ASN:ND2    | 3:sI:89:GLU:OE2   | 2.51                     | 0.43              |
| 5:sX:93:PHE:HE2    | 5:sX:134:TYR:HA   | 1.82                     | 0.43              |
| 6:sG:188:LYS:HD3   | 6:sG:188:LYS:HA   | 1.64                     | 0.43              |
| 12:sH:182:GLY:HA3  | 79:s2:690:G:C8    | 2.54                     | 0.43              |
| 16:sN:33:VAL:O     | 16:sN:37:ILE:HG13 | 2.18                     | 0.43              |
| 17:sO:42:VAL:HG22  | 17:sO:81:VAL:HG11 | 2.01                     | 0.43              |
| 17:sO:80:ASP:OD2   | 17:sO:80:ASP:C    | 2.60                     | 0.43              |
| 19:sb:81:ARG:HD2   | 19:sb:81:ARG:HA   | 1.59                     | 0.43              |
| 20:l7:46:C:H2'     | 20:l7:47:G:H8     | 1.83                     | 0.43              |
| 21:l8:65:A:OP1     | 53:lh:56:ARG:NE   | 2.40                     | 0.43              |
| 21:l8:67:U:C2      | 21:l8:68:G:C8     | 3.06                     | 0.43              |
| 22:lA:34:PHE:CE1   | 85:l5:4087:G:H3'  | 2.53                     | 0.43              |
| 23:lB:36:ASP:N     | 23:lB:36:ASP:OD1  | 2.52                     | 0.43              |
| 26:lE:99:ASP:O     | 26:lE:100:LYS:HG2 | 2.18                     | 0.43              |
| 28:lG:87:LEU:HG    | 28:lG:91:THR:OG1  | 2.19                     | 0.43              |
| 29:lH:170:LYS:HD3  | 29:lH:170:LYS:HA  | 1.80                     | 0.43              |
| 31:lJ:89:VAL:HG12  | 31:lJ:90:ARG:HD2  | 2.00                     | 0.43              |
| 32:lL:154:VAL:O    | 32:lL:155:MET:C   | 2.61                     | 0.43              |
| 35:lO:31:ARG:O     | 35:lO:33:VAL:HG23 | 2.18                     | 0.43              |
| 36:lP:109:VAL:O    | 36:lP:112:LEU:HB2 | 2.19                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 37:lQ:151:HIS:ND1  | 37:lQ:164:LYS:O    | 2.49                     | 0.43              |
| 38:lR:63:CYS:O     | 38:lR:67:THR:HG23  | 2.19                     | 0.43              |
| 38:lR:105:LEU:HD23 | 38:lR:138:LEU:HD23 | 2.00                     | 0.43              |
| 52:lg:11:LEU:HD22  | 52:lg:11:LEU:HA    | 1.71                     | 0.43              |
| 52:lg:54:ARG:NE    | 85:l5:2683:C:H1'   | 2.19                     | 0.43              |
| 55:lj:67:LEU:CG    | 55:lj:71:TYR:HE2   | 2.25                     | 0.43              |
| 56:lk:34:PHE:O     | 56:lk:45:LEU:N     | 2.47                     | 0.43              |
| 62:lr:21:ASN:OD1   | 62:lr:21:ASN:N     | 2.49                     | 0.43              |
| 63:lz:107:TYR:CZ   | 63:lz:110:PHE:CD1  | 3.06                     | 0.43              |
| 64:sR:11:LYS:HB2   | 79:s2:1373:C:C5    | 2.53                     | 0.43              |
| 64:sR:11:LYS:HE2   | 79:s2:1371:U:O2'   | 2.19                     | 0.43              |
| 64:sR:17:ILE:HD11  | 64:sR:54:VAL:HG13  | 2.01                     | 0.43              |
| 66:sF:34:SER:HA    | 73:sc:55:VAL:CG1   | 2.45                     | 0.43              |
| 66:sF:72:LEU:HD22  | 66:sF:151:ILE:CD1  | 2.49                     | 0.43              |
| 68:sP:37:TYR:CD2   | 68:sP:41:GLN:HB2   | 2.41                     | 0.43              |
| 68:sP:53:GLN:OE1   | 68:sP:53:GLN:N     | 2.34                     | 0.43              |
| 68:sP:107:ILE:HD13 | 68:sP:107:ILE:HA   | 1.84                     | 0.43              |
| 69:sQ:31:LEU:HB3   | 69:sQ:67:ASP:HA    | 2.01                     | 0.43              |
| 70:sS:67:VAL:O     | 70:sS:68:ILE:C     | 2.61                     | 0.43              |
| 72:sU:54:VAL:HG12  | 72:sU:88:LEU:HD13  | 2.01                     | 0.43              |
| 74:sd:22:ARG:HG2   | 74:sd:37:ASN:O     | 2.18                     | 0.43              |
| 75:sg:87:LEU:O     | 75:sg:101:PHE:N    | 2.34                     | 0.43              |
| 75:sg:152:SER:H    | 75:sg:169:GLY:HA2  | 1.83                     | 0.43              |
| 76:sM:20:GLU:O     | 76:sM:24:THR:HG23  | 2.19                     | 0.43              |
| 79:s2:26:U:C2      | 79:s2:27:A:C8      | 3.07                     | 0.43              |
| 79:s2:103:A:O4'    | 79:s2:356:C:N4     | 2.52                     | 0.43              |
| 79:s2:387:C:H2'    | 79:s2:388:U:H6     | 1.83                     | 0.43              |
| 79:s2:502:C:H3'    | 79:s2:503:C:C6     | 2.52                     | 0.43              |
| 79:s2:801:U:C2     | 79:s2:802:A:C8     | 3.07                     | 0.43              |
| 79:s2:1016:U:O2    | 79:s2:1016:U:H2'   | 2.18                     | 0.43              |
| 79:s2:1209:A:H2'   | 79:s2:1210:G:H8    | 1.84                     | 0.43              |
| 79:s2:1416:C:H6    | 79:s2:1416:C:O5'   | 2.02                     | 0.43              |
| 80:cB:580:ARG:HB2  | 80:cB:741:MET:HE3  | 1.99                     | 0.43              |
| 80:cB:845:LYS:HA   | 80:cB:845:LYS:HD2  | 1.85                     | 0.43              |
| 81:aP:44:A:H2'     | 81:aP:45:G:O4'     | 2.19                     | 0.43              |
| 85:l5:23:C:H2'     | 85:l5:24:G:O4'     | 2.19                     | 0.43              |
| 85:l5:71:C:N3      | 85:l5:73:A:C4      | 2.87                     | 0.43              |
| 85:l5:276:C:O3'    | 85:l5:277:G:H8     | 2.02                     | 0.43              |
| 85:l5:396:A:H2'    | 85:l5:397:G:C8     | 2.54                     | 0.43              |
| 85:l5:1605:G:H2'   | 85:l5:1606:U:O4'   | 2.19                     | 0.43              |
| 85:l5:1646:A:H2'   | 85:l5:1647:U:H6    | 1.83                     | 0.43              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 85:L5:1664:U:H2'   | 85:L5:1665:C:C6   | 2.54                     | 0.43              |
| 85:L5:2033:A:N3    | 85:L5:2034:G:C8   | 2.87                     | 0.43              |
| 85:L5:3700:C:C2    | 85:L5:3751:G:C2   | 3.06                     | 0.43              |
| 85:L5:3721:U:H2'   | 85:L5:3722:G:H8   | 1.83                     | 0.43              |
| 85:L5:3829:G:C2    | 85:L5:3830:A:N7   | 2.86                     | 0.43              |
| 85:L5:3890:A:N7    | 85:L5:4571:A:H1'  | 2.33                     | 0.43              |
| 85:L5:4651:A:H2'   | 85:L5:4652:G:O4'  | 2.19                     | 0.43              |
| 80:CB:135:VAL:HG23 | 80:CB:181:ILE:CD1 | 2.48                     | 0.43              |
| 80:CB:413:PHE:HE1  | 80:CB:469:ILE:HB  | 1.83                     | 0.43              |
| 80:CB:431:GLY:O    | 80:CB:493:ASN:ND2 | 2.50                     | 0.43              |
| 80:CB:480:VAL:O    | 80:CB:482:THR:N   | 2.49                     | 0.43              |
| 2:SE:2:ALA:HB1     | 79:S2:93:U:OP1    | 2.19                     | 0.43              |
| 2:SE:201:HIS:HB3   | 2:SE:204:SER:HB3  | 2.01                     | 0.43              |
| 3:SI:70:GLU:HG3    | 3:SI:112:TRP:CH2  | 2.53                     | 0.43              |
| 4:SL:128:VAL:HG22  | 4:SL:140:PHE:HB3  | 2.00                     | 0.43              |
| 6:SG:39:ASP:HA     | 6:SG:45:TRP:O     | 2.19                     | 0.43              |
| 86:Se:15:GLN:NE2   | 79:S2:611:G:O3'   | 2.50                     | 0.43              |
| 11:SB:113:MET:O    | 11:SB:115:LYS:HD3 | 2.18                     | 0.43              |
| 17:SO:87:GLU:H     | 17:SO:87:GLU:HG2  | 1.69                     | 0.43              |
| 18:SW:4:MET:HG3    | 18:SW:5:ASN:OD1   | 2.19                     | 0.43              |
| 18:SW:90:GLN:HA    | 18:SW:94:LEU:HD23 | 2.00                     | 0.43              |
| 85:L5:370:U:O3'    | 55:Lj:25:LYS:NZ   | 2.51                     | 0.43              |
| 85:L5:416:U:H4'    | 85:L5:2330:G:H4'  | 2.00                     | 0.43              |
| 85:L5:1468:C:H2'   | 85:L5:1469:C:H6   | 1.83                     | 0.43              |
| 85:L5:1493:G:H2'   | 85:L5:1494:U:O4'  | 2.18                     | 0.43              |
| 85:L5:1613:A:H5''  | 22:LA:183:GLY:HA2 | 2.00                     | 0.43              |
| 85:L5:1624:G:C5    | 85:L5:1643:A:C8   | 3.07                     | 0.43              |
| 85:L5:1737:A:C4    | 85:L5:1738:A:C8   | 3.07                     | 0.43              |
| 85:L5:1912:G:C6    | 85:L5:2057:A:C2   | 3.07                     | 0.43              |
| 85:L5:1951:G:O6    | 85:L5:2033:A:N6   | 2.51                     | 0.43              |
| 85:L5:2267:U:C6    | 85:L5:2270:G:H4'  | 2.54                     | 0.43              |
| 85:L5:2414:G:H2'   | 85:L5:2415:U:C6   | 2.53                     | 0.43              |
| 85:L5:2710:C:C2    | 85:L5:2712:G:C8   | 3.06                     | 0.43              |
| 85:L5:2750:G:C4    | 85:L5:2751:G:C8   | 3.07                     | 0.43              |
| 85:L5:2904:U:H5''  | 85:L5:2905:C:OP1  | 2.19                     | 0.43              |
| 85:L5:3600:G:H2'   | 85:L5:3601:C:H6   | 1.84                     | 0.43              |
| 85:L5:3730:U:H2'   | 85:L5:3731:C:H6   | 1.82                     | 0.43              |
| 85:L5:3835:C:C2    | 85:L5:3836:A:C8   | 3.07                     | 0.43              |
| 85:L5:3947:A:O2'   | 85:L5:3948:C:O5'  | 2.30                     | 0.43              |
| 85:L5:4041:C:O5'   | 85:L5:4042:G:H5'' | 2.19                     | 0.43              |
| 85:L5:4102:C:N1    | 85:L5:4105:A:N3   | 2.64                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 85:L5:4114:C:OP2   | 85:L5:4115:G:C6    | 2.72                     | 0.43              |
| 85:L5:4148:C:O3'   | 45:LZ:59:LYS:NZ    | 2.41                     | 0.43              |
| 85:L5:4195:G:O5'   | 47:Lb:3:LYS:NZ     | 2.30                     | 0.43              |
| 85:L5:4302:U:H2'   | 85:L5:4303:C:O4'   | 2.18                     | 0.43              |
| 85:L5:4627:U:H2'   | 85:L5:4628:U:O4'   | 2.18                     | 0.43              |
| 85:L5:4761:G:H2'   | 85:L5:4762:A:H8    | 1.82                     | 0.43              |
| 85:L5:4945:G:H1'   | 26:LE:158:ARG:NH1  | 2.34                     | 0.43              |
| 85:L5:4970:C:C2    | 85:L5:4971:A:C8    | 3.07                     | 0.43              |
| 24:LC:44:LEU:HB2   | 24:LC:238:LEU:HD21 | 2.00                     | 0.43              |
| 24:LC:139:SER:O    | 62:Lr:15:SER:N     | 2.52                     | 0.43              |
| 25:LD:208:MET:O    | 25:LD:212:MET:SD   | 2.77                     | 0.43              |
| 25:LD:212:MET:HE1  | 25:LD:219:TYR:CD1  | 2.54                     | 0.43              |
| 25:LD:215:ASP:OD1  | 25:LD:216:GLU:N    | 2.51                     | 0.43              |
| 34:LN:51:LEU:HD23  | 34:LN:51:LEU:HA    | 1.84                     | 0.43              |
| 34:LN:84:PRO:HA    | 34:LN:87:HIS:CE1   | 2.54                     | 0.43              |
| 36:LP:111:SER:O    | 36:LP:111:SER:OG   | 2.37                     | 0.43              |
| 40:LT:27:LEU:HD12  | 40:LT:27:LEU:HA    | 1.84                     | 0.43              |
| 41:LU:54:GLY:C     | 41:LU:56:LEU:H     | 2.26                     | 0.43              |
| 42:LV:99:GLU:HB2   | 87:LW:24:THR:HG23  | 2.01                     | 0.43              |
| 42:LV:139:ILE:HD12 | 42:LV:139:ILE:HA   | 1.90                     | 0.43              |
| 48:Lc:63:TYR:O     | 48:Lc:66:LEU:HG    | 2.18                     | 0.43              |
| 50:Le:44:ARG:HA    | 50:Le:47:ARG:HD3   | 1.99                     | 0.43              |
| 65:SD:192:TRP:HD1  | 65:SD:200:PRO:O    | 2.02                     | 0.43              |
| 66:SF:176:GLU:OE1  | 66:SF:188:TYR:N    | 2.51                     | 0.43              |
| 70:SS:50:ILE:CD1   | 70:SS:66:ARG:HH21  | 2.21                     | 0.43              |
| 71:ST:73:GLY:O     | 71:ST:76:THR:OG1   | 2.34                     | 0.43              |
| 75:Sg:270:LEU:HD12 | 75:Sg:270:LEU:HA   | 1.72                     | 0.43              |
| 75:Sg:278:SER:O    | 75:Sg:280:LYS:HE2  | 2.19                     | 0.43              |
| 77:SZ:58:LEU:O     | 77:SZ:63:PRO:HD3   | 2.19                     | 0.43              |
| 79:S2:210:U:H2'    | 79:S2:211:G:C8     | 2.54                     | 0.43              |
| 79:S2:340:C:H2'    | 79:S2:341:C:O4'    | 2.19                     | 0.43              |
| 79:S2:804:U:H2'    | 79:S2:805:U:H6     | 1.81                     | 0.43              |
| 79:S2:926:A:H2'    | 79:S2:927:C:C6     | 2.53                     | 0.43              |
| 79:S2:939:U:H2'    | 79:S2:940:U:C6     | 2.54                     | 0.43              |
| 79:S2:1117:C:H2'   | 79:S2:1118:C:C6    | 2.54                     | 0.43              |
| 79:S2:1518:C:OP1   | 79:S2:1519:U:H2'   | 2.19                     | 0.43              |
| 79:S2:1739:C:H2'   | 79:S2:1740:C:C6    | 2.54                     | 0.43              |
| 82:PE:61:C:H2'     | 82:PE:62:C:C6      | 2.54                     | 0.43              |
| 84:Lt:126:SER:HB3  | 84:Lt:130:LYS:CE   | 2.47                     | 0.43              |
| 1:CH:93:LYS:O      | 1:CH:97:THR:HG23   | 2.19                     | 0.43              |
| 2:sE:21:ASP:OD2    | 2:sE:24:THR:HG23   | 2.19                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:sE:30:ARG:HA     | 2:sE:30:ARG:HD2    | 1.79                     | 0.43              |
| 2:sE:235:TRP:C     | 2:sE:236:ILE:HD12  | 2.43                     | 0.43              |
| 5:sX:12:LYS:HA     | 5:sX:12:LYS:HD2    | 1.81                     | 0.43              |
| 5:sX:79:LYS:HG2    | 5:sX:79:LYS:H      | 1.62                     | 0.43              |
| 5:sX:87:ASN:ND2    | 5:sX:134:TYR:CG    | 2.87                     | 0.43              |
| 6:sG:32:MET:HE1    | 6:sG:66:GLY:N      | 2.34                     | 0.43              |
| 6:sG:164:LYS:O     | 6:sG:167:LYS:HG3   | 2.19                     | 0.43              |
| 10:sA:80:ARG:NH2   | 10:sA:82:THR:OG1   | 2.52                     | 0.43              |
| 11:sB:58:ALA:O     | 11:sB:62:LEU:HD12  | 2.19                     | 0.43              |
| 17:sO:100:THR:OG1  | 17:sO:104:ARG:HB3  | 2.19                     | 0.43              |
| 17:sO:103:ASN:HD22 | 17:sO:142:ARG:CB   | 2.32                     | 0.43              |
| 18:sW:14:ILE:HG23  | 18:sW:65:LEU:HD11  | 2.00                     | 0.43              |
| 21:l8:80:A:H3'     | 21:l8:81:C:H6      | 1.83                     | 0.43              |
| 22:lA:103:PRO:HA   | 22:lA:163:ARG:HA   | 2.00                     | 0.43              |
| 23:lB:47:LEU:HD12  | 23:lB:47:LEU:HA    | 1.81                     | 0.43              |
| 26:lE:270:TYR:CD1  | 33:lM:107:PHE:CD1  | 3.07                     | 0.43              |
| 27:lF:111:LEU:HD23 | 27:lF:111:LEU:HA   | 1.76                     | 0.43              |
| 27:lF:136:VAL:CG2  | 27:lF:139:TYR:HB2  | 2.48                     | 0.43              |
| 35:lO:56:ALA:O     | 35:lO:60:LYS:HG2   | 2.18                     | 0.43              |
| 35:lO:189:ILE:HA   | 35:lO:189:ILE:HD13 | 1.62                     | 0.43              |
| 35:lO:191:LYS:HG2  | 35:lO:192:TYR:N    | 2.34                     | 0.43              |
| 39:lS:136:LYS:HD2  | 39:lS:136:LYS:N    | 2.34                     | 0.43              |
| 41:lU:21:PHE:O     | 41:lU:72:VAL:N     | 2.38                     | 0.43              |
| 41:lU:107:LYS:HZ3  | 85:l5:2717:G:P     | 2.42                     | 0.43              |
| 43:lX:143:ASP:OD2  | 43:lX:144:TYR:N    | 2.51                     | 0.43              |
| 46:la:10:LYS:NZ    | 85:l5:2287:G:N7    | 2.67                     | 0.43              |
| 50:le:124:ASN:OD1  | 50:le:124:ASN:N    | 2.52                     | 0.43              |
| 52:lg:22:LEU:HD23  | 52:lg:22:LEU:H     | 1.84                     | 0.43              |
| 55:lj:18:LEU:HD12  | 55:lj:18:LEU:HA    | 1.72                     | 0.43              |
| 55:lj:28:HIS:CE1   | 55:lj:30:GLN:HB2   | 2.54                     | 0.43              |
| 59:ln:23:ARG:NH2   | 85:l5:3807:A:OP1   | 2.52                     | 0.43              |
| 62:lr:92:SER:O     | 62:lr:96:MET:SD    | 2.77                     | 0.43              |
| 63:lz:85:MET:HE2   | 63:lz:85:MET:HA    | 2.01                     | 0.43              |
| 63:lz:203:ALA:HB1  | 63:lz:215:ARG:HB3  | 2.01                     | 0.43              |
| 64:sR:26:ASN:HB3   | 64:sR:59:LYS:HZ3   | 1.84                     | 0.43              |
| 65:sD:5:ILE:HD11   | 65:sD:9:ARG:HB2    | 2.01                     | 0.43              |
| 66:sF:22:LYS:HB3   | 66:sF:22:LYS:HE2   | 1.71                     | 0.43              |
| 66:sF:89:THR:O     | 66:sF:93:VAL:HG23  | 2.18                     | 0.43              |
| 68:sP:100:LYS:HB2  | 79:s2:1240:A:N1    | 2.34                     | 0.43              |
| 69:sQ:112:LEU:HD12 | 69:sQ:112:LEU:HA   | 1.85                     | 0.43              |
| 70:sS:116:LYS:HA   | 70:sS:116:LYS:HD3  | 1.75                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 71:sT:37:VAL:C     | 71:sT:39:LEU:H     | 2.27                     | 0.43              |
| 71:sT:41:LYS:HZ3   | 79:s2:1569:A:H5'   | 1.84                     | 0.43              |
| 71:sT:82:ARG:NE    | 79:s2:1590:C:H5'   | 2.33                     | 0.43              |
| 75:sg:62:HIS:CD2   | 75:sg:90:TRP:HZ2   | 2.37                     | 0.43              |
| 75:sg:140:TYR:HD2  | 75:sg:182:CYS:SG   | 2.41                     | 0.43              |
| 76:sM:41:ALA:CA    | 76:sM:44:LYS:HZ2   | 2.32                     | 0.43              |
| 79:s2:587:A:N3     | 79:s2:590:A:H2'    | 2.34                     | 0.43              |
| 79:s2:940:U:C2     | 79:s2:1003:U:C4    | 3.06                     | 0.43              |
| 79:s2:1099:G:H2'   | 79:s2:1100:A:O4'   | 2.18                     | 0.43              |
| 79:s2:1305:C:H2'   | 79:s2:1306:U:H6    | 1.84                     | 0.43              |
| 79:s2:1432:U:H4'   | 79:s2:1437:C:O2    | 2.18                     | 0.43              |
| 79:s2:1566:G:C2    | 79:s2:1570:G:C6    | 3.07                     | 0.43              |
| 79:s2:1577:G:H1'   | 79:s2:1582:C:O2    | 2.19                     | 0.43              |
| 79:s2:1735:A:H2'   | 79:s2:1736:G:O4'   | 2.19                     | 0.43              |
| 80:cB:132:VAL:HG11 | 80:cB:162:ARG:NE   | 2.34                     | 0.43              |
| 80:cB:143:LEU:HD11 | 80:cB:188:ILE:CD1  | 2.49                     | 0.43              |
| 80:cB:178:PHE:CD2  | 80:cB:214:PHE:CZ   | 3.07                     | 0.43              |
| 80:cB:603:TYR:O    | 80:cB:705:HIS:N    | 2.46                     | 0.43              |
| 80:cB:731:ALA:HB2  | 80:cB:854:PHE:HB3  | 2.01                     | 0.43              |
| 81:aP:2:U:H2'      | 81:aP:3:C:C6       | 2.54                     | 0.43              |
| 84:lt:129:ILE:HG22 | 84:lt:133:LEU:HD13 | 2.00                     | 0.43              |
| 85:l5:15:A:H2'     | 85:l5:16:G:O4'     | 2.19                     | 0.43              |
| 85:l5:35:U:H4'     | 85:l5:1525:A:C2    | 2.54                     | 0.43              |
| 85:l5:307:A:H2'    | 85:l5:308:G:N3     | 2.34                     | 0.43              |
| 85:l5:512:U:C4     | 85:l5:647:G:O6     | 2.72                     | 0.43              |
| 85:l5:1478:C:H2'   | 85:l5:1479:G:C8    | 2.53                     | 0.43              |
| 85:l5:1629:G:C2    | 85:l5:1631:A:C2    | 3.06                     | 0.43              |
| 85:l5:1770:A:N7    | 85:l5:1771:U:N3    | 2.66                     | 0.43              |
| 85:l5:3672:G:H3'   | 85:l5:3673:C:H5''  | 2.01                     | 0.43              |
| 85:l5:3824:A:H2'   | 85:l5:3825:A:C8    | 2.53                     | 0.43              |
| 85:l5:4092:G:C2    | 85:l5:4093:G:C6    | 3.07                     | 0.43              |
| 85:l5:4561:C:C2    | 85:l5:4562:C:C5    | 3.07                     | 0.43              |
| 85:l5:4578:G:H2'   | 85:l5:4579:U:H6    | 1.83                     | 0.43              |
| 85:l5:4700:A:C2    | 85:l5:4701:A:C8    | 3.07                     | 0.43              |
| 80:CB:58:ASP:HB3   | 80:CB:63:GLU:CB    | 2.49                     | 0.43              |
| 80:CB:161:ASP:O    | 80:CB:165:LEU:HG   | 2.19                     | 0.43              |
| 80:CB:488:PHE:HB3  | 80:CB:491:ALA:HB2  | 2.01                     | 0.43              |
| 2:SE:66:MET:SD     | 79:S2:502:C:C2     | 3.12                     | 0.43              |
| 2:SE:122:LYS:N     | 2:SE:161:GLN:HE22  | 2.16                     | 0.43              |
| 2:SE:163:ASP:O     | 2:SE:166:THR:OG1   | 2.36                     | 0.43              |
| 3:SI:38:ILE:HD13   | 3:SI:38:ILE:HA     | 1.86                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 6:SG:14:LYS:HA     | 79:S2:154:U:H4'    | 2.01                     | 0.43              |
| 7:SJ:93:LYS:N      | 7:SJ:96:TYR:HE2    | 2.16                     | 0.43              |
| 86:Se:28:LYS:O     | 86:Se:33:LYS:HB2   | 2.19                     | 0.43              |
| 86:Se:45:VAL:O     | 86:Se:47:PRO:HD3   | 2.19                     | 0.43              |
| 11:SB:105:LEU:HD11 | 11:SB:110:MET:HE2  | 2.00                     | 0.43              |
| 11:SB:105:LEU:HD11 | 11:SB:110:MET:HA   | 2.00                     | 0.43              |
| 12:SH:107:LYS:HB3  | 12:SH:107:LYS:HE3  | 1.76                     | 0.43              |
| 12:SH:143:ARG:HB2  | 12:SH:155:LYS:CG   | 2.45                     | 0.43              |
| 12:SH:192:PHE:C    | 12:SH:192:PHE:CD1  | 2.97                     | 0.43              |
| 14:Sa:6:ARG:HH21   | 79:S2:1147:C:P     | 2.42                     | 0.43              |
| 15:SC:113:GLN:C    | 15:SC:114:LYS:HD2  | 2.43                     | 0.43              |
| 15:SC:241:PHE:O    | 15:SC:244:ILE:HG13 | 2.19                     | 0.43              |
| 16:SN:18:TYR:CE2   | 18:SW:55:ASP:HA    | 2.54                     | 0.43              |
| 18:SW:2:VAL:HB     | 18:SW:3:ARG:H      | 1.72                     | 0.43              |
| 18:SW:4:MET:HE3    | 18:SW:4:MET:C      | 2.44                     | 0.43              |
| 85:L5:33:A:H5'     | 34:LN:86:HIS:CD2   | 2.54                     | 0.43              |
| 85:L5:127:G:C6     | 85:L5:142:G:C6     | 3.06                     | 0.43              |
| 85:L5:301:G:H2'    | 85:L5:302:C:H6     | 1.82                     | 0.43              |
| 85:L5:1380:G:H4'   | 85:L5:1381:U:H6    | 1.84                     | 0.43              |
| 85:L5:1426:G:N2    | 85:L5:1458:C:OP2   | 2.48                     | 0.43              |
| 85:L5:1437:C:H1'   | 85:L5:2098:G:H3'   | 2.00                     | 0.43              |
| 85:L5:1538:U:H2'   | 85:L5:1539:G:C8    | 2.49                     | 0.43              |
| 85:L5:1615:C:H2'   | 85:L5:1616:U:H6    | 1.83                     | 0.43              |
| 85:L5:1873:A:O5'   | 85:L5:4219:A:H1'   | 2.18                     | 0.43              |
| 85:L5:1948:G:H2'   | 85:L5:1949:U:C6    | 2.54                     | 0.43              |
| 85:L5:2276:A:H2'   | 85:L5:2277:C:H6    | 1.84                     | 0.43              |
| 85:L5:2483:G:C6    | 85:L5:2496:G:C6    | 3.07                     | 0.43              |
| 85:L5:3702:A:C6    | 85:L5:3703:G:C8    | 3.07                     | 0.43              |
| 85:L5:3729:U:H2'   | 85:L5:3730:U:H6    | 1.83                     | 0.43              |
| 85:L5:4250:G:H4'   | 31:LJ:106:GLY:C    | 2.44                     | 0.43              |
| 85:L5:4907:G:C6    | 85:L5:4915:G:C6    | 3.06                     | 0.43              |
| 85:L5:4998:G:OP1   | 49:Ld:115:LYS:HG3  | 2.19                     | 0.43              |
| 20:L7:27:G:H2'     | 20:L7:28:C:C6      | 2.53                     | 0.43              |
| 27:LF:187:MET:HA   | 27:LF:190:LEU:HG   | 2.00                     | 0.43              |
| 30:LI:3:ARG:NH1    | 30:LI:63:GLU:OE1   | 2.52                     | 0.43              |
| 31:LJ:63:ARG:O     | 31:LJ:66:GLU:HG2   | 2.19                     | 0.43              |
| 31:LJ:63:ARG:HG2   | 31:LJ:64:ARG:H     | 1.84                     | 0.43              |
| 32:LL:111:GLN:O    | 32:LL:115:GLN:HG3  | 2.19                     | 0.43              |
| 32:LL:179:PHE:O    | 32:LL:183:ARG:HG2  | 2.19                     | 0.43              |
| 39:LS:95:ARG:HD3   | 39:LS:109:CYS:SG   | 2.59                     | 0.43              |
| 41:LU:83:LEU:HD12  | 41:LU:84:LYS:H     | 1.83                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 43:LX:106:LYS:HE2  | 43:LX:126:THR:HG22 | 2.01                     | 0.43              |
| 43:LX:118:ASP:O    | 43:LX:119:ILE:HD13 | 2.19                     | 0.43              |
| 44:LY:31:SER:HA    | 44:LY:48:PRO:HA    | 2.00                     | 0.43              |
| 45:LZ:21:ARG:HH11  | 45:LZ:47:ASP:HA    | 1.83                     | 0.43              |
| 48:Lc:32:LYS:O     | 48:Lc:36:LYS:HG2   | 2.18                     | 0.43              |
| 48:Lc:54:ALA:HA    | 48:Lc:57:LYS:HG2   | 2.01                     | 0.43              |
| 55:Lj:17:THR:OG1   | 55:Lj:18:LEU:N     | 2.51                     | 0.43              |
| 56:Lk:49:ASP:OD1   | 56:Lk:52:LYS:HG2   | 2.18                     | 0.43              |
| 60:Lo:68:LEU:HD11  | 60:Lo:85:ILE:HD13  | 1.99                     | 0.43              |
| 65:SD:137:VAL:O    | 65:SD:184:ILE:HD12 | 2.19                     | 0.43              |
| 66:SF:45:TYR:O     | 66:SF:45:TYR:CD1   | 2.69                     | 0.43              |
| 67:SK:14:LEU:HD11  | 67:SK:34:GLU:OE1   | 2.18                     | 0.43              |
| 69:SQ:142:GLN:OE1  | 79:S2:1643:U:H1'   | 2.18                     | 0.43              |
| 72:SU:57:PRO:HG3   | 79:S2:1580:A:N3    | 2.34                     | 0.43              |
| 72:SU:116:ILE:HG12 | 72:SU:117:ALA:N    | 2.34                     | 0.43              |
| 75:Sg:155:ARG:HG3  | 75:Sg:198:VAL:HG13 | 2.01                     | 0.43              |
| 76:SM:121:LYS:HB3  | 76:SM:121:LYS:HE3  | 1.78                     | 0.43              |
| 77:SZ:80:ARG:HG2   | 79:S2:1599:U:OP1   | 2.19                     | 0.43              |
| 79:S2:92:A:H61     | 79:S2:444:G:H1'    | 1.82                     | 0.43              |
| 79:S2:414:A:H2'    | 79:S2:415:A:C8     | 2.54                     | 0.43              |
| 79:S2:587:A:N3     | 79:S2:590:A:H2'    | 2.33                     | 0.43              |
| 79:S2:659:G:H2'    | 79:S2:663:C:C6     | 2.54                     | 0.43              |
| 79:S2:659:G:O2'    | 79:S2:662:G:O2'    | 2.29                     | 0.43              |
| 79:S2:913:A:H2'    | 79:S2:913:A:OP1    | 2.19                     | 0.43              |
| 79:S2:1140:G:H2'   | 79:S2:1141:G:H8    | 1.84                     | 0.43              |
| 79:S2:1261:C:OP1   | 79:S2:1518:C:N4    | 2.51                     | 0.43              |
| 82:PE:18:U:H5'     | 82:PE:58:A:C2      | 2.53                     | 0.43              |
| 82:PE:52:G:H3'     | 82:PE:53:G:H8      | 1.82                     | 0.43              |
| 84:Lt:66:ASN:HD21  | 84:Lt:71:ILE:HG13  | 1.83                     | 0.43              |
| 84:Lt:160:VAL:HG12 | 84:Lt:163:PRO:HG2  | 2.00                     | 0.43              |
| 1:cH:46:ALA:HB2    | 9:se:41:ARG:HB3    | 2.00                     | 0.43              |
| 3:sI:73:THR:HG21   | 79:s2:301:A:N3     | 2.33                     | 0.43              |
| 5:sX:64:SER:HB3    | 79:s2:614:C:H1'    | 2.00                     | 0.43              |
| 5:sX:64:SER:HB3    | 79:s2:614:C:O2     | 2.19                     | 0.43              |
| 5:sX:124:LYS:HD2   | 79:s2:28:U:O3'     | 2.19                     | 0.43              |
| 6:sG:5:ILE:HD12    | 6:sG:5:ILE:O       | 2.18                     | 0.43              |
| 6:sG:159:ARG:HD2   | 6:sG:171:THR:OG1   | 2.19                     | 0.43              |
| 6:sG:186:GLN:NE2   | 79:s2:318:A:H61    | 2.17                     | 0.43              |
| 7:sJ:10:ARG:NH1    | 79:s2:827:A:OP2    | 2.50                     | 0.43              |
| 7:sJ:96:TYR:HD1    | 7:sJ:96:TYR:H      | 1.67                     | 0.43              |
| 8:sY:44:LEU:HA     | 8:sY:47:MET:HG3    | 2.01                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 9:se:28:LYS:NZ     | 79:s2:525:A:H3'    | 2.33                     | 0.43              |
| 10:sA:136:GLU:HA   | 10:sA:139:TYR:CD1  | 2.52                     | 0.43              |
| 10:sA:146:ALA:HB2  | 10:sA:157:VAL:HG21 | 2.01                     | 0.43              |
| 10:sA:159:ILE:HD11 | 13:sV:34:MET:SD    | 2.58                     | 0.43              |
| 10:sA:215:GLN:CD   | 10:sA:215:GLN:N    | 2.77                     | 0.43              |
| 10:sA:215:GLN:O    | 10:sA:219:GLU:HG2  | 2.19                     | 0.43              |
| 14:sa:10:ARG:HH12  | 79:s2:1859:A:P     | 2.42                     | 0.43              |
| 17:sO:36:SER:HB2   | 17:sO:100:THR:HG22 | 2.01                     | 0.43              |
| 21:l8:7:U:H2'      | 21:l8:8:U:C6       | 2.54                     | 0.43              |
| 21:l8:151:G:H2'    | 21:l8:152:U:H6     | 1.84                     | 0.43              |
| 22:lA:40:TYR:CE1   | 85:l5:4117:U:N3    | 2.87                     | 0.43              |
| 22:lA:117:GLU:OE2  | 22:lA:163:ARG:NH2  | 2.51                     | 0.43              |
| 23:lB:27:GLY:HA2   | 23:lB:276:HIS:CD2  | 2.54                     | 0.43              |
| 23:lB:175:GLN:OE1  | 85:l5:4985:U:H4'   | 2.19                     | 0.43              |
| 23:lB:317:LEU:HD12 | 23:lB:317:LEU:HA   | 1.86                     | 0.43              |
| 23:lB:324:GLY:N    | 85:l5:5051:C:H5''  | 2.33                     | 0.43              |
| 25:lD:191:ASN:OD1  | 25:lD:194:VAL:HG13 | 2.18                     | 0.43              |
| 31:lJ:24:ILE:HG21  | 31:lJ:40:LEU:HD21  | 2.01                     | 0.43              |
| 44:lY:51:LYS:HG3   | 44:lY:52:ASP:OD2   | 2.19                     | 0.43              |
| 46:la:23:GLY:HA3   | 46:la:24:LYS:HA    | 1.54                     | 0.43              |
| 47:lb:113:ALA:O    | 47:lb:116:LEU:HG   | 2.19                     | 0.43              |
| 51:lf:18:LEU:HD23  | 85:l5:1916:G:O6    | 2.19                     | 0.43              |
| 54:li:16:LYS:HA    | 54:li:16:LYS:HD3   | 1.88                     | 0.43              |
| 54:li:66:ASP:OD2   | 54:li:66:ASP:C     | 2.62                     | 0.43              |
| 65:sD:76:ARG:NH1   | 65:sD:77:PHE:HD1   | 2.15                     | 0.43              |
| 68:sP:90:VAL:HA    | 68:sP:107:ILE:CG2  | 2.49                     | 0.43              |
| 71:sT:62:ARG:NH2   | 79:s2:1542:C:OP1   | 2.47                     | 0.43              |
| 75:sg:217:MET:SD   | 75:sg:217:MET:N    | 2.90                     | 0.43              |
| 77:sZ:102:LYS:HA   | 77:sZ:102:LYS:HD2  | 1.77                     | 0.43              |
| 79:s2:383:G:H2'    | 79:s2:384:U:N1     | 2.34                     | 0.43              |
| 79:s2:584:A:H2'    | 79:s2:585:C:O4'    | 2.17                     | 0.43              |
| 79:s2:1088:U:H4'   | 79:s2:1089:G:OP2   | 2.19                     | 0.43              |
| 79:s2:1158:G:H2'   | 79:s2:1159:G:H8    | 1.83                     | 0.43              |
| 79:s2:1208:A:H4'   | 79:s2:1835:A:N7    | 2.34                     | 0.43              |
| 79:s2:1532:C:H2'   | 79:s2:1637:A:N7    | 2.34                     | 0.43              |
| 79:s2:1777:G:H2'   | 79:s2:1778:C:H6    | 1.84                     | 0.43              |
| 79:s2:1804:U:H2'   | 79:s2:1805:G:H8    | 1.83                     | 0.43              |
| 79:s2:1851:A:H5''  | 79:s2:1852:C:OP2   | 2.18                     | 0.43              |
| 79:s2:1860:A:C6    | 79:s2:1862:G:C6    | 3.07                     | 0.43              |
| 80:cB:260:LEU:HD12 | 80:cB:288:THR:OG1  | 2.18                     | 0.43              |
| 80:cB:568:ILE:HD13 | 80:cB:568:ILE:HA   | 1.85                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 83:ls:91:THR:HG21  | 83:ls:98:ILE:HG13  | 2.01                     | 0.43              |
| 85:l5:274:C:O2'    | 85:l5:275:C:H5'    | 2.19                     | 0.43              |
| 85:l5:759:G:H2'    | 85:l5:759:G:N3     | 2.33                     | 0.43              |
| 85:l5:1258:G:H8    | 85:l5:1258:G:O5'   | 2.02                     | 0.43              |
| 85:l5:1341:U:H2'   | 85:l5:1342:A:C8    | 2.53                     | 0.43              |
| 85:l5:1548:G:O2'   | 85:l5:2812:A:N3    | 2.40                     | 0.43              |
| 85:l5:1721:G:H2'   | 85:l5:1722:C:C6    | 2.54                     | 0.43              |
| 85:l5:1912:G:C5    | 85:l5:2057:A:C4    | 3.07                     | 0.43              |
| 85:l5:2458:C:O2'   | 85:l5:3671:G:N3    | 2.46                     | 0.43              |
| 85:l5:2535:G:H2'   | 85:l5:2536:A:H8    | 1.84                     | 0.43              |
| 85:l5:2689:C:C2    | 85:l5:2690:C:C5    | 3.07                     | 0.43              |
| 85:l5:2838:G:H2'   | 85:l5:2839:U:C6    | 2.53                     | 0.43              |
| 85:l5:3722:G:C2    | 85:l5:3723:A:C5    | 3.07                     | 0.43              |
| 85:l5:4313:A:H2'   | 85:l5:4314:C:O4'   | 2.18                     | 0.43              |
| 85:l5:4619:U:H2'   | 85:l5:4620:U:C6    | 2.54                     | 0.43              |
| 85:l5:4699:U:H4'   | 85:l5:4700:A:OP1   | 2.17                     | 0.43              |
| 85:l5:5030:U:C2    | 85:l5:5031:G:C8    | 3.07                     | 0.43              |
| 80:CB:163:ALA:HA   | 80:CB:167:LEU:HB2  | 2.01                     | 0.43              |
| 3:SI:173:ALA:HA    | 3:SI:189:VAL:HA    | 2.00                     | 0.43              |
| 4:SL:30:LYS:HA     | 4:SL:30:LYS:HD2    | 1.60                     | 0.43              |
| 6:SG:45:TRP:HA     | 6:SG:48:TYR:CD2    | 2.54                     | 0.43              |
| 6:SG:50:VAL:HB     | 6:SG:113:ILE:CD1   | 2.47                     | 0.43              |
| 6:SG:85:ARG:O      | 6:SG:87:ARG:NH1    | 2.52                     | 0.43              |
| 10:SA:121:LEU:HD23 | 10:SA:143:PRO:HG2  | 2.01                     | 0.43              |
| 10:SA:145:ILE:HD12 | 10:SA:146:ALA:H    | 1.84                     | 0.43              |
| 14:Sa:98:PRO:HB2   | 79:S2:1868:U:O4    | 2.19                     | 0.43              |
| 15:SC:271:ASP:O    | 15:SC:274:VAL:HG22 | 2.18                     | 0.43              |
| 17:SO:103:ASN:OD1  | 17:SO:103:ASN:N    | 2.47                     | 0.43              |
| 85:L5:326:C:OP2    | 54:Li:28:ARG:NH2   | 2.30                     | 0.43              |
| 85:L5:470:A:H2'    | 85:L5:471:A:O4'    | 2.19                     | 0.43              |
| 85:L5:658:C:C4     | 85:L5:659:G:C8     | 3.07                     | 0.43              |
| 85:L5:1382:G:H5''  | 32:LL:65:ARG:NH2   | 2.34                     | 0.43              |
| 85:L5:1398:A:OP1   | 46:La:114:LYS:HA   | 2.19                     | 0.43              |
| 85:L5:1427:A:OP2   | 85:L5:1457:G:N2    | 2.50                     | 0.43              |
| 85:L5:1754:U:H2'   | 85:L5:1755:C:C6    | 2.52                     | 0.43              |
| 85:L5:1905:U:OP2   | 51:Lf:76:ARG:NH2   | 2.47                     | 0.43              |
| 85:L5:2652:G:N2    | 61:Lp:58:GLY:O     | 2.49                     | 0.43              |
| 85:L5:2831:G:H2'   | 85:L5:2832:A:H8    | 1.83                     | 0.43              |
| 85:L5:3640:U:C4    | 85:L5:3646:A:C4    | 3.06                     | 0.43              |
| 85:L5:4101:C:OP1   | 85:L5:4108:G:O5'   | 2.37                     | 0.43              |
| 85:L5:4103:C:H5'   | 85:L5:4107:G:P     | 2.58                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 85:L5:4359:U:H2'   | 85:L5:4360:U:H6    | 1.83                     | 0.43              |
| 23:LB:138:GLN:C    | 23:LB:143:LYS:HZ1  | 2.26                     | 0.43              |
| 23:LB:218:ASP:CG   | 23:LB:280:ILE:HG22 | 2.44                     | 0.43              |
| 24:LC:104:PRO:HB2  | 24:LC:106:LYS:NZ   | 2.34                     | 0.43              |
| 24:LC:236:ASN:OD1  | 24:LC:239:LYS:HG3  | 2.19                     | 0.43              |
| 24:LC:349:LEU:HD13 | 24:LC:349:LEU:HA   | 1.92                     | 0.43              |
| 26:LE:68:MET:HE2   | 26:LE:71:ARG:HG3   | 2.01                     | 0.43              |
| 26:LE:266:GLN:NE2  | 33:LM:111:LYS:HD3  | 2.34                     | 0.43              |
| 28:LG:78:PRO:HD3   | 28:LG:237:TRP:CD2  | 2.54                     | 0.43              |
| 29:LH:59:LYS:HG2   | 29:LH:67:LEU:HD23  | 2.01                     | 0.43              |
| 30:LI:183:ASP:N    | 30:LI:183:ASP:OD1  | 2.48                     | 0.43              |
| 32:LL:108:GLU:HA   | 32:LL:111:GLN:HG2  | 2.01                     | 0.43              |
| 35:LO:171:LYS:HA   | 35:LO:174:LEU:HD23 | 2.01                     | 0.43              |
| 39:LS:44:PHE:O     | 39:LS:48:VAL:HG13  | 2.19                     | 0.43              |
| 42:LV:107:ASN:OD1  | 42:LV:111:GLU:N    | 2.52                     | 0.43              |
| 49:Ld:51:LYS:HE3   | 49:Ld:51:LYS:HB3   | 1.90                     | 0.43              |
| 62:Lr:65:LYS:HE3   | 62:Lr:70:GLN:HE22  | 1.84                     | 0.43              |
| 65:SD:95:GLY:HA2   | 65:SD:101:GLN:HE22 | 1.84                     | 0.43              |
| 65:SD:136:VAL:HG22 | 65:SD:152:PHE:HB2  | 2.00                     | 0.43              |
| 66:SF:168:THR:HG22 | 66:SF:171:GLU:CD   | 2.43                     | 0.43              |
| 68:SP:62:LYS:HA    | 68:SP:65:LYS:HG2   | 2.01                     | 0.43              |
| 69:SQ:28:GLY:O     | 69:SQ:65:GLY:HA2   | 2.19                     | 0.43              |
| 69:SQ:68:ILE:HD12  | 69:SQ:68:ILE:HA    | 1.84                     | 0.43              |
| 69:SQ:116:ASP:OD1  | 69:SQ:118:THR:HG23 | 2.19                     | 0.43              |
| 79:S2:23:G:H2'     | 79:S2:24:C:C6      | 2.54                     | 0.43              |
| 79:S2:476:A:H2'    | 79:S2:477:G:O4'    | 2.18                     | 0.43              |
| 79:S2:907:G:C2     | 79:S2:908:A:C5     | 3.07                     | 0.43              |
| 79:S2:942:G:H2'    | 79:S2:943:U:C6     | 2.54                     | 0.43              |
| 79:S2:943:U:C2     | 79:S2:944:A:C8     | 3.05                     | 0.43              |
| 79:S2:991:G:C6     | 79:S2:1134:G:H4'   | 2.53                     | 0.43              |
| 79:S2:1019:C:H3'   | 79:S2:1020:A:H8    | 1.83                     | 0.43              |
| 79:S2:1243:U:OP2   | 79:S2:1518:C:O2'   | 2.20                     | 0.43              |
| 79:S2:1316:C:C2    | 79:S2:1317:C:C5    | 3.07                     | 0.43              |
| 82:PE:3:C:H2'      | 82:PE:4:C:O4'      | 2.19                     | 0.43              |
| 82:PE:65:G:C6      | 82:PE:66:U:C4      | 3.07                     | 0.43              |
| 83:Ls:28:PHE:CD1   | 83:Ls:189:ILE:HD12 | 2.54                     | 0.43              |
| 83:Ls:61:MET:SD    | 83:Ls:61:MET:N     | 2.92                     | 0.43              |
| 1:cH:36:GLU:N      | 1:cH:36:GLU:OE1    | 2.51                     | 0.42              |
| 2:sE:222:LEU:C     | 2:sE:222:LEU:HD23  | 2.44                     | 0.42              |
| 4:sL:105:ARG:NH2   | 79:s2:355:G:H5''   | 2.34                     | 0.42              |
| 6:sG:72:ARG:NH2    | 79:s2:466:G:O2'    | 2.52                     | 0.42              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 8:sY:16:ARG:C     | 8:sY:19:GLN:H      | 2.27                     | 0.42              |
| 8:sY:19:GLN:NE2   | 8:sY:85:ASN:ND2    | 2.67                     | 0.42              |
| 10:sA:17:LYS:NZ   | 64:sR:91:LEU:HG    | 2.33                     | 0.42              |
| 10:sA:33:GLN:OE1  | 10:sA:154:LEU:HD13 | 2.19                     | 0.42              |
| 11:sB:93:GLY:HA2  | 28:lG:264:LYS:HA   | 2.01                     | 0.42              |
| 16:sN:128:TYR:O   | 16:sN:131:THR:OG1  | 2.35                     | 0.42              |
| 17:sO:26:ASN:ND2  | 17:sO:92:ALA:HB2   | 2.34                     | 0.42              |
| 17:sO:93:LEU:N    | 17:sO:125:LYS:O    | 2.51                     | 0.42              |
| 19:sb:42:LYS:HD3  | 19:sb:42:LYS:N     | 2.34                     | 0.42              |
| 21:l8:110:U:O4    | 85:l5:2509:C:H5"   | 2.19                     | 0.42              |
| 24:lC:345:ARG:O   | 24:lC:348:LYS:HG3  | 2.19                     | 0.42              |
| 25:lD:85:LYS:HG2  | 25:lD:85:LYS:O     | 2.18                     | 0.42              |
| 26:lE:111:LYS:HB2 | 26:lE:111:LYS:HE2  | 1.80                     | 0.42              |
| 28:lG:154:LEU:O   | 28:lG:204:PHE:N    | 2.48                     | 0.42              |
| 28:lG:244:PRO:O   | 28:lG:247:VAL:HG22 | 2.19                     | 0.42              |
| 29:lH:91:LYS:HE3  | 29:lH:183:GLU:HB3  | 2.00                     | 0.42              |
| 30:lI:46:PHE:HB2  | 30:lI:139:ARG:NE   | 2.34                     | 0.42              |
| 30:lI:62:SER:O    | 30:lI:65:LEU:HG    | 2.18                     | 0.42              |
| 34:lN:154:PRO:HB2 | 85:l5:57:G:H5"     | 1.99                     | 0.42              |
| 40:lT:89:ILE:HD12 | 40:lT:89:ILE:C     | 2.44                     | 0.42              |
| 42:IV:36:ASN:O    | 42:IV:37:LEU:HD23  | 2.19                     | 0.42              |
| 44:lY:86:GLN:HG3  | 44:lY:94:THR:OG1   | 2.18                     | 0.42              |
| 45:lZ:13:VAL:HG13 | 45:lZ:75:TYR:CE1   | 2.54                     | 0.42              |
| 45:lZ:83:THR:HG22 | 45:lZ:85:TYR:CD1   | 2.54                     | 0.42              |
| 45:lZ:113:GLU:OE2 | 45:lZ:117:LYS:CG   | 2.67                     | 0.42              |
| 52:lg:16:ALA:O    | 52:lg:19:LYS:HG2   | 2.18                     | 0.42              |
| 54:li:57:ALA:O    | 54:li:61:LEU:HG    | 2.19                     | 0.42              |
| 58:lm:79:GLU:CD   | 58:lm:79:GLU:C     | 2.87                     | 0.42              |
| 60:lo:21:HIS:CD2  | 60:lo:72:CYS:HA    | 2.54                     | 0.42              |
| 62:lr:11:ARG:NH2  | 85:l5:2269:C:C4    | 2.87                     | 0.42              |
| 64:sR:11:LYS:HD2  | 64:sR:11:LYS:O     | 2.19                     | 0.42              |
| 64:sR:41:ILE:C    | 79:s2:1388:A:C8    | 2.97                     | 0.42              |
| 65:sD:52:ALA:O    | 65:sD:90:LYS:HA    | 2.19                     | 0.42              |
| 66:sF:66:CYS:SG   | 66:sF:70:GLU:HG2   | 2.59                     | 0.42              |
| 68:sP:95:GLY:HA2  | 68:sP:103:ASN:O    | 2.19                     | 0.42              |
| 69:sQ:134:GLY:HA2 | 69:sQ:141:TYR:CE2  | 2.53                     | 0.42              |
| 70:sS:48:ALA:O    | 70:sS:50:ILE:HG23  | 2.18                     | 0.42              |
| 75:sg:94:THR:OG1  | 75:sg:96:THR:HG23  | 2.19                     | 0.42              |
| 75:sg:150:TRP:N   | 75:sg:150:TRP:CD1  | 2.87                     | 0.42              |
| 76:sM:53:ALA:HB2  | 76:sM:85:LEU:HD13  | 2.01                     | 0.42              |
| 77:sZ:88:LEU:HD13 | 77:sZ:109:TYR:CE1  | 2.54                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 77:sZ:99:LEU:HD11  | 77:sZ:102:LYS:N    | 2.34                     | 0.42              |
| 79:s2:185:G:H2'    | 79:s2:186:C:C6     | 2.53                     | 0.42              |
| 79:s2:200:G:H2'    | 79:s2:201:C:H6     | 1.84                     | 0.42              |
| 79:s2:415:A:H2'    | 79:s2:416:U:C6     | 2.54                     | 0.42              |
| 79:s2:854:A:C4     | 79:s2:855:G:C8     | 3.07                     | 0.42              |
| 79:s2:986:G:H3'    | 79:s2:987:A:H8     | 1.84                     | 0.42              |
| 79:s2:1064:C:C2    | 79:s2:1065:G:C8    | 3.07                     | 0.42              |
| 79:s2:1159:G:H2'   | 79:s2:1160:U:C6    | 2.54                     | 0.42              |
| 79:s2:1164:G:O2'   | 79:s2:1165:G:H5'   | 2.19                     | 0.42              |
| 79:s2:1388:A:C8    | 79:s2:1389:C:C6    | 3.07                     | 0.42              |
| 79:s2:1533:A:C8    | 79:s2:1604:G:H1'   | 2.54                     | 0.42              |
| 79:s2:1567:G:C6    | 79:s2:1568:C:C4    | 3.07                     | 0.42              |
| 79:s2:1738:C:H2'   | 79:s2:1739:C:C6    | 2.53                     | 0.42              |
| 80:cB:429:ILE:CD1  | 80:cB:485:ILE:HG12 | 2.49                     | 0.42              |
| 80:cB:479:LEU:HD23 | 80:cB:479:LEU:HA   | 1.80                     | 0.42              |
| 80:cB:594:LYS:HD2  | 80:cB:595:SER:O    | 2.19                     | 0.42              |
| 80:cB:629:LYS:O    | 80:cB:633:ARG:HG2  | 2.19                     | 0.42              |
| 85:l5:69:A:H5'     | 85:l5:100:C:O2'    | 2.19                     | 0.42              |
| 85:l5:133:C:O2     | 85:l5:136:C:H1'    | 2.19                     | 0.42              |
| 85:l5:190:G:H2'    | 85:l5:191:G:C8     | 2.54                     | 0.42              |
| 85:l5:218:A:H1'    | 85:l5:219:G:C8     | 2.53                     | 0.42              |
| 85:l5:433:A:H2'    | 85:l5:434:A:O4'    | 2.18                     | 0.42              |
| 85:l5:928:C:H2'    | 85:l5:929:A:H8     | 1.84                     | 0.42              |
| 85:l5:1855:G:C6    | 85:l5:1880:G:N2    | 2.86                     | 0.42              |
| 85:l5:1964:A:H2'   | 85:l5:1965:G:H8    | 1.83                     | 0.42              |
| 85:l5:1979:A:C6    | 85:l5:1980:U:H5    | 2.37                     | 0.42              |
| 85:l5:2025:A:N3    | 85:l5:2026:A:H1'   | 2.33                     | 0.42              |
| 85:l5:2446:C:H2'   | 85:l5:2447:U:C6    | 2.54                     | 0.42              |
| 85:l5:2599:G:C6    | 85:l5:2600:A:C6    | 3.07                     | 0.42              |
| 85:l5:3723:A:H2'   | 85:l5:3724:A:C8    | 2.54                     | 0.42              |
| 85:l5:4176:C:H2'   | 85:l5:4177:C:H6    | 1.83                     | 0.42              |
| 85:l5:4177:C:C2    | 85:l5:4178:A:C8    | 3.06                     | 0.42              |
| 85:l5:4710:C:H2'   | 85:l5:4711:C:C6    | 2.54                     | 0.42              |
| 80:CB:19:ILE:HG22  | 80:CB:21:ASN:HD21  | 1.84                     | 0.42              |
| 80:CB:452:LEU:O    | 80:CB:459:GLU:N    | 2.29                     | 0.42              |
| 80:CB:761:GLY:O    | 80:CB:765:ARG:HD3  | 2.19                     | 0.42              |
| 2:SE:33:THR:O      | 79:S2:120:U:H1'    | 2.18                     | 0.42              |
| 3:SI:31:ARG:NH2    | 79:S2:380:G:H5''   | 2.34                     | 0.42              |
| 3:SI:78:ILE:HG23   | 3:SI:102:VAL:HG11  | 2.01                     | 0.42              |
| 4:SL:38:LYS:N      | 4:SL:62:PHE:O      | 2.52                     | 0.42              |
| 6:SG:50:VAL:CB     | 6:SG:113:ILE:HD13  | 2.48                     | 0.42              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 6:SG:173:ALA:HB3  | 79:S2:78:C:H5'     | 2.01                     | 0.42              |
| 11:SB:208:HIS:CG  | 11:SB:209:ASP:N    | 2.87                     | 0.42              |
| 12:SH:53:VAL:CG2  | 12:SH:175:GLY:HA3  | 2.44                     | 0.42              |
| 13:SV:54:ALA:HB2  | 15:SC:261:PHE:CE1  | 2.54                     | 0.42              |
| 15:SC:130:ILE:C   | 15:SC:216:MET:HE1  | 2.44                     | 0.42              |
| 15:SC:186:GLY:HA3 | 15:SC:243:ALA:HB2  | 2.01                     | 0.42              |
| 15:SC:238:LYS:NZ  | 79:S2:1356:G:O4'   | 2.51                     | 0.42              |
| 18:SW:82:GLN:HB3  | 79:S2:805:U:OP1    | 2.18                     | 0.42              |
| 85:L5:735:G:H2'   | 85:L5:736:C:C6     | 2.54                     | 0.42              |
| 85:L5:736:C:OP1   | 33:LM:71:LYS:HB2   | 2.19                     | 0.42              |
| 85:L5:944:A:OP1   | 27:LF:62:ARG:HD2   | 2.20                     | 0.42              |
| 85:L5:1074:G:H3'  | 85:L5:1075:G:H8    | 1.84                     | 0.42              |
| 85:L5:1313:C:H3'  | 50:Le:44:ARG:HH22  | 1.84                     | 0.42              |
| 85:L5:1394:G:H5'  | 32:LL:186:ARG:CZ   | 2.49                     | 0.42              |
| 85:L5:1413:C:H2'  | 85:L5:1414:C:C1'   | 2.49                     | 0.42              |
| 85:L5:1545:G:H2'  | 85:L5:1546:C:H6    | 1.84                     | 0.42              |
| 85:L5:1726:U:C4'  | 27:LF:132:MET:HE1  | 2.49                     | 0.42              |
| 85:L5:2051:C:H1'  | 35:LO:87:MET:HE1   | 2.01                     | 0.42              |
| 85:L5:2094:G:H2'  | 85:L5:2095:A:C4    | 2.54                     | 0.42              |
| 85:L5:3908:A:N7   | 85:L5:4449:A:N6    | 2.66                     | 0.42              |
| 85:L5:3953:G:H2'  | 85:L5:3954:A:H5'   | 2.00                     | 0.42              |
| 85:L5:4600:G:H1'  | 85:L5:4601:U:H5    | 1.83                     | 0.42              |
| 85:L5:4896:G:H2'  | 85:L5:4897:G:H8    | 1.81                     | 0.42              |
| 20:L7:7:G:OP1     | 25:LD:33:ARG:HD2   | 2.19                     | 0.42              |
| 20:L7:51:G:H2'    | 20:L7:52:C:C6      | 2.54                     | 0.42              |
| 20:L7:75:G:N2     | 20:L7:100:A:OP2    | 2.51                     | 0.42              |
| 21:L8:4:C:H2'     | 21:L8:5:U:C6       | 2.54                     | 0.42              |
| 23:LB:56:ILE:HD13 | 23:LB:365:LEU:HD12 | 2.00                     | 0.42              |
| 23:LB:109:HIS:HB2 | 23:LB:202:GLU:OE2  | 2.19                     | 0.42              |
| 24:LC:121:ARG:NE  | 24:LC:274:LYS:HD3  | 2.34                     | 0.42              |
| 24:LC:293:LEU:O   | 24:LC:299:GLN:NE2  | 2.49                     | 0.42              |
| 24:LC:331:TYR:HD2 | 27:LF:51:TYR:HE1   | 1.67                     | 0.42              |
| 26:LE:93:THR:O    | 26:LE:93:THR:OG1   | 2.33                     | 0.42              |
| 29:LH:123:ILE:CD1 | 29:LH:125:ARG:HH21 | 2.31                     | 0.42              |
| 30:LI:53:VAL:O    | 30:LI:164:LYS:N    | 2.41                     | 0.42              |
| 30:LI:56:GLU:HG3  | 30:LI:58:GLU:HG2   | 2.01                     | 0.42              |
| 31:LJ:35:ARG:HE   | 31:LJ:123:ILE:C    | 2.26                     | 0.42              |
| 31:LJ:40:LEU:O    | 31:LJ:43:LEU:HD23  | 2.19                     | 0.42              |
| 32:LL:181:SER:HA  | 32:LL:184:MET:SD   | 2.59                     | 0.42              |
| 33:LM:105:THR:OG1 | 33:LM:106:ASP:N    | 2.50                     | 0.42              |
| 34:LN:39:ALA:HB3  | 34:LN:61:ILE:HG13  | 2.00                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:LO:30:GLY:HA2   | 35:LO:101:ARG:CZ   | 2.48                     | 0.42              |
| 36:LP:32:THR:HG23  | 36:LP:91:LEU:HD11  | 2.00                     | 0.42              |
| 44:LY:39:ARG:HH22  | 44:LY:45:ARG:HH12  | 1.66                     | 0.42              |
| 49:Ld:85:ARG:HD3   | 49:Ld:117:LEU:HD13 | 2.00                     | 0.42              |
| 50:Le:11:LYS:HB3   | 50:Le:11:LYS:HE3   | 1.73                     | 0.42              |
| 50:Le:117:GLN:OE1  | 50:Le:118:LEU:HG   | 2.19                     | 0.42              |
| 54:Li:46:GLU:OE1   | 54:Li:46:GLU:C     | 2.61                     | 0.42              |
| 55:Lj:65:ARG:HE    | 55:Lj:65:ARG:HB3   | 1.67                     | 0.42              |
| 63:Lz:1:MET:O      | 63:Lz:207:LYS:HG3  | 2.18                     | 0.42              |
| 63:Lz:171:HIS:CE1  | 63:Lz:173:LYS:HB2  | 2.54                     | 0.42              |
| 65:SD:50:ILE:HG22  | 65:SD:52:ALA:H     | 1.84                     | 0.42              |
| 66:SF:67:PRO:O     | 66:SF:71:ARG:HG3   | 2.18                     | 0.42              |
| 67:SK:35:LEU:HD11  | 67:SK:40:VAL:HG21  | 2.00                     | 0.42              |
| 70:SS:40:TYR:HA    | 70:SS:43:VAL:HG22  | 2.01                     | 0.42              |
| 73:Sc:36:ASP:OD1   | 73:Sc:37:ASP:N     | 2.49                     | 0.42              |
| 75:Sg:206:LEU:HD22 | 75:Sg:241:PHE:CE2  | 2.54                     | 0.42              |
| 75:Sg:302:TYR:HB2  | 75:Sg:304:ASP:OD1  | 2.19                     | 0.42              |
| 77:SZ:47:LEU:HD23  | 77:SZ:80:ARG:HB2   | 2.00                     | 0.42              |
| 79:S2:130:G:O2'    | 79:S2:131:C:O3'    | 2.37                     | 0.42              |
| 79:S2:807:G:H2'    | 79:S2:808:A:C8     | 2.53                     | 0.42              |
| 79:S2:880:G:C8     | 79:S2:907:G:C2     | 3.07                     | 0.42              |
| 79:S2:1049:A:C8    | 79:S2:1050:A:C8    | 3.07                     | 0.42              |
| 79:S2:1318:G:C6    | 79:S2:1319:U:C4    | 3.07                     | 0.42              |
| 79:S2:1332:A:H2    | 79:S2:1500:G:H1'   | 1.84                     | 0.42              |
| 79:S2:1359:U:H2'   | 79:S2:1360:U:H6    | 1.83                     | 0.42              |
| 79:S2:1413:G:H2'   | 79:S2:1414:A:C8    | 2.54                     | 0.42              |
| 79:S2:1670:C:H2'   | 79:S2:1671:G:O4'   | 2.19                     | 0.42              |
| 79:S2:1700:C:C4    | 79:S2:1702:G:C2    | 3.07                     | 0.42              |
| 79:S2:1839:U:H2'   | 79:S2:1840:U:H6    | 1.84                     | 0.42              |
| 81:AP:10:G:H2'     | 81:AP:11:U:C6      | 2.54                     | 0.42              |
| 83:Ls:95:LEU:HD12  | 83:Ls:192:VAL:HG11 | 2.00                     | 0.42              |
| 84:Lt:119:ARG:NH1  | 84:Lt:129:ILE:HB   | 2.34                     | 0.42              |
| 84:Lt:147:HIS:CG   | 84:Lt:148:PRO:HD2  | 2.53                     | 0.42              |
| 87:LW:97:LYS:HG3   | 87:LW:98:PRO:HD3   | 2.00                     | 0.42              |
| 1:CH:37:ASP:O      | 1:CH:38:VAL:HB     | 2.18                     | 0.42              |
| 1:cH:49:ASN:CG     | 9:se:56:ASN:HD22   | 2.26                     | 0.42              |
| 2:sE:9:LEU:HG      | 2:sE:28:ALA:HB3    | 2.02                     | 0.42              |
| 5:sX:124:LYS:NZ    | 79:s2:29:G:OP1     | 2.34                     | 0.42              |
| 6:sG:49:VAL:HG12   | 6:sG:115:LYS:HG2   | 2.00                     | 0.42              |
| 6:sG:147:LEU:HD22  | 87:IW:101:ARG:NH1  | 2.34                     | 0.42              |
| 7:sJ:27:GLN:OE1    | 7:sJ:30:LYS:HE2    | 2.18                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:sJ:137:VAL:HG22  | 7:sJ:138:ARG:H     | 1.84                     | 0.42              |
| 10:sA:85:ARG:HE    | 10:sA:85:ARG:C     | 2.27                     | 0.42              |
| 10:sA:111:GLN:HG2  | 10:sA:112:ILE:HD12 | 2.01                     | 0.42              |
| 11:sB:147:ASN:OD1  | 11:sB:147:ASN:N    | 2.51                     | 0.42              |
| 13:sV:29:HIS:NE2   | 15:sC:87:PRO:HA    | 2.34                     | 0.42              |
| 16:sN:20:ARG:HD3   | 16:sN:65:PHE:CE1   | 2.54                     | 0.42              |
| 17:sO:86:LYS:HE2   | 17:sO:86:LYS:HB2   | 1.84                     | 0.42              |
| 18:sW:52:ILE:HG22  | 18:sW:61:ILE:HG23  | 2.02                     | 0.42              |
| 20:l7:50:A:C4      | 20:l7:51:G:C8      | 3.07                     | 0.42              |
| 24:lC:166:GLU:H    | 24:lC:166:GLU:HG2  | 1.55                     | 0.42              |
| 27:lF:124:LYS:HZ1  | 85:l5:1839:U:P     | 2.42                     | 0.42              |
| 28:lG:31:LEU:HD11  | 45:lZ:122:TYR:OH   | 2.18                     | 0.42              |
| 28:lG:123:ALA:HA   | 28:lG:124:GLY:HA2  | 1.72                     | 0.42              |
| 29:lH:134:CYS:SG   | 29:lH:146:LEU:HB3  | 2.59                     | 0.42              |
| 32:lL:81:LEU:HD21  | 32:lL:98:VAL:HG22  | 2.01                     | 0.42              |
| 33:lM:94:LYS:HA    | 35:lO:203:VAL:HG21 | 2.01                     | 0.42              |
| 35:lO:93:LYS:CG    | 35:lO:94:ARG:N     | 2.78                     | 0.42              |
| 37:lQ:89:ASP:HA    | 85:l5:1502:G:N1    | 2.34                     | 0.42              |
| 37:lQ:113:ILE:HD12 | 37:lQ:113:ILE:HA   | 1.79                     | 0.42              |
| 38:lR:43:LYS:O     | 38:lR:46:LYS:HG3   | 2.19                     | 0.42              |
| 39:lS:159:LEU:HD23 | 39:lS:159:LEU:C    | 2.43                     | 0.42              |
| 41:lU:92:LYS:HG2   | 85:l5:2626:U:C6    | 2.54                     | 0.42              |
| 43:lX:83:THR:HG21  | 85:l5:2435:G:OP1   | 2.20                     | 0.42              |
| 44:lY:74:TYR:CD1   | 44:lY:77:LYS:HD2   | 2.54                     | 0.42              |
| 46:la:110:LYS:HD2  | 46:la:128:PHE:HB2  | 2.00                     | 0.42              |
| 48:lc:32:LYS:NZ    | 85:l5:2675:G:O2'   | 2.53                     | 0.42              |
| 48:lc:104:ILE:HG23 | 48:lc:106:ARG:NH1  | 2.20                     | 0.42              |
| 52:lg:60:ARG:HH11  | 52:lg:60:ARG:HG2   | 1.84                     | 0.42              |
| 52:lg:102:ILE:O    | 52:lg:106:VAL:HG13 | 2.20                     | 0.42              |
| 63:lz:178:GLU:HA   | 63:lz:181:TYR:CZ   | 2.53                     | 0.42              |
| 64:sR:27:ASP:HB3   | 79:s2:1455:A:P     | 2.59                     | 0.42              |
| 64:sR:102:THR:O    | 64:sR:105:MET:SD   | 2.77                     | 0.42              |
| 65:sD:75:LYS:HB3   | 65:sD:75:LYS:HE2   | 1.33                     | 0.42              |
| 69:sQ:15:ARG:HA    | 69:sQ:19:ALA:O     | 2.19                     | 0.42              |
| 78:sf:124:ASP:OD1  | 78:sf:124:ASP:N    | 2.52                     | 0.42              |
| 79:s2:222:U:H2'    | 79:s2:223:C:H6     | 1.84                     | 0.42              |
| 79:s2:575:A:H2'    | 79:s2:576:A:O4'    | 2.19                     | 0.42              |
| 79:s2:1036:A:C4    | 79:s2:1037:G:C8    | 3.06                     | 0.42              |
| 79:s2:1102:G:H2'   | 79:s2:1103:C:C6    | 2.54                     | 0.42              |
| 79:s2:1860:A:HO2'  | 79:s2:1862:G:H8    | 1.67                     | 0.42              |
| 80:cB:18:ASN:O     | 80:cB:98:PHE:HD1   | 2.02                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 80:cB:111:PHE:CD2  | 80:cB:501:VAL:HG22 | 2.54                     | 0.42              |
| 80:cB:507:VAL:HA   | 80:cB:575:PRO:HD3  | 2.01                     | 0.42              |
| 81:aP:53:G:O2'     | 81:aP:54:U:H5'     | 2.18                     | 0.42              |
| 85:l5:290:U:H2'    | 85:l5:291:U:C6     | 2.53                     | 0.42              |
| 85:l5:297:U:H2'    | 85:l5:298:G:O4'    | 2.19                     | 0.42              |
| 85:l5:671:G:C6     | 85:l5:672:C:C4     | 3.07                     | 0.42              |
| 85:l5:739:G:O2'    | 85:l5:740:G:C8     | 2.69                     | 0.42              |
| 85:l5:1758:G:C8    | 85:l5:1775:A:C4    | 3.06                     | 0.42              |
| 85:l5:1999:A:H4'   | 85:l5:2018:C:O2'   | 2.19                     | 0.42              |
| 85:l5:2249:C:H2'   | 85:l5:2250:C:C5    | 2.53                     | 0.42              |
| 85:l5:2676:A:C4    | 85:l5:2677:G:C8    | 3.06                     | 0.42              |
| 85:l5:3648:A:H1'   | 85:l5:3785:A:N6    | 2.34                     | 0.42              |
| 85:l5:3952:A:H8    | 85:l5:3952:A:O5'   | 2.01                     | 0.42              |
| 85:l5:4454:G:HO2'  | 85:l5:4500:U:HO2'  | 1.67                     | 0.42              |
| 85:l5:4762:A:H2'   | 85:l5:4763:U:O4'   | 2.18                     | 0.42              |
| 80:CB:171:PRO:HA   | 80:CB:174:LEU:CD1  | 2.45                     | 0.42              |
| 80:CB:504:VAL:N    | 80:CB:548:GLY:O    | 2.51                     | 0.42              |
| 2:SE:141:THR:OG1   | 2:SE:142:HIS:N     | 2.53                     | 0.42              |
| 3:SI:202:ILE:O     | 3:SI:205:ARG:NH2   | 2.52                     | 0.42              |
| 7:SJ:15:THR:HG21   | 79:S2:23:G:OP1     | 2.19                     | 0.42              |
| 7:SJ:132:GLN:HA    | 7:SJ:133:ARG:HH21  | 1.84                     | 0.42              |
| 86:Se:12:VAL:HG13  | 79:S2:616:A:H1'    | 2.00                     | 0.42              |
| 86:Se:36:MET:SD    | 86:Se:40:ARG:NH2   | 2.92                     | 0.42              |
| 10:SA:10:MET:SD    | 10:SA:11:LYS:N     | 2.92                     | 0.42              |
| 10:SA:124:VAL:O    | 10:SA:146:ALA:HA   | 2.19                     | 0.42              |
| 11:SB:171:ILE:HB   | 11:SB:174:ARG:NH2  | 2.34                     | 0.42              |
| 12:SH:30:LEU:HD12  | 12:SH:86:LYS:NZ    | 2.34                     | 0.42              |
| 12:SH:145:ARG:HA   | 12:SH:145:ARG:HD3  | 1.63                     | 0.42              |
| 15:SC:114:LYS:HG3  | 79:S2:1358:U:H5'   | 2.01                     | 0.42              |
| 15:SC:140:GLY:HA3  | 15:SC:158:ALA:HB2  | 2.01                     | 0.42              |
| 15:SC:176:LYS:HD2  | 15:SC:176:LYS:HA   | 1.86                     | 0.42              |
| 15:SC:193:VAL:HG21 | 15:SC:240:THR:HA   | 2.01                     | 0.42              |
| 16:SN:129:TYR:HB3  | 16:SN:135:LEU:HG   | 2.00                     | 0.42              |
| 17:SO:39:ASP:OD1   | 17:SO:40:THR:N     | 2.52                     | 0.42              |
| 18:SW:102:ILE:HB   | 18:SW:113:HIS:CD2  | 2.52                     | 0.42              |
| 18:SW:122:GLY:N    | 79:S2:804:U:O2'    | 2.51                     | 0.42              |
| 85:L5:62:A:P       | 34:LN:172:ARG:HH12 | 2.39                     | 0.42              |
| 85:L5:72:C:O4'     | 54:Li:15:HIS:HB3   | 2.18                     | 0.42              |
| 85:L5:119:G:C5     | 28:LG:132:ARG:CZ   | 3.02                     | 0.42              |
| 85:L5:163:A:H2'    | 85:L5:164:G:H8     | 1.84                     | 0.42              |
| 85:L5:453:G:N3     | 85:L5:453:G:H2'    | 2.34                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 85:L5:677:G:H2'   | 85:L5:678:C:C6    | 2.54                     | 0.42              |
| 85:L5:1072:C:C2   | 85:L5:1073:G:C8   | 3.07                     | 0.42              |
| 85:L5:1383:G:H2'  | 85:L5:1384:C:C6   | 2.54                     | 0.42              |
| 85:L5:1406:G:C4   | 85:L5:1412:G:C2   | 3.07                     | 0.42              |
| 85:L5:1416:G:H2'  | 85:L5:1417:C:C6   | 2.53                     | 0.42              |
| 85:L5:1485:C:O4'  | 85:L5:4349:C:N4   | 2.52                     | 0.42              |
| 85:L5:1598:C:C2   | 85:L5:1599:A:C8   | 3.07                     | 0.42              |
| 85:L5:1673:U:H2'  | 85:L5:1674:C:H6   | 1.82                     | 0.42              |
| 85:L5:1779:U:H2'  | 85:L5:1780:A:C8   | 2.53                     | 0.42              |
| 85:L5:1962:A:H2   | 85:L5:2024:G:H21  | 1.64                     | 0.42              |
| 85:L5:2085:G:H2'  | 85:L5:2086:G:H8   | 1.84                     | 0.42              |
| 85:L5:2090:U:O2'  | 62:Lr:105:ASP:OD1 | 2.34                     | 0.42              |
| 85:L5:2321:G:H5'  | 50:Le:35:TRP:HB3  | 2.01                     | 0.42              |
| 85:L5:2751:G:N3   | 85:L5:2752:G:C8   | 2.87                     | 0.42              |
| 85:L5:2823:G:OP1  | 38:LR:19:LYS:HG3  | 2.19                     | 0.42              |
| 85:L5:2837:U:H2'  | 85:L5:2838:G:O4'  | 2.18                     | 0.42              |
| 85:L5:2865:U:H2'  | 85:L5:2866:C:H6   | 1.84                     | 0.42              |
| 85:L5:3748:A:H5'' | 22:LA:243:THR:HB  | 2.00                     | 0.42              |
| 85:L5:3936:A:N6   | 85:L5:4175:G:O6   | 2.52                     | 0.42              |
| 85:L5:4090:G:C6   | 85:L5:4091:G:C5   | 3.07                     | 0.42              |
| 85:L5:4097:G:H3'  | 85:L5:4111:U:C2   | 2.54                     | 0.42              |
| 85:L5:4113:U:H5'  | 85:L5:4114:C:O2'  | 2.18                     | 0.42              |
| 85:L5:4494:G:C6   | 85:L5:4495:G:C5   | 3.07                     | 0.42              |
| 85:L5:4500:U:H2'  | 85:L5:4501:U:C6   | 2.54                     | 0.42              |
| 85:L5:4878:C:H2'  | 85:L5:4879:C:H6   | 1.84                     | 0.42              |
| 21:L8:7:U:H2'     | 21:L8:8:U:H6      | 1.83                     | 0.42              |
| 21:L8:131:G:H4'   | 43:LX:111:GLN:NE2 | 2.33                     | 0.42              |
| 22:LA:23:ARG:NH1  | 22:LA:52:PRO:O    | 2.51                     | 0.42              |
| 23:LB:35:ASP:OD1  | 23:LB:36:ASP:N    | 2.52                     | 0.42              |
| 23:LB:394:LYS:HG2 | 23:LB:395:ASP:N   | 2.34                     | 0.42              |
| 24:LC:189:MET:HE1 | 24:LC:200:ARG:CD  | 2.48                     | 0.42              |
| 24:LC:267:TRP:NE1 | 24:LC:280:PRO:O   | 2.39                     | 0.42              |
| 25:LD:119:TYR:CE1 | 25:LD:134:SER:HA  | 2.54                     | 0.42              |
| 25:LD:164:LYS:HZ3 | 25:LD:168:ASP:CG  | 2.27                     | 0.42              |
| 31:LJ:35:ARG:HH21 | 31:LJ:123:ILE:C   | 2.28                     | 0.42              |
| 33:LM:6:PHE:H     | 33:LM:11:ARG:HH21 | 1.68                     | 0.42              |
| 35:LO:7:LEU:HD12  | 35:LO:7:LEU:HA    | 1.88                     | 0.42              |
| 36:LP:22:LEU:HD12 | 36:LP:90:PHE:CE2  | 2.53                     | 0.42              |
| 38:LR:32:ILE:H    | 38:LR:32:ILE:HG13 | 1.65                     | 0.42              |
| 40:LT:156:TYR:CD1 | 40:LT:156:TYR:C   | 2.97                     | 0.42              |
| 50:Le:87:VAL:HG23 | 62:Lr:34:ALA:HB1  | 2.01                     | 0.42              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 66:SF:91:ARG:NH2  | 77:SZ:105:ALA:HB3  | 2.28                     | 0.42              |
| 66:SF:123:GLU:OE1 | 66:SF:138:ALA:HB1  | 2.18                     | 0.42              |
| 66:SF:204:ARG:NH2 | 73:Sc:63:ARG:HA    | 2.34                     | 0.42              |
| 67:SK:23:ALA:HB3  | 67:SK:69:TRP:HH2   | 1.85                     | 0.42              |
| 69:SQ:10:VAL:HG21 | 69:SQ:94:ALA:HB1   | 2.00                     | 0.42              |
| 75:Sg:20:GLN:OE1  | 75:Sg:69:VAL:HG12  | 2.18                     | 0.42              |
| 77:SZ:112:ASN:O   | 77:SZ:114:LYS:NZ   | 2.40                     | 0.42              |
| 79:S2:108:G:C6    | 79:S2:109:U:C4     | 3.07                     | 0.42              |
| 79:S2:387:C:C2    | 79:S2:388:U:C5     | 3.08                     | 0.42              |
| 79:S2:566:U:H3'   | 79:S2:567:C:H6     | 1.84                     | 0.42              |
| 79:S2:610:G:H2'   | 79:S2:611:G:C8     | 2.52                     | 0.42              |
| 79:S2:824:C:H2'   | 79:S2:825:A:H8     | 1.84                     | 0.42              |
| 79:S2:1501:C:C2   | 79:S2:1502:C:C5    | 3.07                     | 0.42              |
| 83:Ls:170:SER:O   | 83:Ls:173:THR:HG22 | 2.20                     | 0.42              |
| 84:Lt:54:LYS:HA   | 84:Lt:54:LYS:HD2   | 1.60                     | 0.42              |
| 87:IW:119:LYS:HA  | 87:IW:119:LYS:HD3  | 1.77                     | 0.42              |
| 1:cH:82:GLN:OE1   | 1:cH:83:GLN:HG3    | 2.20                     | 0.42              |
| 3:sI:37:LYS:O     | 3:sI:59:ARG:HA     | 2.19                     | 0.42              |
| 3:sI:75:LYS:HE3   | 79:s2:303:C:H4'    | 2.00                     | 0.42              |
| 3:sI:141:ARG:HB3  | 3:sI:145:ILE:HB    | 2.01                     | 0.42              |
| 4:sL:136:LYS:NZ   | 79:s2:385:G:O2'    | 2.52                     | 0.42              |
| 5:sX:33:GLY:O     | 5:sX:37:LYS:HG2    | 2.20                     | 0.42              |
| 6:sG:160:LYS:NZ   | 6:sG:174:PRO:HD3   | 2.34                     | 0.42              |
| 6:sG:201:LYS:HE3  | 6:sG:201:LYS:HB3   | 1.88                     | 0.42              |
| 7:sJ:133:ARG:NH2  | 79:s2:563:G:OP1    | 2.52                     | 0.42              |
| 8:sY:19:GLN:NE2   | 8:sY:85:ASN:HD21   | 2.18                     | 0.42              |
| 8:sY:68:LYS:HD3   | 8:sY:69:THR:N      | 2.35                     | 0.42              |
| 12:sH:142:LYS:HA  | 12:sH:155:LYS:O    | 2.19                     | 0.42              |
| 14:sa:23:CYS:SG   | 14:sa:74:CYS:HB3   | 2.59                     | 0.42              |
| 16:sN:74:ILE:O    | 16:sN:77:SER:OG    | 2.20                     | 0.42              |
| 16:sN:96:VAL:O    | 16:sN:100:LYS:HG2  | 2.19                     | 0.42              |
| 16:sN:99:ARG:HB3  | 16:sN:100:LYS:NZ   | 2.33                     | 0.42              |
| 18:sW:75:ILE:HG22 | 18:sW:126:LEU:O    | 2.19                     | 0.42              |
| 19:sb:68:GLY:HA2  | 79:s2:929:G:H1'    | 2.01                     | 0.42              |
| 23:lB:26:ARG:NH2  | 85:l5:4581:G:OP2   | 2.53                     | 0.42              |
| 24:lC:33:ARG:NH1  | 24:lC:35:ASP:OD2   | 2.52                     | 0.42              |
| 27:lF:46:ARG:HE   | 85:l5:1705:G:H21   | 1.67                     | 0.42              |
| 27:lF:74:MET:HE3  | 27:lF:74:MET:HB2   | 1.64                     | 0.42              |
| 29:lH:68:ALA:O    | 85:l5:4691:A:O2'   | 2.37                     | 0.42              |
| 32:lL:178:ALA:O   | 32:lL:181:SER:OG   | 2.30                     | 0.42              |
| 33:lM:14:TYR:CZ   | 33:lM:22:GLY:HA2   | 2.54                     | 0.42              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 33:IM:125:ASN:OD1 | 33:IM:125:ASN:C    | 2.62                     | 0.42              |
| 34:IN:22:LEU:HD23 | 34:IN:22:LEU:HA    | 1.81                     | 0.42              |
| 34:IN:44:ARG:NH1  | 34:IN:47:LYS:HD3   | 2.34                     | 0.42              |
| 34:IN:120:TRP:CD1 | 34:IN:120:TRP:C    | 2.95                     | 0.42              |
| 36:IP:131:ARG:HG3 | 36:IP:137:ASN:ND2  | 2.34                     | 0.42              |
| 36:IP:138:PRO:HB3 | 36:IP:140:MET:SD   | 2.59                     | 0.42              |
| 37:IQ:25:LEU:HA   | 37:IQ:28:LEU:HD23  | 2.02                     | 0.42              |
| 37:IQ:70:MET:HE1  | 37:IQ:137:VAL:CG2  | 2.41                     | 0.42              |
| 39:IS:50:GLN:HA   | 39:IS:50:GLN:OE1   | 2.20                     | 0.42              |
| 41:IU:52:LYS:NZ   | 41:IU:57:GLY:H     | 2.16                     | 0.42              |
| 42:IV:20:LEU:HD12 | 42:IV:20:LEU:HA    | 1.82                     | 0.42              |
| 42:IV:65:VAL:HG13 | 42:IV:73:ARG:HA    | 2.00                     | 0.42              |
| 43:IX:116:LEU:HG  | 43:IX:117:TYR:CE1  | 2.54                     | 0.42              |
| 44:IY:55:VAL:HG23 | 44:IY:106:ILE:HG22 | 2.01                     | 0.42              |
| 45:IZ:67:LYS:HE2  | 45:IZ:67:LYS:HB3   | 1.78                     | 0.42              |
| 47:lb:41:ARG:NH2  | 85:l5:1492:G:H4'   | 2.30                     | 0.42              |
| 47:lb:45:PHE:CE1  | 85:l5:1815:G:C6    | 3.07                     | 0.42              |
| 50:le:70:LEU:HD21 | 50:le:76:LYS:HG3   | 2.02                     | 0.42              |
| 50:le:75:ARG:N    | 50:le:94:SER:O     | 2.48                     | 0.42              |
| 53:lh:56:ARG:O    | 53:lh:59:THR:OG1   | 2.33                     | 0.42              |
| 54:li:33:LEU:HD12 | 54:li:34:THR:N     | 2.34                     | 0.42              |
| 55:lj:63:ARG:HD3  | 55:lj:65:ARG:HG2   | 2.02                     | 0.42              |
| 55:lj:65:ARG:HA   | 55:lj:65:ARG:HD3   | 1.83                     | 0.42              |
| 60:lo:60:ALA:N    | 85:l5:4372:U:OP1   | 2.52                     | 0.42              |
| 60:lo:61:LYS:HZ3  | 85:l5:4337:C:H42   | 1.62                     | 0.42              |
| 61:lp:58:GLY:O    | 85:l5:2652:G:N2    | 2.39                     | 0.42              |
| 62:lr:69:GLY:HA2  | 62:lr:72:LYS:NZ    | 2.35                     | 0.42              |
| 63:lz:67:VAL:HA   | 63:lz:68:LEU:HA    | 1.74                     | 0.42              |
| 64:sR:67:ARG:HH21 | 79:s2:1375:G:H5''  | 1.83                     | 0.42              |
| 64:sR:92:ASP:OD1  | 64:sR:92:ASP:N     | 2.52                     | 0.42              |
| 65:sD:161:GLY:C   | 65:sD:163:PRO:HD2  | 2.44                     | 0.42              |
| 67:sK:32:HIS:ND1  | 67:sK:34:GLU:OE1   | 2.53                     | 0.42              |
| 67:sK:43:LEU:HD23 | 67:sK:47:LYS:HE2   | 2.02                     | 0.42              |
| 68:sP:23:ASP:HA   | 68:sP:26:LEU:HD23  | 2.02                     | 0.42              |
| 71:sT:114:GLU:O   | 71:sT:121:ARG:HB3  | 2.18                     | 0.42              |
| 74:sd:56:ASP:OD1  | 79:s2:1480:A:H2    | 2.01                     | 0.42              |
| 75:sg:38:LYS:HE2  | 75:sg:38:LYS:HB3   | 1.66                     | 0.42              |
| 75:sg:74:ASP:OD1  | 75:sg:74:ASP:N     | 2.50                     | 0.42              |
| 75:sg:191:HIS:HE2 | 75:sg:211:GLY:N    | 2.17                     | 0.42              |
| 76:sM:25:ALA:O    | 76:sM:29:ASP:N     | 2.52                     | 0.42              |
| 79:s2:394:G:C2    | 79:s2:395:G:C8     | 3.07                     | 0.42              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 79:s2:600:G:C2     | 79:s2:601:G:C5    | 3.07                     | 0.42              |
| 79:s2:806:U:C2     | 79:s2:807:G:C8    | 3.08                     | 0.42              |
| 79:s2:964:A:H2'    | 79:s2:965:U:H6    | 1.84                     | 0.42              |
| 79:s2:1364:U:C4    | 79:s2:1365:G:C5   | 3.08                     | 0.42              |
| 79:s2:1500:G:H2'   | 79:s2:1501:C:H6   | 1.85                     | 0.42              |
| 80:cB:56:PHE:HA    | 80:cB:456:ARG:NE  | 2.34                     | 0.42              |
| 80:cB:63:GLU:O     | 80:cB:67:CYS:N    | 2.52                     | 0.42              |
| 80:cB:746:LEU:HD13 | 80:cB:771:PHE:HZ  | 1.84                     | 0.42              |
| 84:lt:9:GLU:HG2    | 84:lt:9:GLU:O     | 2.19                     | 0.42              |
| 84:lt:104:ILE:HB   | 84:lt:106:PHE:CE2 | 2.54                     | 0.42              |
| 85:l5:929:A:H2'    | 85:l5:930:G:C8    | 2.55                     | 0.42              |
| 85:l5:947:C:H2'    | 85:l5:948:C:C6    | 2.54                     | 0.42              |
| 85:l5:1415:G:H2'   | 85:l5:1416:G:H8   | 1.84                     | 0.42              |
| 85:l5:1416:G:H2'   | 85:l5:1417:C:C6   | 2.54                     | 0.42              |
| 85:l5:1614:C:H2'   | 85:l5:1615:C:C6   | 2.54                     | 0.42              |
| 85:l5:1709:C:O2    | 85:l5:1716:G:O6   | 2.37                     | 0.42              |
| 85:l5:1754:U:H2'   | 85:l5:1755:C:C6   | 2.53                     | 0.42              |
| 85:l5:1839:U:H2'   | 85:l5:1840:G:C8   | 2.54                     | 0.42              |
| 85:l5:2897:G:C4    | 85:l5:3603:G:N2   | 2.86                     | 0.42              |
| 85:l5:3947:A:N1    | 85:l5:4068:U:H1'  | 2.34                     | 0.42              |
| 85:l5:4343:U:H2'   | 85:l5:4344:U:C6   | 2.54                     | 0.42              |
| 85:l5:4411:G:H2'   | 85:l5:4412:C:H6   | 1.82                     | 0.42              |
| 80:CB:353:MET:HE2  | 80:CB:353:MET:C   | 2.45                     | 0.42              |
| 80:CB:748:GLU:HB3  | 80:CB:811:GLN:HB3 | 2.01                     | 0.42              |
| 80:CB:775:GLN:HG2  | 80:CB:782:PHE:CE1 | 2.53                     | 0.42              |
| 2:SE:90:ILE:O      | 2:SE:99:PHE:N     | 2.52                     | 0.42              |
| 3:SI:92:ARG:NH1    | 85:L5:3611:A:O3'  | 2.51                     | 0.42              |
| 4:SL:94:HIS:HB2    | 4:SL:105:ARG:HD2  | 2.01                     | 0.42              |
| 11:SB:71:LEU:HD12  | 11:SB:71:LEU:HA   | 1.88                     | 0.42              |
| 13:SV:74:LYS:HE3   | 13:SV:74:LYS:HA   | 2.02                     | 0.42              |
| 14:Sa:41:ILE:O     | 14:Sa:67:LEU:HG   | 2.18                     | 0.42              |
| 14:Sa:50:VAL:O     | 14:Sa:54:SER:N    | 2.41                     | 0.42              |
| 15:SC:113:GLN:O    | 15:SC:114:LYS:HD2 | 2.19                     | 0.42              |
| 17:SO:35:ALA:O     | 17:SO:109:GLY:N   | 2.50                     | 0.42              |
| 85:L5:323:C:H2'    | 85:L5:324:A:C8    | 2.51                     | 0.42              |
| 85:L5:921:C:H2'    | 85:L5:922:C:H6    | 1.83                     | 0.42              |
| 85:L5:1405:C:N3    | 85:L5:1413:C:N4   | 2.66                     | 0.42              |
| 85:L5:1730:U:O3'   | 40:LT:100:LYS:NZ  | 2.51                     | 0.42              |
| 85:L5:1843:A:H2'   | 85:L5:1844:G:H8   | 1.84                     | 0.42              |
| 85:L5:2705:G:H2'   | 85:L5:2706:G:C8   | 2.54                     | 0.42              |
| 85:L5:2752:G:C6    | 85:L5:2753:G:C6   | 3.07                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 85:L5:2892:C:H5    | 38:LR:74:ARG:NH1   | 2.13                     | 0.42              |
| 85:L5:4110:C:C3'   | 85:L5:4111:U:H3'   | 2.48                     | 0.42              |
| 85:L5:4121:G:N2    | 22:LA:46:LYS:HA    | 2.34                     | 0.42              |
| 85:L5:4122:G:C5    | 85:L5:4123:C:C5    | 3.08                     | 0.42              |
| 85:L5:4174:U:H2'   | 85:L5:4175:G:C8    | 2.40                     | 0.42              |
| 85:L5:4240:G:H2'   | 85:L5:4241:C:C6    | 2.55                     | 0.42              |
| 85:L5:4361:U:H2'   | 85:L5:4362:A:C8    | 2.54                     | 0.42              |
| 85:L5:4592:C:H2'   | 85:L5:4593:C:H6    | 1.84                     | 0.42              |
| 85:L5:4673:U:H2'   | 85:L5:4674:C:H6    | 1.84                     | 0.42              |
| 85:L5:5050:C:C2    | 85:L5:5051:C:C5    | 3.07                     | 0.42              |
| 20:L7:49:A:H3'     | 25:LD:225:GLN:HE21 | 1.84                     | 0.42              |
| 21:L8:65:A:C6      | 21:L8:66:A:C5      | 3.08                     | 0.42              |
| 21:L8:67:U:H2'     | 21:L8:68:G:C8      | 2.55                     | 0.42              |
| 23:LB:356:LYS:HD3  | 23:LB:356:LYS:HA   | 1.73                     | 0.42              |
| 24:LC:212:ASN:ND2  | 24:LC:213:GLU:OE2  | 2.51                     | 0.42              |
| 25:LD:52:ILE:HB    | 25:LD:63:GLN:HG2   | 2.01                     | 0.42              |
| 31:LJ:95:ARG:HG2   | 31:LJ:96:LYS:H     | 1.84                     | 0.42              |
| 31:LJ:104:ASN:CG   | 31:LJ:133:VAL:HG12 | 2.45                     | 0.42              |
| 34:LN:143:ARG:H    | 34:LN:143:ARG:HG2  | 1.61                     | 0.42              |
| 35:LO:109:PRO:HA   | 35:LO:110:PRO:HD3  | 1.90                     | 0.42              |
| 37:LQ:91:ARG:O     | 37:LQ:93:GLN:NE2   | 2.53                     | 0.42              |
| 38:LR:23:TRP:HB2   | 38:LR:53:LYS:HG3   | 2.00                     | 0.42              |
| 38:LR:131:VAL:HG23 | 38:LR:132:PHE:CD2  | 2.54                     | 0.42              |
| 39:LS:143:LYS:HA   | 39:LS:146:HIS:CD2  | 2.55                     | 0.42              |
| 41:LU:40:GLU:OE2   | 41:LU:65:ARG:HB3   | 2.20                     | 0.42              |
| 45:LZ:83:THR:HA    | 48:Lc:62:TYR:OH    | 2.18                     | 0.42              |
| 48:Lc:13:SER:O     | 48:Lc:17:ARG:HG2   | 2.19                     | 0.42              |
| 54:Li:58:MET:HA    | 54:Li:61:LEU:CG    | 2.50                     | 0.42              |
| 55:Lj:34:CYS:SG    | 55:Lj:36:LYS:N     | 2.92                     | 0.42              |
| 60:Lo:56:PHE:O     | 60:Lo:58:LYS:HG2   | 2.20                     | 0.42              |
| 61:Lp:26:VAL:HA    | 61:Lp:29:ILE:HG22  | 2.00                     | 0.42              |
| 63:Lz:68:LEU:HD13  | 63:Lz:90:LEU:HB2   | 2.01                     | 0.42              |
| 64:SR:5:ARG:HH12   | 79:S2:1454:A:H5''  | 1.83                     | 0.42              |
| 74:Sd:14:PHE:HZ    | 79:S2:1617:G:HO2'  | 1.63                     | 0.42              |
| 75:Sg:10:THR:HB    | 75:Sg:306:LEU:HD22 | 2.01                     | 0.42              |
| 75:Sg:178:ASN:ND2  | 75:Sg:181:ASN:H    | 2.17                     | 0.42              |
| 77:SZ:52:LYS:O     | 77:SZ:52:LYS:HD3   | 2.20                     | 0.42              |
| 78:Sf:145:CYS:O    | 78:Sf:146:LEU:HD23 | 2.19                     | 0.42              |
| 79:S2:15:U:H2'     | 79:S2:16:G:O4'     | 2.20                     | 0.42              |
| 79:S2:945:U:H2'    | 79:S2:946:U:H6     | 1.83                     | 0.42              |
| 79:S2:1218:C:H2'   | 79:S2:1219:C:H6    | 1.83                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 79:S2:1278:A:H2'   | 79:S2:1279:C:H6    | 1.83                     | 0.42              |
| 79:S2:1424:G:H3'   | 79:S2:1425:G:H8    | 1.84                     | 0.42              |
| 79:S2:1532:C:H3'   | 79:S2:1637:A:H62   | 1.84                     | 0.42              |
| 1:CH:130:LEU:HD11  | 1:CH:138:GLY:CA    | 2.50                     | 0.42              |
| 1:CH:143:LYS:HD2   | 1:CH:143:LYS:HA    | 1.80                     | 0.42              |
| 2:sE:17:HIS:CE1    | 2:sE:18:TRP:CZ3    | 3.08                     | 0.42              |
| 5:sX:8:ARG:O       | 79:s2:681:U:H5''   | 2.19                     | 0.42              |
| 5:sX:107:ARG:HE    | 5:sX:107:ARG:HB2   | 1.39                     | 0.42              |
| 5:sX:130:LEU:HA    | 5:sX:133:LEU:HD13  | 2.00                     | 0.42              |
| 6:sG:195:LYS:O     | 6:sG:198:ARG:HG2   | 2.19                     | 0.42              |
| 10:sA:39:TYR:CD1   | 10:sA:40:LYS:HB3   | 2.54                     | 0.42              |
| 11:sB:84:PHE:HB3   | 11:sB:86:LEU:HD13  | 2.02                     | 0.42              |
| 12:sH:60:ILE:O     | 12:sH:92:VAL:HA    | 2.19                     | 0.42              |
| 13:sV:32:ILE:HD12  | 13:sV:32:ILE:HA    | 1.40                     | 0.42              |
| 16:sN:16:LEU:HD22  | 16:sN:62:GLN:HG3   | 2.01                     | 0.42              |
| 16:sN:89:TYR:HE1   | 16:sN:150:VAL:HA   | 1.84                     | 0.42              |
| 16:sN:100:LYS:HA   | 16:sN:100:LYS:HD3  | 1.77                     | 0.42              |
| 20:l7:29:C:OP1     | 31:lJ:138:GLY:N    | 2.52                     | 0.42              |
| 20:l7:43:U:OP1     | 31:lJ:140:SER:OG   | 2.29                     | 0.42              |
| 20:l7:73:U:O5'     | 20:l7:74:A:H2'     | 2.20                     | 0.42              |
| 22:lA:108:PRO:HG2  | 61:lp:86:LEU:HD13  | 2.00                     | 0.42              |
| 22:lA:175:ILE:HD11 | 85:l5:3683:C:C1'   | 2.49                     | 0.42              |
| 23:lB:66:LYS:HD2   | 42:lV:12:ALA:O     | 2.19                     | 0.42              |
| 24:lC:196:MET:SD   | 24:lC:196:MET:C    | 3.03                     | 0.42              |
| 24:lC:317:ASN:HB2  | 85:l5:716:C:P      | 2.59                     | 0.42              |
| 24:lC:324:ILE:HD13 | 24:lC:324:ILE:HA   | 1.87                     | 0.42              |
| 28:lG:75:LYS:HD2   | 28:lG:240:ASN:HD22 | 1.84                     | 0.42              |
| 29:lH:180:TYR:HB3  | 58:lm:89:TYR:CD1   | 2.54                     | 0.42              |
| 31:lJ:17:ILE:HD11  | 31:lJ:165:TRP:CZ2  | 2.55                     | 0.42              |
| 32:lL:103:ARG:NH1  | 85:l5:75:G:O6      | 2.53                     | 0.42              |
| 33:lM:7:VAL:HG21   | 39:lS:154:LEU:CD2  | 2.50                     | 0.42              |
| 36:lP:67:VAL:HB    | 36:lP:80:GLN:NE2   | 2.34                     | 0.42              |
| 37:lQ:128:LEU:HD23 | 37:lQ:128:LEU:HA   | 1.86                     | 0.42              |
| 39:lS:160:ARG:HA   | 39:lS:162:GLN:NE2  | 2.35                     | 0.42              |
| 40:lT:18:PRO:HB2   | 40:lT:21:LYS:HD2   | 2.01                     | 0.42              |
| 40:lT:158:PHE:CE1  | 40:lT:160:ALA:C    | 2.97                     | 0.42              |
| 41:lU:26:THR:O     | 41:lU:29:VAL:HG22  | 2.19                     | 0.42              |
| 41:lU:89:LYS:NZ    | 85:l5:2630:U:O4    | 2.45                     | 0.42              |
| 43:lX:143:ASP:OD2  | 43:lX:143:ASP:C    | 2.62                     | 0.42              |
| 45:lZ:6:LYS:HA     | 45:lZ:6:LYS:HD3    | 1.87                     | 0.42              |
| 46:la:133:ALA:O    | 46:la:137:ILE:HG22 | 2.20                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 47:lb:112:ILE:O    | 47:lb:116:LEU:HD23 | 2.18                     | 0.42              |
| 58:lm:94:MET:HE1   | 58:lm:122:ARG:C    | 2.45                     | 0.42              |
| 60:lo:58:LYS:HA    | 60:lo:58:LYS:HD3   | 1.80                     | 0.42              |
| 62:lr:47:LYS:HB3   | 62:lr:102:TYR:CZ   | 2.54                     | 0.42              |
| 64:sR:3:ARG:HD2    | 79:s2:1367:U:H5''  | 2.01                     | 0.42              |
| 64:sR:53:TYR:HB2   | 79:s2:1466:G:O5'   | 2.18                     | 0.42              |
| 64:sR:57:LEU:HG    | 79:s2:1465:A:H5'   | 2.02                     | 0.42              |
| 66:sF:175:ASP:OD2  | 66:sF:176:GLU:N    | 2.52                     | 0.42              |
| 67:sK:11:ILE:HG13  | 67:sK:12:TYR:HD1   | 1.83                     | 0.42              |
| 67:sK:67:PHE:HB2   | 67:sK:69:TRP:CH2   | 2.54                     | 0.42              |
| 69:sQ:113:ILE:HD12 | 69:sQ:113:ILE:HA   | 1.85                     | 0.42              |
| 74:sd:33:LYS:HE3   | 79:s2:1658:G:H5'   | 2.00                     | 0.42              |
| 75:sg:44:LYS:HG3   | 75:sg:56:GLN:OE1   | 2.19                     | 0.42              |
| 76:sM:22:LEU:HD21  | 76:sM:88:TRP:CE3   | 2.54                     | 0.42              |
| 77:sZ:96:LEU:HD23  | 77:sZ:97:ILE:HG12  | 2.02                     | 0.42              |
| 79:s2:475:C:C4     | 79:s2:476:A:N7     | 2.87                     | 0.42              |
| 79:s2:676:C:H2'    | 79:s2:677:G:O4'    | 2.19                     | 0.42              |
| 79:s2:1364:U:C2    | 79:s2:1365:G:C8    | 3.08                     | 0.42              |
| 79:s2:1367:U:O5'   | 79:s2:1367:U:H6    | 2.03                     | 0.42              |
| 80:cB:27:HIS:ND1   | 80:cB:28:VAL:HG22  | 2.34                     | 0.42              |
| 80:cB:252:LYS:HA   | 80:cB:255:ASP:OD2  | 2.19                     | 0.42              |
| 80:cB:600:ASN:HA   | 80:cB:708:THR:O    | 2.20                     | 0.42              |
| 85:l5:280:G:H1'    | 85:l5:305:A:N1     | 2.33                     | 0.42              |
| 85:l5:1168:G:C6    | 85:l5:1194:G:C6    | 3.07                     | 0.42              |
| 85:l5:2286:G:H2'   | 85:l5:2287:G:H8    | 1.84                     | 0.42              |
| 85:l5:2532:C:C2    | 85:l5:2533:C:C5    | 3.08                     | 0.42              |
| 85:l5:2538:U:H2'   | 85:l5:2539:C:H6    | 1.85                     | 0.42              |
| 85:l5:2610:G:H2'   | 85:l5:2611:A:H8    | 1.84                     | 0.42              |
| 85:l5:2750:G:C4    | 85:l5:2751:G:C8    | 3.07                     | 0.42              |
| 85:l5:2844:A:O2'   | 85:l5:4631:G:H4'   | 2.20                     | 0.42              |
| 85:l5:3615:G:H1'   | 87:IW:44:ARG:HD2   | 2.01                     | 0.42              |
| 85:l5:3772:U:H2'   | 85:l5:3773:U:H5''  | 2.01                     | 0.42              |
| 85:l5:3824:A:H2'   | 85:l5:3825:A:H8    | 1.85                     | 0.42              |
| 85:l5:3867:A:C2    | 85:l5:3880:G:C6    | 3.07                     | 0.42              |
| 85:l5:3951:G:C2    | 85:l5:4062:A:N1    | 2.87                     | 0.42              |
| 85:l5:4627:U:C4    | 85:l5:4628:U:C4    | 3.07                     | 0.42              |
| 85:l5:4893:A:H2'   | 85:l5:4894:A:C8    | 2.54                     | 0.42              |
| 85:l5:5059:C:H2'   | 85:l5:5060:A:C8    | 2.55                     | 0.42              |
| 80:CB:12:ILE:HG21  | 80:CB:99:LEU:HB2   | 2.01                     | 0.42              |
| 80:CB:14:ASP:OD1   | 80:CB:15:LYS:N     | 2.53                     | 0.42              |
| 80:CB:162:ARG:NH2  | 85:L5:4601:U:O3'   | 2.52                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 80:CB:182:VAL:HG22 | 80:CB:186:ASN:ND2  | 2.33                     | 0.42              |
| 80:CB:369:CYS:SG   | 80:CB:386:LYS:HG3  | 2.59                     | 0.42              |
| 80:CB:372:LEU:C    | 80:CB:495:ARG:HD2  | 2.45                     | 0.42              |
| 80:CB:422:SER:HB2  | 80:CB:425:LEU:HD11 | 2.02                     | 0.42              |
| 2:SE:18:TRP:NE1    | 2:SE:41:CYS:O      | 2.45                     | 0.42              |
| 2:SE:164:LEU:C     | 2:SE:166:THR:N     | 2.77                     | 0.42              |
| 2:SE:246:LEU:HB2   | 2:SE:250:GLU:HG3   | 2.02                     | 0.42              |
| 4:SL:4:ILE:HG21    | 4:SL:55:TYR:HA     | 2.01                     | 0.42              |
| 4:SL:84:ARG:HG2    | 4:SL:112:HIS:CE1   | 2.54                     | 0.42              |
| 6:SG:138:ALA:HB3   | 6:SG:178:ARG:O     | 2.19                     | 0.42              |
| 11:SB:140:VAL:HG23 | 11:SB:213:ARG:HD2  | 2.01                     | 0.42              |
| 12:SH:84:GLU:OE1   | 12:SH:91:HIS:HA    | 2.19                     | 0.42              |
| 14:Sa:52:ASP:OD2   | 14:Sa:53:ILE:N     | 2.46                     | 0.42              |
| 14:Sa:73:TYR:HE1   | 14:Sa:83:VAL:HG21  | 1.82                     | 0.42              |
| 15:SC:173:LYS:H    | 15:SC:173:LYS:HG2  | 1.68                     | 0.42              |
| 17:SO:43:HIS:HE1   | 79:S2:974:C:O2     | 2.02                     | 0.42              |
| 17:SO:131:ASP:OD2  | 17:SO:131:ASP:C    | 2.62                     | 0.42              |
| 85:L5:14:C:O4'     | 43:LX:54:LEU:HD21  | 2.19                     | 0.42              |
| 85:L5:154:G:C4'    | 53:Lh:105:LYS:HZ1  | 2.32                     | 0.42              |
| 85:L5:163:A:H2'    | 85:L5:164:G:C8     | 2.54                     | 0.42              |
| 85:L5:199:G:C4     | 85:L5:201:C:C5     | 3.07                     | 0.42              |
| 85:L5:666:G:H2'    | 85:L5:668:C:OP1    | 2.19                     | 0.42              |
| 85:L5:1628:C:H3'   | 22:LA:9:ARG:HH22   | 1.85                     | 0.42              |
| 85:L5:1661:C:H5''  | 85:L5:2345:G:O2'   | 2.20                     | 0.42              |
| 85:L5:1730:U:H2'   | 85:L5:1731:C:C6    | 2.55                     | 0.42              |
| 85:L5:1972:G:C6    | 85:L5:1995:G:C6    | 3.07                     | 0.42              |
| 85:L5:2423:A:H2'   | 85:L5:2424:G:C8    | 2.54                     | 0.42              |
| 85:L5:2539:C:H2'   | 85:L5:2540:C:H6    | 1.84                     | 0.42              |
| 85:L5:2682:G:H2'   | 85:L5:2683:C:H6    | 1.84                     | 0.42              |
| 85:L5:3641:U:H5    | 85:L5:3646:A:N7    | 2.18                     | 0.42              |
| 85:L5:3932:U:H2'   | 85:L5:3933:G:H8    | 1.84                     | 0.42              |
| 85:L5:3933:G:H2'   | 85:L5:3934:G:H8    | 1.84                     | 0.42              |
| 85:L5:4147:G:H2'   | 85:L5:4148:C:H6    | 1.84                     | 0.42              |
| 85:L5:4160:C:H2'   | 85:L5:4161:G:H8    | 1.83                     | 0.42              |
| 85:L5:4474:A:OP1   | 58:Lm:124:LYS:HG3  | 2.20                     | 0.42              |
| 85:L5:4504:C:H2'   | 85:L5:4505:C:H6    | 1.83                     | 0.42              |
| 85:L5:4699:U:H4'   | 85:L5:4700:A:OP1   | 2.19                     | 0.42              |
| 85:L5:4957:C:H2'   | 85:L5:4958:C:H6    | 1.84                     | 0.42              |
| 20:L7:24:C:H2'     | 20:L7:25:G:O4'     | 2.20                     | 0.42              |
| 22:LA:225:ILE:HG22 | 22:LA:237:LEU:O    | 2.19                     | 0.42              |
| 22:LA:237:LEU:HG   | 22:LA:240:ALA:HB2  | 2.02                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:LB:223:THR:HG23 | 23:LB:275:HIS:O    | 2.19                     | 0.42              |
| 24:LC:121:ARG:HD2  | 24:LC:277:TYR:CD1  | 2.55                     | 0.42              |
| 25:LD:69:ILE:H     | 25:LD:69:ILE:HG12  | 1.71                     | 0.42              |
| 26:LE:209:PRO:HD2  | 26:LE:212:LEU:HD11 | 2.00                     | 0.42              |
| 27:LF:66:ARG:O     | 27:LF:69:ILE:HG12  | 2.18                     | 0.42              |
| 28:LG:156:VAL:HG22 | 28:LG:202:VAL:HB   | 2.00                     | 0.42              |
| 29:LH:1:MET:HE1    | 29:LH:3:THR:HA     | 2.00                     | 0.42              |
| 30:LI:43:VAL:O     | 30:LI:171:TRP:NE1  | 2.49                     | 0.42              |
| 30:LI:143:GLN:HG2  | 30:LI:144:ASN:OD1  | 2.19                     | 0.42              |
| 30:LI:210:ARG:HB2  | 30:LI:210:ARG:NH1  | 2.33                     | 0.42              |
| 38:LR:89:MET:SD    | 38:LR:89:MET:N     | 2.92                     | 0.42              |
| 39:LS:80:ILE:HB    | 39:LS:129:VAL:HG22 | 2.00                     | 0.42              |
| 45:LZ:122:TYR:HB2  | 45:LZ:131:PHE:CE1  | 2.54                     | 0.42              |
| 49:Ld:27:ILE:HD11  | 49:Ld:52:PHE:CE1   | 2.55                     | 0.42              |
| 52:Lg:99:GLU:OE1   | 52:Lg:100:GLN:N    | 2.53                     | 0.42              |
| 57:Ll:41:ARG:HA    | 57:Ll:41:ARG:HD2   | 1.80                     | 0.42              |
| 65:SD:1:MET:O      | 65:SD:4:GLN:HG2    | 2.19                     | 0.42              |
| 65:SD:96:LEU:HD12  | 65:SD:96:LEU:HA    | 1.78                     | 0.42              |
| 65:SD:138:VAL:O    | 65:SD:149:SER:HA   | 2.19                     | 0.42              |
| 70:SS:13:LEU:HB2   | 70:SS:20:ILE:HG13  | 2.02                     | 0.42              |
| 71:ST:20:ALA:HB1   | 71:ST:24:LYS:HZ1   | 1.83                     | 0.42              |
| 71:ST:126:GLN:HA   | 71:ST:129:ARG:HB3  | 2.00                     | 0.42              |
| 72:SU:23:THR:HA    | 72:SU:88:LEU:HA    | 2.00                     | 0.42              |
| 75:Sg:79:LEU:CD1   | 75:Sg:113:PHE:HE1  | 2.32                     | 0.42              |
| 75:Sg:172:LYS:CA   | 75:Sg:194:TYR:HA   | 2.49                     | 0.42              |
| 75:Sg:217:MET:HA   | 75:Sg:229:THR:HA   | 1.99                     | 0.42              |
| 79:S2:322:C:C2     | 79:S2:330:G:N2     | 2.87                     | 0.42              |
| 79:S2:420:G:O2'    | 79:S2:421:G:OP1    | 2.33                     | 0.42              |
| 79:S2:559:G:N3     | 79:S2:560:A:C8     | 2.87                     | 0.42              |
| 79:S2:651:U:H2'    | 79:S2:652:U:H6     | 1.84                     | 0.42              |
| 79:S2:946:U:C2     | 79:S2:947:G:C8     | 3.08                     | 0.42              |
| 79:S2:1243:U:H2'   | 79:S2:1244:U:O4'   | 2.19                     | 0.42              |
| 79:S2:1700:C:C2    | 79:S2:1702:G:C5    | 3.08                     | 0.42              |
| 79:S2:1701:C:N3    | 82:PE:34:U:H1'     | 2.35                     | 0.42              |
| 79:S2:1758:G:O6    | 79:S2:1772:C:N4    | 2.52                     | 0.42              |
| 81:AP:41:G:H2'     | 81:AP:42:A:C8      | 2.54                     | 0.42              |
| 83:Ls:66:ARG:HB2   | 83:Ls:79:LEU:HD11  | 2.00                     | 0.42              |
| 83:Ls:161:ILE:HD12 | 83:Ls:161:ILE:HA   | 1.90                     | 0.42              |
| 87:IW:90:ILE:HA    | 87:IW:93:LYS:NZ    | 2.32                     | 0.42              |
| 1:cH:43:LYS:NZ     | 1:cH:44:TRP:HB2    | 2.34                     | 0.42              |
| 2:sE:240:ARG:HG2   | 2:sE:241:GLY:N     | 2.34                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:sI:3:ILE:HG22    | 3:sI:30:GLY:HA3    | 2.01                     | 0.42              |
| 3:sI:12:ARG:NH1    | 79:s2:103:A:H5'    | 2.35                     | 0.42              |
| 4:sL:125:ILE:HD12  | 4:sL:148:ALA:HB2   | 2.02                     | 0.42              |
| 10:sA:120:ARG:HE   | 15:sC:65:LYS:HZ3   | 1.67                     | 0.42              |
| 12:sH:78:ARG:HA    | 12:sH:78:ARG:HD2   | 1.84                     | 0.42              |
| 13:sV:43:THR:HG23  | 13:sV:45:ARG:H     | 1.85                     | 0.42              |
| 15:sC:75:ILE:HD11  | 15:sC:80:GLU:OE1   | 2.19                     | 0.42              |
| 15:sC:206:SER:OG   | 15:sC:207:ALA:O    | 2.37                     | 0.42              |
| 16:sN:71:ILE:HG13  | 16:sN:72:LEU:HD12  | 2.02                     | 0.42              |
| 20:l7:47:G:H4'     | 25:lD:204:VAL:HG12 | 2.01                     | 0.42              |
| 20:l7:71:G:C6      | 20:l7:72:U:N3      | 2.88                     | 0.42              |
| 21:l8:109:C:C4     | 55:lJ:20:ARG:NH2   | 2.84                     | 0.42              |
| 22:lA:9:ARG:HD2    | 85:l5:1628:C:OP2   | 2.18                     | 0.42              |
| 27:lF:44:LYS:HZ2   | 27:lF:44:LYS:HG2   | 1.72                     | 0.42              |
| 27:lF:104:LYS:O    | 27:lF:108:VAL:HG12 | 2.19                     | 0.42              |
| 27:lF:238:ASP:N    | 27:lF:238:ASP:OD2  | 2.52                     | 0.42              |
| 28:lG:162:ASP:C    | 28:lG:162:ASP:OD2  | 2.62                     | 0.42              |
| 31:lJ:24:ILE:HD13  | 31:lJ:127:GLY:O    | 2.19                     | 0.42              |
| 35:lO:178:ARG:O    | 35:lO:181:ALA:HB3  | 2.20                     | 0.42              |
| 48:lC:32:LYS:HE2   | 85:l5:2675:G:C4    | 2.54                     | 0.42              |
| 51:lF:9:ALA:HB3    | 51:lF:101:ILE:HG23 | 2.01                     | 0.42              |
| 53:lH:15:GLU:C     | 53:lH:15:GLU:OE2   | 2.62                     | 0.42              |
| 56:lK:54:GLU:OE2   | 56:lK:57:LYS:HD3   | 2.19                     | 0.42              |
| 58:lM:79:GLU:CD    | 58:lM:81:SER:H     | 2.23                     | 0.42              |
| 64:sR:53:TYR:CB    | 79:s2:1465:A:H3'   | 2.49                     | 0.42              |
| 64:sR:53:TYR:CE1   | 79:s2:1466:G:C5    | 3.08                     | 0.42              |
| 65:sD:65:ARG:HA    | 65:sD:68:GLU:OE1   | 2.19                     | 0.42              |
| 67:sK:1:MET:CG     | 67:sK:47:LYS:HD2   | 2.44                     | 0.42              |
| 67:sK:24:LYS:NZ    | 67:sK:65:ARG:HD2   | 2.34                     | 0.42              |
| 69:sQ:11:GLN:HG3   | 69:sQ:24:HIS:CD2   | 2.54                     | 0.42              |
| 69:sQ:20:THR:HG21  | 79:s2:1444:U:OP1   | 2.19                     | 0.42              |
| 70:sS:106:LYS:HD2  | 70:sS:106:LYS:HA   | 1.85                     | 0.42              |
| 71:sT:134:ILE:HA   | 71:sT:137:GLN:CD   | 2.44                     | 0.42              |
| 74:sd:10:HIS:ND1   | 74:sd:12:ARG:NH1   | 2.67                     | 0.42              |
| 75:sg:66:VAL:HA    | 75:sg:82:SER:HA    | 2.02                     | 0.42              |
| 75:sg:235:ILE:HD12 | 75:sg:236:ILE:N    | 2.34                     | 0.42              |
| 76:sM:19:GLN:OE1   | 76:sM:22:LEU:HD11  | 2.20                     | 0.42              |
| 76:sM:42:LEU:C     | 76:sM:42:LEU:HD23  | 2.44                     | 0.42              |
| 79:s2:480:G:C5     | 79:s2:481:C:C4     | 3.08                     | 0.42              |
| 79:s2:881:G:C2     | 79:s2:906:U:C2     | 3.07                     | 0.42              |
| 79:s2:1589:A:C4    | 79:s2:1590:C:C6    | 3.08                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 79:s2:1688:C:H2'   | 79:s2:1689:C:C6    | 2.54                     | 0.42              |
| 80:cB:19:ILE:O     | 80:cB:20:ARG:HD2   | 2.19                     | 0.42              |
| 80:cB:135:VAL:N    | 80:cB:181:ILE:HD11 | 2.35                     | 0.42              |
| 80:cB:259:LYS:HE2  | 80:cB:273:PHE:CD2  | 2.54                     | 0.42              |
| 80:cB:406:ASP:O    | 80:cB:407:LYS:HB3  | 2.18                     | 0.42              |
| 80:cB:481:LYS:H    | 80:cB:529:LYS:HD2  | 1.85                     | 0.42              |
| 81:aP:66:C:H5'     | 81:aP:67:G:OP2     | 2.19                     | 0.42              |
| 82:pE:48:C:OP2     | 82:pE:48:C:H4'     | 2.19                     | 0.42              |
| 82:pE:52:G:H3'     | 82:pE:53:G:H8      | 1.84                     | 0.42              |
| 85:l5:221:C:C2     | 85:l5:222:C:C5     | 3.07                     | 0.42              |
| 85:l5:271:C:C2     | 85:l5:272:U:C5     | 3.07                     | 0.42              |
| 85:l5:400:A:H2'    | 85:l5:401:G:O4'    | 2.19                     | 0.42              |
| 85:l5:1094:G:C5    | 85:l5:1203:G:C2    | 3.07                     | 0.42              |
| 85:l5:1170:G:H2'   | 85:l5:1171:G:C8    | 2.55                     | 0.42              |
| 85:l5:1354:A:N6    | 85:l5:1503:A:O4'   | 2.53                     | 0.42              |
| 85:l5:1449:C:H2'   | 85:l5:1450:C:H6    | 1.84                     | 0.42              |
| 85:l5:1554:A:H61   | 85:l5:1573:G:H1'   | 1.82                     | 0.42              |
| 85:l5:1554:A:N6    | 85:l5:1573:G:O2'   | 2.52                     | 0.42              |
| 85:l5:1601:A:N7    | 85:l5:3643:A:C4    | 2.86                     | 0.42              |
| 85:l5:1789:C:H2'   | 85:l5:1790:U:C6    | 2.54                     | 0.42              |
| 85:l5:2693:G:H2'   | 85:l5:2694:G:N2    | 2.34                     | 0.42              |
| 85:l5:2759:G:O2'   | 85:l5:2760:G:O4'   | 2.22                     | 0.42              |
| 85:l5:2862:G:C2    | 85:l5:3624:A:C4    | 3.07                     | 0.42              |
| 85:l5:4146:G:H2'   | 85:l5:4147:G:C8    | 2.55                     | 0.42              |
| 85:l5:4458:C:H2'   | 85:l5:4459:U:H6    | 1.84                     | 0.42              |
| 2:SE:94:LYS:CE     | 8:SY:16:ARG:HB2    | 2.49                     | 0.42              |
| 2:SE:199:GLU:HB3   | 2:SE:207:VAL:HG12  | 2.01                     | 0.42              |
| 5:SX:22:TRP:O      | 5:SX:28:LYS:HE2    | 2.19                     | 0.42              |
| 6:SG:195:LYS:O     | 6:SG:199:THR:HG22  | 2.19                     | 0.42              |
| 7:SJ:125:HIS:O     | 7:SJ:128:VAL:HG12  | 2.19                     | 0.42              |
| 10:SA:5:LEU:HB2    | 10:SA:8:LEU:HG     | 2.00                     | 0.42              |
| 10:SA:90:PHE:CE2   | 10:SA:94:THR:HG21  | 2.55                     | 0.42              |
| 10:SA:159:ILE:HG22 | 10:SA:159:ILE:O    | 2.19                     | 0.42              |
| 11:SB:166:LYS:O    | 11:SB:170:GLU:HG3  | 2.18                     | 0.42              |
| 12:SH:95:ILE:HD13  | 12:SH:95:ILE:HA    | 1.86                     | 0.42              |
| 13:SV:18:SER:N     | 13:SV:54:ALA:O     | 2.51                     | 0.42              |
| 15:SC:88:ILE:HG23  | 15:SC:160:LEU:HD13 | 2.01                     | 0.42              |
| 15:SC:91:SER:HB2   | 15:SC:159:LYS:HE2  | 2.02                     | 0.42              |
| 18:SW:80:ASP:OD1   | 79:S2:803:C:H4'    | 2.19                     | 0.42              |
| 85:L5:125:C:H2'    | 85:L5:126:C:C6     | 2.54                     | 0.42              |
| 85:L5:171:U:H5''   | 85:L5:172:C:C5     | 2.54                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 85:L5:500:G:N3     | 85:L5:504:G:H2'    | 2.34                     | 0.42              |
| 85:L5:743:G:N1     | 85:L5:922:C:N3     | 2.68                     | 0.42              |
| 85:L5:1071:C:C5    | 26:LE:67:ALA:HB2   | 2.54                     | 0.42              |
| 85:L5:1520:C:H2'   | 85:L5:1521:C:H6    | 1.84                     | 0.42              |
| 85:L5:2508:U:H2'   | 85:L5:2509:C:C6    | 2.54                     | 0.42              |
| 85:L5:2528:G:H3'   | 85:L5:2528:G:N3    | 2.34                     | 0.42              |
| 85:L5:2741:U:H4'   | 85:L5:2742:G:O4'   | 2.20                     | 0.42              |
| 85:L5:3690:U:OP2   | 22:LA:200:ARG:HD2  | 2.19                     | 0.42              |
| 85:L5:3748:A:O2'   | 22:LA:223:SER:OG   | 2.23                     | 0.42              |
| 85:L5:3814:U:H2'   | 85:L5:3815:G:C8    | 2.54                     | 0.42              |
| 85:L5:3824:A:H2'   | 85:L5:3825:A:C8    | 2.55                     | 0.42              |
| 85:L5:3965:A:O2'   | 85:L5:4050:A:OP2   | 2.31                     | 0.42              |
| 85:L5:4196:G:C4    | 85:L5:4197:G:C8    | 3.07                     | 0.42              |
| 85:L5:4236:G:H2'   | 85:L5:4237:C:H6    | 1.84                     | 0.42              |
| 85:L5:4313:A:OP1   | 40:LT:50:LYS:HE3   | 2.19                     | 0.42              |
| 85:L5:4337:C:N3    | 60:Lo:61:LYS:NZ    | 2.65                     | 0.42              |
| 85:L5:4421:C:H6    | 85:L5:4421:C:O5'   | 2.03                     | 0.42              |
| 85:L5:4605:A:H2'   | 85:L5:4606:G:C8    | 2.54                     | 0.42              |
| 85:L5:4617:G:H2'   | 85:L5:4618:G:H8    | 1.84                     | 0.42              |
| 20:L7:13:A:C4      | 20:L7:110:G:C5     | 3.08                     | 0.42              |
| 20:L7:59:G:C4      | 20:L7:60:G:C8      | 3.07                     | 0.42              |
| 20:L7:67:C:H2'     | 20:L7:68:C:H6      | 1.85                     | 0.42              |
| 22:LA:117:GLU:HG3  | 22:LA:163:ARG:HG2  | 2.02                     | 0.42              |
| 23:LB:84:MET:SD    | 23:LB:85:VAL:N     | 2.92                     | 0.42              |
| 24:LC:109:ARG:HB3  | 24:LC:111:TRP:CE2  | 2.54                     | 0.42              |
| 24:LC:149:GLU:OE2  | 62:Lr:72:LYS:NZ    | 2.29                     | 0.42              |
| 24:LC:221:PHE:HD1  | 24:LC:229:LEU:HD11 | 1.84                     | 0.42              |
| 25:LD:38:ILE:HD12  | 40:LT:30:TYR:CD2   | 2.53                     | 0.42              |
| 27:LF:30:ILE:O     | 27:LF:33:LEU:HG    | 2.19                     | 0.42              |
| 27:LF:62:ARG:HH21  | 27:LF:66:ARG:N     | 2.18                     | 0.42              |
| 27:LF:98:ILE:HG21  | 37:LQ:4:ASP:HB3    | 2.01                     | 0.42              |
| 27:LF:146:ASN:OD1  | 27:LF:149:SER:OG   | 2.38                     | 0.42              |
| 28:LG:252:LYS:HB2  | 28:LG:252:LYS:HE2  | 1.92                     | 0.42              |
| 29:LH:187:VAL:HG23 | 29:LH:188:GLN:OE1  | 2.19                     | 0.42              |
| 31:LJ:13:ARG:NH1   | 31:LJ:154:LYS:O    | 2.52                     | 0.42              |
| 32:LL:171:GLU:OE1  | 32:LL:175:ASN:ND2  | 2.45                     | 0.42              |
| 33:LM:92:ALA:O     | 33:LM:95:ILE:HG13  | 2.19                     | 0.42              |
| 34:LN:150:TRP:CD1  | 34:LN:150:TRP:H    | 2.37                     | 0.42              |
| 35:LO:7:LEU:HB3    | 35:LO:33:VAL:HG22  | 2.00                     | 0.42              |
| 35:LO:61:ARG:HA    | 35:LO:70:PRO:HD2   | 2.01                     | 0.42              |
| 40:LT:45:MET:CE    | 40:LT:94:GLU:HB2   | 2.43                     | 0.42              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 40:LT:63:ARG:HG2  | 40:LT:75:VAL:HG22  | 2.00                     | 0.42              |
| 41:LU:19:LEU:C    | 41:LU:20:LYS:HG3   | 2.44                     | 0.42              |
| 42:LV:26:ILE:HB   | 42:LV:101:ASN:O    | 2.18                     | 0.42              |
| 43:LX:94:ASN:OD1  | 43:LX:140:LEU:HB2  | 2.19                     | 0.42              |
| 53:Lh:96:ASN:OD1  | 53:Lh:98:HIS:N     | 2.52                     | 0.42              |
| 58:Lm:94:MET:HE3  | 58:Lm:123:PRO:HA   | 2.02                     | 0.42              |
| 62:Lr:20:ARG:HD3  | 62:Lr:20:ARG:HA    | 1.80                     | 0.42              |
| 63:Lz:73:HIS:CE1  | 63:Lz:111:LEU:HD21 | 2.53                     | 0.42              |
| 65:SD:53:THR:OG1  | 65:SD:54:ARG:N     | 2.52                     | 0.42              |
| 66:SF:35:LEU:HA   | 66:SF:38:TYR:HD2   | 1.83                     | 0.42              |
| 67:SK:55:ARG:HD2  | 79:S2:1277:C:H4'   | 2.01                     | 0.42              |
| 75:Sg:192:THR:OG1 | 75:Sg:213:ASP:OD2  | 2.36                     | 0.42              |
| 75:Sg:241:PHE:CG  | 75:Sg:248:LEU:HD23 | 2.53                     | 0.42              |
| 79:S2:160:U:O2'   | 79:S2:161:U:H3'    | 2.19                     | 0.42              |
| 79:S2:1078:C:C2   | 79:S2:1079:C:C5    | 3.08                     | 0.42              |
| 79:S2:1102:G:C6   | 79:S2:1131:G:C6    | 3.07                     | 0.42              |
| 79:S2:1135:C:H2'  | 79:S2:1136:U:C6    | 2.54                     | 0.42              |
| 79:S2:1348:G:C8   | 79:S2:1349:G:C8    | 3.07                     | 0.42              |
| 79:S2:1500:G:C4   | 79:S2:1501:C:C5    | 3.08                     | 0.42              |
| 1:CH:139:LYS:HE2  | 1:CH:139:LYS:HB2   | 1.78                     | 0.42              |
| 1:cH:51:GLN:O     | 1:cH:52:HIS:HB3    | 2.19                     | 0.42              |
| 2:sE:191:ARG:CZ   | 2:sE:245:ARG:HD2   | 2.50                     | 0.42              |
| 3:sI:37:LYS:HB2   | 3:sI:59:ARG:HG3    | 2.01                     | 0.42              |
| 3:sI:67:TRP:CZ3   | 3:sI:69:SER:HB2    | 2.41                     | 0.42              |
| 3:sI:116:HIS:HB3  | 3:sI:117:TYR:CE1   | 2.54                     | 0.42              |
| 3:sI:141:ARG:HB2  | 3:sI:146:GLN:OE1   | 2.19                     | 0.42              |
| 4:sL:103:GLU:OE1  | 5:sX:11:ARG:HB2    | 2.19                     | 0.42              |
| 5:sX:20:GLN:OE1   | 79:s2:1165:G:N1    | 2.45                     | 0.42              |
| 5:sX:48:LYS:HB2   | 79:s2:483:C:OP2    | 2.20                     | 0.42              |
| 6:sG:2:LYS:HG3    | 6:sG:108:VAL:HG12  | 2.00                     | 0.42              |
| 6:sG:147:LEU:HB3  | 6:sG:151:ASP:OD2   | 2.20                     | 0.42              |
| 11:sB:32:ASP:OD1  | 11:sB:32:ASP:N     | 2.46                     | 0.42              |
| 12:sH:122:LEU:HA  | 12:sH:125:VAL:HG22 | 2.01                     | 0.42              |
| 12:sH:143:ARG:NH1 | 12:sH:157:HIS:CE1  | 2.87                     | 0.42              |
| 14:sa:40:VAL:O    | 14:sa:41:ILE:HD13  | 2.20                     | 0.42              |
| 16:sN:40:LEU:O    | 16:sN:43:LYS:HB3   | 2.19                     | 0.42              |
| 19:sb:22:LYS:HG2  | 79:s2:921:G:N1     | 2.34                     | 0.42              |
| 21:l8:132:G:P     | 43:lX:108:GLN:HE22 | 2.43                     | 0.42              |
| 22:lA:82:ILE:HB   | 22:lA:86:GLN:NE2   | 2.34                     | 0.42              |
| 23:lB:63:PRO:CA   | 23:lB:68:ASN:HD21  | 2.29                     | 0.42              |
| 23:lB:113:GLU:H   | 23:lB:113:GLU:HG2  | 1.57                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:1B:181:MET:HE2  | 23:1B:181:MET:HB3  | 1.84                     | 0.42              |
| 23:1B:302:ASN:CG   | 23:1B:303:ALA:H    | 2.28                     | 0.42              |
| 24:1C:172:LYS:HA   | 24:1C:177:TRP:HB2  | 2.00                     | 0.42              |
| 24:1C:175:LYS:HE2  | 24:1C:175:LYS:HB2  | 1.68                     | 0.42              |
| 29:1H:41:ILE:HG21  | 29:1H:73:ILE:HD11  | 2.01                     | 0.42              |
| 30:1I:143:GLN:C    | 30:1I:144:ASN:HD22 | 2.28                     | 0.42              |
| 32:1L:16:LYS:O     | 32:1L:21:ARG:NH2   | 2.52                     | 0.42              |
| 35:1O:34:VAL:HG21  | 35:1O:112:TYR:CE2  | 2.55                     | 0.42              |
| 35:1O:179:LYS:HE2  | 85:15:4873:G:C8    | 2.53                     | 0.42              |
| 37:1Q:43:PHE:CE1   | 37:1Q:133:GLY:HA3  | 2.54                     | 0.42              |
| 40:1T:12:ARG:HH11  | 85:15:4209:G:H4'   | 1.83                     | 0.42              |
| 40:1T:127:GLN:HE22 | 40:1T:129:LYS:C    | 2.11                     | 0.42              |
| 41:1U:101:ARG:HH21 | 85:15:2702:C:H5''  | 1.85                     | 0.42              |
| 52:1g:86:CYS:HA    | 52:1g:89:ASP:OD1   | 2.19                     | 0.42              |
| 53:1h:94:ARG:HE    | 53:1h:94:ARG:HB2   | 1.59                     | 0.42              |
| 62:1r:53:PRO:HD3   | 62:1r:117:ILE:HD11 | 2.02                     | 0.42              |
| 62:1r:94:ARG:NH1   | 85:15:2262:G:OP1   | 2.52                     | 0.42              |
| 63:1z:32:VAL:HG12  | 63:1z:170:GLY:C    | 2.45                     | 0.42              |
| 63:1z:55:LEU:HD12  | 63:1z:55:LEU:HA    | 1.84                     | 0.42              |
| 63:1z:59:PRO:HB2   | 63:1z:170:GLY:HA3  | 2.02                     | 0.42              |
| 66:sF:144:LEU:HD23 | 66:sF:144:LEU:HA   | 1.69                     | 0.42              |
| 68:sP:21:ASP:O     | 68:sP:25:LEU:HD23  | 2.20                     | 0.42              |
| 69:sQ:10:VAL:HG22  | 69:sQ:11:GLN:N     | 2.35                     | 0.42              |
| 69:sQ:32:ILE:HG23  | 69:sQ:68:ILE:HD11  | 2.01                     | 0.42              |
| 69:sQ:96:TYR:HA    | 69:sQ:100:VAL:HG12 | 2.01                     | 0.42              |
| 69:sQ:100:VAL:O    | 75:sg:57:ARG:NH2   | 2.52                     | 0.42              |
| 70:sS:63:GLU:H     | 70:sS:63:GLU:CD    | 2.22                     | 0.42              |
| 70:sS:142:ARG:HH22 | 79:s2:1228:A:C5'   | 2.31                     | 0.42              |
| 72:sU:23:THR:HG23  | 72:sU:113:GLU:OE1  | 2.19                     | 0.42              |
| 79:s2:350:C:H2'    | 79:s2:351:G:O4'    | 2.19                     | 0.42              |
| 79:s2:359:U:O2     | 79:s2:403:G:N2     | 2.46                     | 0.42              |
| 79:s2:534:G:C2     | 79:s2:550:C:C2     | 3.07                     | 0.42              |
| 79:s2:636:C:H2'    | 79:s2:637:U:C6     | 2.54                     | 0.42              |
| 79:s2:831:G:C2     | 79:s2:844:U:C2     | 3.07                     | 0.42              |
| 79:s2:833:C:H2'    | 79:s2:834:C:C1'    | 2.49                     | 0.42              |
| 79:s2:951:C:H2'    | 79:s2:952:G:C8     | 2.55                     | 0.42              |
| 79:s2:1301:A:H2'   | 79:s2:1303:C:C6    | 2.55                     | 0.42              |
| 79:s2:1349:G:H2'   | 79:s2:1350:U:O4'   | 2.19                     | 0.42              |
| 79:s2:1370:A:C2    | 79:s2:1387:G:H1'   | 2.55                     | 0.42              |
| 79:s2:1599:U:H5''  | 79:s2:1600:G:C4    | 2.53                     | 0.42              |
| 80:cB:41:CYS:O     | 80:cB:49:ALA:HA    | 2.19                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 80:cB:185:VAL:HA   | 80:cB:188:ILE:HG12 | 2.02                     | 0.42              |
| 80:cB:404:THR:HA   | 80:cB:411:TYR:CE2  | 2.55                     | 0.42              |
| 80:cB:652:PHE:O    | 80:cB:658:GLY:N    | 2.52                     | 0.42              |
| 80:cB:822:GLY:N    | 80:cB:830:ARG:HH22 | 2.03                     | 0.42              |
| 82:pE:54:U:H5''    | 82:pE:55:U:OP2     | 2.20                     | 0.42              |
| 85:l5:1076:C:H2'   | 85:l5:1077:C:H6    | 1.80                     | 0.42              |
| 85:l5:1600:A:C5    | 85:l5:1638:A:C6    | 3.07                     | 0.42              |
| 85:l5:2080:U:H2'   | 85:l5:2081:C:C6    | 2.55                     | 0.42              |
| 85:l5:2274:C:H2'   | 85:l5:2275:G:H8    | 1.84                     | 0.42              |
| 85:l5:2538:U:H2'   | 85:l5:2539:C:C6    | 2.54                     | 0.42              |
| 85:l5:2597:G:H2'   | 85:l5:2598:A:C8    | 2.55                     | 0.42              |
| 85:l5:4054:C:H5''  | 85:l5:4055:U:C4    | 2.55                     | 0.42              |
| 85:l5:4111:U:H2'   | 85:l5:4112:C:H5    | 1.84                     | 0.42              |
| 85:l5:4258:C:C2    | 85:l5:4259:C:C5    | 3.08                     | 0.42              |
| 80:CB:35:LEU:O     | 80:CB:39:LEU:HG    | 2.20                     | 0.42              |
| 80:CB:45:ILE:HD13  | 80:CB:78:PHE:N     | 2.34                     | 0.42              |
| 80:CB:56:PHE:CD2   | 80:CB:456:ARG:HG3  | 2.55                     | 0.42              |
| 2:SE:59:ASP:O      | 2:SE:63:LYS:HG2    | 2.19                     | 0.42              |
| 3:SI:8:TRP:CZ3     | 3:SI:20:PRO:HB3    | 2.54                     | 0.42              |
| 5:SX:81:ILE:HG13   | 5:SX:82:THR:N      | 2.35                     | 0.42              |
| 5:SX:85:VAL:HB     | 5:SX:90:CYS:SG     | 2.60                     | 0.42              |
| 7:SJ:60:LEU:HD21   | 7:SJ:73:GLU:CD     | 2.45                     | 0.42              |
| 10:SA:31:ASP:OD1   | 10:SA:32:PHE:N     | 2.52                     | 0.42              |
| 10:SA:124:VAL:HG11 | 10:SA:134:LEU:HD21 | 2.00                     | 0.42              |
| 11:SB:30:TRP:CD1   | 11:SB:48:LEU:HB3   | 2.55                     | 0.42              |
| 11:SB:214:LYS:HD3  | 11:SB:215:VAL:C    | 2.45                     | 0.42              |
| 13:SV:15:ARG:HH21  | 15:SC:84:PHE:HA    | 1.84                     | 0.42              |
| 14:Sa:38:LYS:HD2   | 79:S2:1867:U:O2'   | 2.20                     | 0.42              |
| 17:SO:29:GLY:C     | 17:SO:93:LEU:HD12  | 2.44                     | 0.42              |
| 19:Sb:31:TYR:H     | 19:Sb:48:SER:HB2   | 1.84                     | 0.42              |
| 85:L5:27:C:O3'     | 85:L5:60:G:N2      | 2.51                     | 0.42              |
| 85:L5:28:C:O2'     | 34:LN:162:ARG:O    | 2.32                     | 0.42              |
| 85:L5:53:C:H2'     | 85:L5:54:G:H8      | 1.84                     | 0.42              |
| 85:L5:214:G:H2'    | 85:L5:215:C:C6     | 2.55                     | 0.42              |
| 85:L5:476:G:H2'    | 85:L5:477:C:C6     | 2.55                     | 0.42              |
| 85:L5:1281:G:H5'   | 24:LC:323:ARG:HB2  | 2.00                     | 0.42              |
| 85:L5:1552:G:H1'   | 85:L5:1575:A:N6    | 2.34                     | 0.42              |
| 85:L5:1643:A:H2'   | 85:L5:1644:C:H6    | 1.84                     | 0.42              |
| 85:L5:1751:A:H5'   | 30:LI:194:GLY:HA2  | 2.02                     | 0.42              |
| 85:L5:1913:C:H2'   | 85:L5:1914:C:C6    | 2.55                     | 0.42              |
| 85:L5:2017:A:H2'   | 85:L5:2017:A:OP2   | 2.20                     | 0.42              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 85:L5:2832:A:H2'   | 85:L5:2833:A:C8   | 2.54                     | 0.42              |
| 85:L5:2845:A:N3    | 85:L5:2845:A:H2'  | 2.34                     | 0.42              |
| 85:L5:3661:G:N2    | 85:L5:3681:G:O2'  | 2.53                     | 0.42              |
| 85:L5:3804:G:H2'   | 85:L5:3805:U:C6   | 2.54                     | 0.42              |
| 85:L5:4101:C:OP2   | 85:L5:4108:G:H1'  | 2.20                     | 0.42              |
| 85:L5:4129:G:H2'   | 85:L5:4130:C:C6   | 2.54                     | 0.42              |
| 85:L5:4175:G:H2'   | 85:L5:4176:C:C6   | 2.54                     | 0.42              |
| 85:L5:4220:A:H5'   | 47:Lb:6:ASN:ND2   | 2.34                     | 0.42              |
| 85:L5:4223:C:H2'   | 85:L5:4224:A:H8   | 1.84                     | 0.42              |
| 85:L5:4454:G:H2'   | 85:L5:4455:G:C8   | 2.53                     | 0.42              |
| 85:L5:4769:G:H2'   | 85:L5:4770:U:H6   | 1.83                     | 0.42              |
| 85:L5:4910:G:N2    | 35:LO:106:ASP:O   | 2.52                     | 0.42              |
| 85:L5:4996:C:P     | 49:Ld:32:ARG:HH22 | 2.42                     | 0.42              |
| 20:L7:7:G:H2'      | 20:L7:8:G:H8      | 1.85                     | 0.42              |
| 21:L8:83:C:P       | 21:L8:83:C:H6     | 2.43                     | 0.42              |
| 21:L8:111:U:O3'    | 21:L8:112:G:H8    | 2.03                     | 0.42              |
| 22:LA:63:PHE:HB2   | 22:LA:74:GLU:OE1  | 2.19                     | 0.42              |
| 22:LA:102:LEU:HG   | 22:LA:107:MET:HE2 | 2.00                     | 0.42              |
| 22:LA:117:GLU:HB2  | 22:LA:162:ASN:HB3 | 2.01                     | 0.42              |
| 23:LB:212:GLY:N    | 23:LB:215:GLU:OE2 | 2.50                     | 0.42              |
| 24:LC:189:MET:SD   | 24:LC:190:ARG:N   | 2.93                     | 0.42              |
| 26:LE:138:ARG:NH2  | 26:LE:170:SER:HA  | 2.34                     | 0.42              |
| 28:LG:121:LYS:HE3  | 28:LG:121:LYS:HB3 | 1.75                     | 0.42              |
| 31:LJ:160:GLU:HA   | 31:LJ:163:MET:SD  | 2.59                     | 0.42              |
| 32:LL:189:ALA:HB2  | 54:Li:10:GLY:HA2  | 2.01                     | 0.42              |
| 33:LM:108:ASP:OD1  | 33:LM:111:LYS:NZ  | 2.52                     | 0.42              |
| 34:LN:9:GLU:HG3    | 54:Li:44:ILE:HG21 | 2.02                     | 0.42              |
| 36:LP:24:VAL:HG12  | 36:LP:86:LYS:HG2  | 2.02                     | 0.42              |
| 36:LP:96:LYS:O     | 36:LP:99:GLU:HG3  | 2.19                     | 0.42              |
| 37:LQ:93:GLN:HB3   | 46:La:87:ARG:NH2  | 2.35                     | 0.42              |
| 40:LT:80:VAL:HG22  | 40:LT:83:LYS:O    | 2.18                     | 0.42              |
| 41:LU:113:ARG:HG2  | 41:LU:114:TYR:H   | 1.84                     | 0.42              |
| 45:LZ:57:MET:HB3   | 45:LZ:61:LYS:HD2  | 2.02                     | 0.42              |
| 48:Lc:77:ASN:OD1   | 48:Lc:77:ASN:C    | 2.62                     | 0.42              |
| 60:Lo:25:GLN:OE1   | 60:Lo:26:TYR:N    | 2.53                     | 0.42              |
| 65:SD:204:LEU:HD23 | 65:SD:206:ASP:N   | 2.34                     | 0.42              |
| 70:SS:133:GLY:HA3  | 79:S2:1623:A:O5'  | 2.20                     | 0.42              |
| 71:ST:8:ASP:N      | 71:ST:8:ASP:OD1   | 2.35                     | 0.42              |
| 72:SU:80:PHE:HB3   | 74:Sd:52:PHE:CD2  | 2.54                     | 0.42              |
| 73:Sc:11:LEU:HD13  | 73:Sc:55:VAL:HG11 | 2.00                     | 0.42              |
| 74:Sd:13:LYS:NZ    | 79:S2:1556:A:N3   | 2.59                     | 0.42              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 74:Sd:14:PHE:HD2  | 79:S2:1661:A:C8    | 2.38                     | 0.42              |
| 75:Sg:42:MET:HE1  | 75:Sg:56:GLN:HG2   | 2.02                     | 0.42              |
| 75:Sg:168:CYS:HB2 | 75:Sg:198:VAL:HB   | 2.01                     | 0.42              |
| 79:S2:112:U:H4'   | 79:S2:114:G:OP1    | 2.19                     | 0.42              |
| 79:S2:347:G:C4    | 79:S2:348:A:C8     | 3.08                     | 0.42              |
| 79:S2:1330:G:N7   | 79:S2:1492:U:H3'   | 2.34                     | 0.42              |
| 79:S2:1653:U:H2'  | 79:S2:1654:G:C8    | 2.55                     | 0.42              |
| 79:S2:1685:U:C4   | 79:S2:1686:G:N7    | 2.88                     | 0.42              |
| 79:S2:1831:A:O2'  | 79:S2:1852:C:H5'   | 2.19                     | 0.42              |
| 81:AP:37:A:H2'    | 81:AP:38:C:O4'     | 2.20                     | 0.42              |
| 84:Lt:65:GLN:OE1  | 84:Lt:66:ASN:N     | 2.53                     | 0.42              |
| 84:Lt:123:ARG:HG3 | 84:Lt:125:LEU:N    | 2.34                     | 0.42              |
| 1:CH:121:LEU:HD11 | 1:CH:132:LEU:HD21  | 2.02                     | 0.42              |
| 2:sE:160:ILE:HB   | 2:sE:169:ILE:HG23  | 2.02                     | 0.42              |
| 2:sE:188:ASN:ND2  | 2:sE:220:THR:HG1   | 2.17                     | 0.42              |
| 3:sI:8:TRP:CE3    | 3:sI:20:PRO:HB3    | 2.54                     | 0.42              |
| 4:sL:13:GLN:HG2   | 4:sL:36:TYR:HB3    | 2.02                     | 0.42              |
| 4:sL:32:LYS:HD2   | 4:sL:32:LYS:HA     | 1.65                     | 0.42              |
| 5:sX:87:ASN:HB3   | 5:sX:90:CYS:SG     | 2.60                     | 0.42              |
| 6:sG:167:LYS:HD2  | 79:s2:67:C:N4      | 2.35                     | 0.42              |
| 8:sY:66:GLY:HA2   | 79:s2:581:U:H4'    | 2.02                     | 0.42              |
| 10:sA:216:ALA:O   | 10:sA:220:LYS:HG2  | 2.20                     | 0.42              |
| 13:sV:23:ILE:HD11 | 15:sC:249:SER:C    | 2.44                     | 0.42              |
| 14:sa:76:SER:OG   | 79:s2:1863:A:N1    | 2.52                     | 0.42              |
| 15:sC:78:LEU:HB2  | 15:sC:97:PHE:CD2   | 2.54                     | 0.42              |
| 16:sN:114:ARG:NH1 | 79:s2:996:A:OP1    | 2.53                     | 0.42              |
| 21:l8:124:U:OP1   | 21:l8:126:C:N4     | 2.48                     | 0.42              |
| 21:l8:143:G:C6    | 85:l5:15:A:N6      | 2.88                     | 0.42              |
| 22:lA:178:PRO:HD3 | 61:lp:25:MET:HE1   | 2.01                     | 0.42              |
| 24:lC:167:ALA:HB1 | 24:lC:221:PHE:HE1  | 1.84                     | 0.42              |
| 24:lC:286:ASN:ND2 | 24:lC:292:ILE:HD11 | 2.34                     | 0.42              |
| 24:lC:336:ARG:O   | 24:lC:339:THR:HG22 | 2.19                     | 0.42              |
| 26:lE:200:LYS:NZ  | 26:lE:201:ILE:O    | 2.38                     | 0.42              |
| 29:lH:7:ASN:HB2   | 29:lH:56:ARG:HD3   | 2.02                     | 0.42              |
| 33:lM:13:ALA:HA   | 33:lM:58:THR:HG23  | 2.01                     | 0.42              |
| 34:lN:160:GLU:HG2 | 34:lN:161:MET:N    | 2.34                     | 0.42              |
| 36:lP:28:ASN:O    | 36:lP:32:THR:HG22  | 2.19                     | 0.42              |
| 40:lT:20:ARG:HG2  | 40:lT:20:ARG:O     | 2.20                     | 0.42              |
| 43:lX:50:LYS:HD2  | 85:l5:2475:G:C2    | 2.55                     | 0.42              |
| 47:lb:42:ASN:ND2  | 85:l5:1816:C:C1'   | 2.82                     | 0.42              |
| 49:ld:19:GLU:HB2  | 49:ld:92:ARG:HH21  | 1.83                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 50:le:24:GLN:OE1   | 50:le:27:ARG:HD3   | 2.20                     | 0.42              |
| 52:lg:82:MET:HE3   | 52:lg:82:MET:HB2   | 1.82                     | 0.42              |
| 56:lk:8:ILE:O      | 56:lk:12:LEU:HG    | 2.19                     | 0.42              |
| 60:lo:61:LYS:NZ    | 85:l5:4337:C:N4    | 2.67                     | 0.42              |
| 62:lr:95:HIS:O     | 62:lr:96:MET:C     | 2.62                     | 0.42              |
| 63:lz:103:LEU:HG   | 63:lz:105:LYS:N    | 2.31                     | 0.42              |
| 63:lz:189:PHE:CD2  | 63:lz:189:PHE:C    | 2.97                     | 0.42              |
| 63:lz:194:LEU:O    | 63:lz:194:LEU:HD12 | 2.19                     | 0.42              |
| 64:sR:94:GLU:O     | 64:sR:116:ASN:ND2  | 2.52                     | 0.42              |
| 65:sD:156:LEU:CD1  | 79:s2:1383:A:H4'   | 2.50                     | 0.42              |
| 66:sF:59:LYS:HG2   | 66:sF:62:ARG:HD2   | 2.02                     | 0.42              |
| 70:sS:8:LYS:HE3    | 70:sS:59:LEU:O     | 2.20                     | 0.42              |
| 70:sS:41:ALA:O     | 70:sS:45:LEU:HD23  | 2.19                     | 0.42              |
| 71:sT:25:SER:OG    | 71:sT:27:LYS:HE2   | 2.19                     | 0.42              |
| 72:sU:61:LEU:O     | 72:sU:81:GLN:HA    | 2.19                     | 0.42              |
| 73:sc:12:ALA:HA    | 73:sc:33:GLU:O     | 2.20                     | 0.42              |
| 73:sc:33:GLU:N     | 73:sc:33:GLU:CD    | 2.77                     | 0.42              |
| 75:sg:38:LYS:HZ1   | 75:sg:64:HIS:HD2   | 1.67                     | 0.42              |
| 75:sg:244:ASN:ND2  | 75:sg:245:ARG:HE   | 2.18                     | 0.42              |
| 77:sZ:77:LEU:H     | 77:sZ:77:LEU:HD12  | 1.84                     | 0.42              |
| 79:s2:174:C:H2'    | 79:s2:175:A:O4'    | 2.20                     | 0.42              |
| 79:s2:444:G:H22    | 79:s2:447:A:P      | 2.42                     | 0.42              |
| 79:s2:455:A:H2'    | 79:s2:456:C:H6     | 1.85                     | 0.42              |
| 79:s2:831:G:N1     | 79:s2:832:G:C5     | 2.88                     | 0.42              |
| 79:s2:872:A:C6     | 79:s2:915:G:C5     | 3.07                     | 0.42              |
| 79:s2:906:U:H2'    | 79:s2:907:G:H8     | 1.85                     | 0.42              |
| 79:s2:1283:C:H2'   | 79:s2:1284:A:H2    | 1.85                     | 0.42              |
| 79:s2:1351:G:C2    | 79:s2:1352:G:C8    | 3.08                     | 0.42              |
| 79:s2:1706:G:N3    | 79:s2:1850:A:O2'   | 2.52                     | 0.42              |
| 80:cB:214:PHE:HB2  | 80:cB:223:PHE:CE1  | 2.54                     | 0.42              |
| 80:cB:538:ILE:CD1  | 80:cB:544:HIS:HD1  | 2.32                     | 0.42              |
| 80:cB:650:TRP:NE1  | 80:cB:676:LYS:HE2  | 2.35                     | 0.42              |
| 80:cB:858:LEU:HD23 | 80:cB:858:LEU:H    | 1.83                     | 0.42              |
| 83:ls:162:LYS:NZ   | 83:ls:163:THR:HG23 | 2.35                     | 0.42              |
| 84:lt:125:LEU:HD12 | 84:lt:126:SER:H    | 1.84                     | 0.42              |
| 85:l5:423:G:H2'    | 85:l5:424:U:C6     | 2.54                     | 0.42              |
| 85:l5:675:C:H2'    | 85:l5:676:C:C6     | 2.54                     | 0.42              |
| 85:l5:752:G:O6     | 85:l5:912:G:N2     | 2.52                     | 0.42              |
| 85:l5:1466:G:H2'   | 85:l5:1467:C:C6    | 2.55                     | 0.42              |
| 85:l5:1636:U:H5''  | 85:l5:1637:A:H5'   | 2.01                     | 0.42              |
| 85:l5:1952:G:H2'   | 85:l5:1953:U:C6    | 2.54                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 85:L5:2419:C:H2'   | 85:L5:2420:A:H8    | 1.85                     | 0.42              |
| 85:L5:2578:G:H2'   | 85:L5:2579:G:H8    | 1.83                     | 0.42              |
| 85:L5:2635:U:H2'   | 85:L5:2636:U:C6    | 2.55                     | 0.42              |
| 85:L5:2635:U:H2'   | 85:L5:2636:U:H6    | 1.84                     | 0.42              |
| 85:L5:2653:C:H2'   | 85:L5:2654:C:C6    | 2.54                     | 0.42              |
| 85:L5:2889:G:H2'   | 85:L5:2890:C:C6    | 2.55                     | 0.42              |
| 85:L5:3717:A:C4    | 85:L5:3718:A:C8    | 3.08                     | 0.42              |
| 85:L5:4046:A:O2'   | 85:L5:4047:A:H5'   | 2.19                     | 0.42              |
| 85:L5:4062:A:H2'   | 85:L5:4063:U:C6    | 2.54                     | 0.42              |
| 85:L5:4970:C:C2    | 85:L5:5064:G:C2    | 3.07                     | 0.42              |
| 85:L5:4975:G:C4    | 85:L5:4977:A:C5    | 3.08                     | 0.42              |
| 85:L5:4977:A:H2'   | 85:L5:4978:G:C8    | 2.55                     | 0.42              |
| 80:CB:99:LEU:HD23  | 80:CB:100:ILE:N    | 2.35                     | 0.42              |
| 80:CB:181:ILE:O    | 80:CB:185:VAL:HG13 | 2.20                     | 0.42              |
| 80:CB:745:TYR:HA   | 80:CB:815:ASP:H    | 1.84                     | 0.42              |
| 80:CB:820:LEU:HD23 | 80:CB:831:PRO:HG3  | 2.02                     | 0.42              |
| 3:SI:76:THR:HG21   | 3:SI:109:TYR:CE2   | 2.55                     | 0.42              |
| 4:SL:85:THR:HA     | 4:SL:113:LEU:H     | 1.85                     | 0.42              |
| 7:SJ:163:SER:C     | 7:SJ:165:TYR:H     | 2.28                     | 0.42              |
| 8:SY:9:THR:H       | 79:S2:837:A:H61    | 1.68                     | 0.42              |
| 8:SY:15:ASN:HD21   | 8:SY:20:ARG:HG2    | 1.84                     | 0.42              |
| 10:SA:184:ARG:HG2  | 10:SA:189:ILE:HB   | 2.00                     | 0.42              |
| 10:SA:185:MET:HE3  | 13:SV:46:PHE:CE1   | 2.54                     | 0.42              |
| 13:SV:34:MET:HE2   | 13:SV:34:MET:HA    | 2.01                     | 0.42              |
| 15:SC:81:ILE:O     | 15:SC:85:SER:N     | 2.52                     | 0.42              |
| 85:L5:179:G:H2'    | 85:L5:180:C:H6     | 1.83                     | 0.42              |
| 85:L5:370:U:O2'    | 85:L5:371:A:H5'    | 2.19                     | 0.42              |
| 85:L5:417:G:O2'    | 21:L8:16:G:N2      | 2.51                     | 0.42              |
| 85:L5:1097:C:H2'   | 85:L5:1098:G:H8    | 1.84                     | 0.42              |
| 85:L5:1361:G:H2'   | 85:L5:1362:G:C8    | 2.55                     | 0.42              |
| 85:L5:1383:G:C6    | 85:L5:1384:C:C4    | 3.08                     | 0.42              |
| 85:L5:1462:A:H2'   | 85:L5:1463:C:C6    | 2.55                     | 0.42              |
| 85:L5:1577:G:C2    | 85:L5:3637:U:H1'   | 2.55                     | 0.42              |
| 85:L5:1621:A:H2'   | 85:L5:1622:U:C6    | 2.54                     | 0.42              |
| 85:L5:1624:G:C4    | 85:L5:1626:G:C6    | 3.08                     | 0.42              |
| 85:L5:1815:G:C4    | 47:Lb:45:PHE:HE2   | 2.37                     | 0.42              |
| 85:L5:1896:A:OP1   | 27:LF:97:GLY:N     | 2.53                     | 0.42              |
| 85:L5:2028:C:H2'   | 85:L5:2029:A:C8    | 2.55                     | 0.42              |
| 85:L5:2328:G:H2'   | 85:L5:2329:U:H6    | 1.84                     | 0.42              |
| 85:L5:2683:C:H2'   | 85:L5:2684:C:H6    | 1.84                     | 0.42              |
| 85:L5:3704:U:H2'   | 85:L5:3705:G:O4'   | 2.20                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 85:L5:3748:A:H2'   | 85:L5:3749:C:H6    | 1.85                     | 0.42              |
| 85:L5:4665:A:H2'   | 85:L5:4666:G:C8    | 2.55                     | 0.42              |
| 85:L5:4894:A:C3'   | 85:L5:4895:C:H5'   | 2.46                     | 0.42              |
| 22:LA:131:GLY:N    | 22:LA:169:VAL:HG23 | 2.28                     | 0.42              |
| 24:LC:46:LYS:HB3   | 24:LC:49:ARG:HH21  | 1.84                     | 0.42              |
| 24:LC:56:GLU:HG3   | 32:LL:20:ARG:HH12  | 1.84                     | 0.42              |
| 24:LC:153:VAL:HG22 | 24:LC:257:PHE:CE1  | 2.54                     | 0.42              |
| 24:LC:322:LEU:O    | 24:LC:326:LEU:HG   | 2.19                     | 0.42              |
| 25:LD:60:ILE:HB    | 25:LD:80:ALA:HB2   | 2.02                     | 0.42              |
| 25:LD:78:ALA:HB2   | 25:LD:105:LEU:HB2  | 2.01                     | 0.42              |
| 26:LE:111:LYS:HG2  | 62:Lr:87:ARG:HD3   | 2.02                     | 0.42              |
| 26:LE:119:GLU:OE1  | 50:Le:7:LEU:CD1    | 2.67                     | 0.42              |
| 28:LG:55:VAL:HG21  | 43:LX:41:ARG:HH11  | 1.84                     | 0.42              |
| 30:LI:87:MET:SD    | 30:LI:88:ARG:N     | 2.93                     | 0.42              |
| 30:LI:91:LEU:HD23  | 30:LI:135:ILE:HA   | 2.01                     | 0.42              |
| 31:LJ:52:LYS:HA    | 31:LJ:66:GLU:O     | 2.19                     | 0.42              |
| 32:LL:154:VAL:O    | 32:LL:155:MET:C    | 2.62                     | 0.42              |
| 37:LQ:18:PRO:HG2   | 37:LQ:26:ARG:NH1   | 2.35                     | 0.42              |
| 38:LR:173:ARG:NH1  | 79:S2:909:G:H5'    | 2.35                     | 0.42              |
| 45:LZ:21:ARG:HA    | 45:LZ:21:ARG:HD3   | 1.71                     | 0.42              |
| 50:Le:23:HIS:CD2   | 50:Le:24:GLN:HG3   | 2.55                     | 0.42              |
| 50:Le:78:LEU:O     | 62:Lr:20:ARG:NH1   | 2.52                     | 0.42              |
| 53:Lh:87:LYS:H     | 53:Lh:87:LYS:HG2   | 1.55                     | 0.42              |
| 53:Lh:108:GLN:OE1  | 53:Lh:108:GLN:C    | 2.62                     | 0.42              |
| 64:SR:36:GLU:H     | 64:SR:36:GLU:CD    | 2.22                     | 0.42              |
| 64:SR:41:ILE:O     | 64:SR:41:ILE:HG13  | 2.18                     | 0.42              |
| 65:SD:40:ARG:HG3   | 72:SU:108:PRO:CG   | 2.50                     | 0.42              |
| 65:SD:104:SER:O    | 65:SD:108:LYS:NZ   | 2.51                     | 0.42              |
| 66:SF:30:ILE:HG13  | 66:SF:36:GLN:HE22  | 1.85                     | 0.42              |
| 67:SK:16:PHE:HE2   | 67:SK:80:ARG:HA    | 1.80                     | 0.42              |
| 70:SS:60:THR:HB    | 70:SS:63:GLU:OE2   | 2.19                     | 0.42              |
| 71:ST:10:ASN:HD21  | 71:ST:13:GLU:CG    | 2.30                     | 0.42              |
| 72:SU:42:GLY:O     | 72:SU:46:LYS:NZ    | 2.34                     | 0.42              |
| 72:SU:75:LYS:NZ    | 79:S2:1252:C:OP1   | 2.51                     | 0.42              |
| 75:Sg:201:SER:HA   | 75:Sg:241:PHE:CE2  | 2.55                     | 0.42              |
| 79:S2:830:A:C2     | 79:S2:845:G:C6     | 3.07                     | 0.42              |
| 79:S2:1047:C:H2'   | 79:S2:1048:G:O4'   | 2.20                     | 0.42              |
| 79:S2:1231:C:H2'   | 79:S2:1232:U:H6    | 1.85                     | 0.42              |
| 79:S2:1398:G:H1    | 79:S2:1448:A:H2    | 1.59                     | 0.42              |
| 79:S2:1406:G:N3    | 79:S2:1443:C:N4    | 2.67                     | 0.42              |
| 79:S2:1801:A:H2'   | 79:S2:1802:C:C6    | 2.54                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 82:PE:26:A:N1      | 82:PE:44:G:C6      | 2.88                     | 0.42              |
| 1:CH:114:ALA:O     | 1:CH:115:ILE:C     | 2.62                     | 0.42              |
| 4:sL:109:MET:HG3   | 4:sL:111:VAL:HG13  | 2.01                     | 0.42              |
| 5:sX:21:LYS:HE2    | 5:sX:21:LYS:HB2    | 1.78                     | 0.42              |
| 8:sY:26:ASP:OD1    | 8:sY:68:LYS:NZ     | 2.49                     | 0.42              |
| 10:sA:22:GLY:C     | 10:sA:24:HIS:H     | 2.28                     | 0.42              |
| 10:sA:41:ARG:HD3   | 10:sA:45:GLY:HA2   | 2.01                     | 0.42              |
| 11:sB:187:LYS:C    | 11:sB:190:PRO:HD2  | 2.44                     | 0.42              |
| 16:sN:25:TRP:CE3   | 19:sb:82:LYS:HE2   | 2.55                     | 0.42              |
| 17:sO:55:ARG:NH1   | 79:s2:973:C:O2     | 2.51                     | 0.42              |
| 18:sW:109:GLY:C    | 18:sW:110:ILE:HD13 | 2.45                     | 0.42              |
| 22:lA:245:ARG:NH2  | 85:l5:3656:A:H4'   | 2.31                     | 0.42              |
| 23:lB:382:MET:O    | 23:lB:386:LYS:HG2  | 2.20                     | 0.42              |
| 24:lC:84:THR:HG23  | 24:lC:86:ARG:H     | 1.85                     | 0.42              |
| 24:lC:293:LEU:HD13 | 24:lC:298:ILE:HG21 | 2.02                     | 0.42              |
| 25:lD:244:HIS:O    | 25:lD:248:ARG:HG2  | 2.20                     | 0.42              |
| 25:lD:271:MET:HB2  | 25:lD:275:GLN:CG   | 2.50                     | 0.42              |
| 26:lE:188:ARG:NH1  | 26:lE:217:PHE:HB2  | 2.35                     | 0.42              |
| 26:lE:258:LEU:O    | 26:lE:262:LYS:HG3  | 2.19                     | 0.42              |
| 27:lF:94:ARG:CB    | 27:lF:114:LEU:HD12 | 2.50                     | 0.42              |
| 27:lF:149:SER:HB3  | 27:lF:245:ARG:NH1  | 2.31                     | 0.42              |
| 27:lF:226:HIS:HA   | 27:lF:233:ALA:HB3  | 2.01                     | 0.42              |
| 31:lJ:63:ARG:HD3   | 60:lo:105:GLN:O    | 2.19                     | 0.42              |
| 33:lM:6:PHE:CE1    | 39:lS:152:PHE:CA   | 3.02                     | 0.42              |
| 34:lN:120:TRP:CE3  | 85:l5:280:G:H2'    | 2.54                     | 0.42              |
| 36:lP:64:ASN:ND2   | 85:l5:3891:A:O2'   | 2.52                     | 0.42              |
| 37:lQ:75:ARG:HG3   | 37:lQ:137:VAL:HG11 | 2.02                     | 0.42              |
| 38:lR:78:ILE:HD12  | 38:lR:81:ARG:HD2   | 2.01                     | 0.42              |
| 40:lT:159:MET:SD   | 40:lT:160:ALA:N    | 2.90                     | 0.42              |
| 42:lV:40:ILE:HA    | 42:lV:40:ILE:HD12  | 1.65                     | 0.42              |
| 42:lV:68:GLY:N     | 42:lV:73:ARG:HH12  | 2.18                     | 0.42              |
| 45:lZ:76:ASN:HB3   | 45:lZ:79:HIS:HE1   | 1.79                     | 0.42              |
| 45:lZ:76:ASN:OD1   | 45:lZ:77:TYR:N     | 2.53                     | 0.42              |
| 47:lb:118:LEU:C    | 47:lb:118:LEU:HD12 | 2.45                     | 0.42              |
| 50:le:72:SER:O     | 50:le:72:SER:OG    | 2.32                     | 0.42              |
| 52:lg:43:LYS:N     | 52:lg:52:ARG:HH11  | 2.18                     | 0.42              |
| 52:lg:110:GLN:C    | 52:lg:110:GLN:OE1  | 2.63                     | 0.42              |
| 59:ln:2:ARG:NH2    | 59:ln:4:LYS:HD2    | 2.35                     | 0.42              |
| 60:lo:99:ARG:N     | 60:lo:99:ARG:CD    | 2.81                     | 0.42              |
| 61:lp:17:ARG:HB2   | 61:lp:18:TYR:CE2   | 2.54                     | 0.42              |
| 61:lp:19:GLY:HA2   | 85:l5:3692:A:H2    | 1.85                     | 0.42              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 61:lp:29:ILE:HD11  | 61:lp:69:TRP:HB3  | 1.98                     | 0.42              |
| 63:lz:31:THR:HA    | 63:lz:171:HIS:HD2 | 1.84                     | 0.42              |
| 64:sR:6:THR:HG1    | 64:sR:9:VAL:H     | 1.66                     | 0.42              |
| 65:sD:64:ARG:NH1   | 67:sK:94:LEU:HA   | 2.34                     | 0.42              |
| 67:sK:55:ARG:NH1   | 79:s2:1278:A:H5'  | 2.34                     | 0.42              |
| 69:sQ:50:LYS:O     | 69:sQ:53:GLU:HG2  | 2.19                     | 0.42              |
| 70:sS:86:ARG:HH22  | 79:s2:1610:G:C2'  | 2.30                     | 0.42              |
| 75:sg:14:HIS:CD2   | 75:sg:35:SER:HB2  | 2.55                     | 0.42              |
| 75:sg:238:ALA:HB1  | 75:sg:289:LEU:HB3 | 2.02                     | 0.42              |
| 76:sM:61:TYR:CE1   | 76:sM:107:SER:CB  | 3.03                     | 0.42              |
| 76:sM:122:ASP:OD1  | 76:sM:122:ASP:N   | 2.53                     | 0.42              |
| 79:s2:42:A:C6      | 79:s2:426:A:C6    | 3.08                     | 0.42              |
| 79:s2:325:C:H3'    | 79:s2:326:C:H4'   | 2.02                     | 0.42              |
| 79:s2:828:G:H2'    | 79:s2:829:C:C6    | 2.54                     | 0.42              |
| 79:s2:841:G:O2'    | 79:s2:842:C:H6    | 2.03                     | 0.42              |
| 79:s2:1564:C:H2'   | 79:s2:1565:C:H6   | 1.84                     | 0.42              |
| 79:s2:1630:A:N3    | 79:s2:1630:A:H2'  | 2.35                     | 0.42              |
| 79:s2:1653:U:H2'   | 79:s2:1654:G:C8   | 2.53                     | 0.42              |
| 79:s2:1685:U:H2'   | 79:s2:1686:G:O4'  | 2.19                     | 0.42              |
| 79:s2:1842:C:H2'   | 79:s2:1843:G:H8   | 1.84                     | 0.42              |
| 80:cB:88:PHE:HE1   | 80:cB:226:LYS:NZ  | 2.17                     | 0.42              |
| 80:cB:174:LEU:HD12 | 80:cB:178:PHE:CE1 | 2.55                     | 0.42              |
| 80:cB:370:GLU:OE1  | 80:cB:371:LEU:HG  | 2.20                     | 0.42              |
| 80:cB:538:ILE:HD13 | 80:cB:538:ILE:HA  | 1.86                     | 0.42              |
| 80:cB:753:GLU:OE1  | 80:cB:780:PRO:HA  | 2.20                     | 0.42              |
| 80:cB:767:ARG:HA   | 85:l5:1981:G:O6   | 2.20                     | 0.42              |
| 82:pE:2:C:H2'      | 82:pE:3:C:C6      | 2.55                     | 0.42              |
| 83:ls:138:PHE:HB3  | 83:ls:143:ILE:HB  | 2.02                     | 0.42              |
| 85:l5:112:C:C2     | 85:l5:113:A:C8    | 3.08                     | 0.42              |
| 85:l5:122:U:H2'    | 85:l5:123:C:C6    | 2.54                     | 0.42              |
| 85:l5:481:G:H2'    | 85:l5:482:G:C8    | 2.54                     | 0.42              |
| 85:l5:963:G:O2'    | 85:l5:964:A:O4'   | 2.33                     | 0.42              |
| 85:l5:1194:G:C2    | 85:l5:1195:G:C5   | 3.07                     | 0.42              |
| 85:l5:1315:C:H2'   | 85:l5:1316:G:H8   | 1.85                     | 0.42              |
| 85:l5:2018:C:H2'   | 85:l5:2019:C:C6   | 2.54                     | 0.42              |
| 85:l5:2032:U:H2'   | 85:l5:2033:A:C8   | 2.54                     | 0.42              |
| 85:l5:2293:U:H2'   | 85:l5:2294:G:C8   | 2.55                     | 0.42              |
| 85:l5:2328:G:C6    | 85:l5:2329:U:C4   | 3.08                     | 0.42              |
| 85:l5:2496:G:H2'   | 85:l5:2497:C:C6   | 2.55                     | 0.42              |
| 85:l5:2777:G:H5''  | 85:l5:2778:G:H5'  | 2.01                     | 0.42              |
| 85:l5:2817:C:C2    | 85:l5:2818:C:C5   | 3.08                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 85:L5:2877:G:H2'   | 85:L5:2878:G:O4'   | 2.20                     | 0.42              |
| 85:L5:3662:A:N7    | 85:L5:3664:G:C2    | 2.88                     | 0.42              |
| 85:L5:3850:C:H2'   | 85:L5:3851:U:O4'   | 2.19                     | 0.42              |
| 85:L5:4101:C:N4    | 85:L5:4107:G:C6    | 2.87                     | 0.42              |
| 85:L5:4175:G:H2'   | 85:L5:4176:C:C6    | 2.54                     | 0.42              |
| 85:L5:4638:U:H3'   | 85:L5:4639:G:H21   | 1.85                     | 0.42              |
| 80:CB:120:ARG:HG2  | 80:CB:397:TYR:HE2  | 1.85                     | 0.42              |
| 80:CB:195:GLY:O    | 80:CB:200:MET:HB2  | 2.20                     | 0.42              |
| 80:CB:404:THR:HG22 | 80:CB:411:TYR:CE1  | 2.54                     | 0.42              |
| 80:CB:413:PHE:CE1  | 80:CB:469:ILE:HB   | 2.55                     | 0.42              |
| 4:SL:4:ILE:HD13    | 4:SL:55:TYR:HA     | 2.01                     | 0.42              |
| 8:SY:88:LYS:HA     | 8:SY:88:LYS:HD3    | 1.93                     | 0.42              |
| 10:SA:24:HIS:HA    | 10:SA:49:ILE:HG12  | 2.01                     | 0.42              |
| 11:SB:133:TYR:CD2  | 11:SB:181:LEU:HD22 | 2.55                     | 0.42              |
| 11:SB:133:TYR:CD1  | 11:SB:221:PRO:HD2  | 2.55                     | 0.42              |
| 12:SH:57:ARG:NH2   | 12:SH:58:LYS:O     | 2.52                     | 0.42              |
| 14:Sa:10:ARG:HB2   | 14:Sa:33:ASP:HB2   | 2.00                     | 0.42              |
| 14:Sa:46:GLU:HB3   | 14:Sa:49:ALA:HB3   | 2.01                     | 0.42              |
| 17:SO:23:GLU:HG3   | 17:SO:24:GLY:N     | 2.35                     | 0.42              |
| 17:SO:54:CYS:SG    | 17:SO:81:VAL:HG23  | 2.60                     | 0.42              |
| 18:SW:9:ASP:OD1    | 79:S2:1093:A:H1'   | 2.20                     | 0.42              |
| 19:Sb:19:HIS:ND1   | 79:S2:1128:C:O2'   | 2.53                     | 0.42              |
| 85:L5:259:C:H2'    | 85:L5:260:C:C6     | 2.55                     | 0.42              |
| 85:L5:302:C:P      | 34:LN:68:ARG:HH21  | 2.42                     | 0.42              |
| 85:L5:473:C:H2'    | 85:L5:474:C:H6     | 1.84                     | 0.42              |
| 85:L5:663:G:H2'    | 85:L5:664:G:O4'    | 2.19                     | 0.42              |
| 85:L5:717:U:H3     | 85:L5:951:G:H1     | 1.68                     | 0.42              |
| 85:L5:733:A:C2     | 85:L5:734:G:H1'    | 2.55                     | 0.42              |
| 85:L5:1171:G:OP2   | 85:L5:1171:G:H8    | 2.03                     | 0.42              |
| 85:L5:1175:A:H2    | 85:L5:1185:G:N1    | 2.17                     | 0.42              |
| 85:L5:1455:G:H2'   | 85:L5:1456:C:H6    | 1.84                     | 0.42              |
| 85:L5:1576:G:O2'   | 85:L5:1578:U:H6    | 2.03                     | 0.42              |
| 85:L5:1624:G:C4    | 85:L5:1643:A:C8    | 3.07                     | 0.42              |
| 85:L5:1633:G:H5'   | 85:L5:1634:A:OP1   | 2.20                     | 0.42              |
| 85:L5:1648:C:OP2   | 85:L5:1649:U:O2'   | 2.28                     | 0.42              |
| 85:L5:1789:C:H2'   | 85:L5:1790:U:C6    | 2.55                     | 0.42              |
| 85:L5:1923:A:OP1   | 39:LS:160:ARG:NH2  | 2.52                     | 0.42              |
| 85:L5:2328:G:H2'   | 85:L5:2329:U:C6    | 2.55                     | 0.42              |
| 85:L5:2629:C:H2'   | 85:L5:2630:U:O4'   | 2.19                     | 0.42              |
| 85:L5:2716:C:H2'   | 85:L5:2717:G:C8    | 2.54                     | 0.42              |
| 85:L5:2762:G:C6    | 85:L5:2764:A:C4    | 3.08                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 85:L5:2853:C:H2'   | 85:L5:2854:G:O4'   | 2.20                     | 0.42              |
| 85:L5:3927:U:H2'   | 85:L5:3928:A:C8    | 2.55                     | 0.42              |
| 85:L5:3966:A:H2'   | 85:L5:4047:A:H62   | 1.84                     | 0.42              |
| 85:L5:4085:A:H62   | 28:LG:62:ARG:CZ    | 2.33                     | 0.42              |
| 85:L5:4195:G:N3    | 47:Lb:3:LYS:NZ     | 2.68                     | 0.42              |
| 85:L5:4400:G:C6    | 85:L5:4401:G:N7    | 2.88                     | 0.42              |
| 85:L5:4438:U:H2'   | 85:L5:4439:U:O4'   | 2.19                     | 0.42              |
| 85:L5:4584:A:C2    | 85:L5:4719:G:C4    | 3.08                     | 0.42              |
| 85:L5:4673:U:H2'   | 85:L5:4674:C:C6    | 2.54                     | 0.42              |
| 85:L5:4704:C:O2'   | 29:LH:160:LEU:HD21 | 2.20                     | 0.42              |
| 20:L7:5:A:H2'      | 20:L7:6:C:C6       | 2.54                     | 0.42              |
| 20:L7:15:C:H2'     | 20:L7:16:A:H8      | 1.85                     | 0.42              |
| 20:L7:63:C:OP1     | 30:LI:206:LEU:HD22 | 2.20                     | 0.42              |
| 20:L7:67:C:H2'     | 20:L7:68:C:C6      | 2.54                     | 0.42              |
| 22:LA:124:GLY:O    | 22:LA:128:ARG:NH1  | 2.53                     | 0.42              |
| 25:LD:89:LYS:HG3   | 25:LD:90:VAL:HG12  | 2.02                     | 0.42              |
| 26:LE:140:LEU:HA   | 26:LE:191:GLN:OE1  | 2.20                     | 0.42              |
| 27:LF:178:SER:C    | 27:LF:179:LEU:HD23 | 2.43                     | 0.42              |
| 30:LI:205:PRO:HB2  | 30:LI:207:ASP:OD1  | 2.20                     | 0.42              |
| 36:LP:41:ILE:HG12  | 36:LP:112:LEU:O    | 2.20                     | 0.42              |
| 41:LU:24:ASP:N     | 41:LU:110:TYR:O    | 2.26                     | 0.42              |
| 43:LX:124:VAL:HG23 | 43:LX:138:VAL:HA   | 2.02                     | 0.42              |
| 45:LZ:13:VAL:HG12  | 45:LZ:19:SER:HA    | 2.01                     | 0.42              |
| 45:LZ:60:LYS:H     | 45:LZ:60:LYS:HZ2   | 1.68                     | 0.42              |
| 46:La:23:GLY:HA3   | 46:La:24:LYS:HA    | 1.50                     | 0.42              |
| 51:Lf:77:ALA:HA    | 51:Lf:84:VAL:HG12  | 2.01                     | 0.42              |
| 56:Lk:24:LYS:HB3   | 56:Lk:69:LEU:HD11  | 2.01                     | 0.42              |
| 62:Lr:6:GLN:O      | 62:Lr:10:VAL:HG23  | 2.20                     | 0.42              |
| 63:Lz:120:ILE:HD13 | 63:Lz:120:ILE:HA   | 1.75                     | 0.42              |
| 64:SR:98:VAL:O     | 64:SR:120:THR:HG22 | 2.19                     | 0.42              |
| 66:SF:167:LYS:NZ   | 66:SF:172:CYS:SG   | 2.87                     | 0.42              |
| 71:ST:91:HIS:NE2   | 79:S2:1665:G:OP1   | 2.53                     | 0.42              |
| 74:Sd:3:HIS:NE2    | 79:S2:1301:A:O2'   | 2.52                     | 0.42              |
| 75:Sg:3:GLU:H      | 75:Sg:3:GLU:HG3    | 1.72                     | 0.42              |
| 75:Sg:20:GLN:CD    | 75:Sg:69:VAL:H     | 2.26                     | 0.42              |
| 75:Sg:89:LEU:HB3   | 75:Sg:99:ARG:HG2   | 2.01                     | 0.42              |
| 76:SM:128:PHE:HA   | 76:SM:131:LYS:HG2  | 2.01                     | 0.42              |
| 77:SZ:47:LEU:HD13  | 77:SZ:79:ILE:HA    | 2.00                     | 0.42              |
| 78:Sf:95:ARG:NH1   | 79:S2:1305:C:O5'   | 2.53                     | 0.42              |
| 79:S2:102:A:H4'    | 79:S2:104:A:C8     | 2.55                     | 0.42              |
| 79:S2:788:G:H1'    | 79:S2:789:G:N7     | 2.35                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 79:S2:996:A:H2'    | 79:S2:997:A:H8     | 1.84                     | 0.42              |
| 79:S2:1317:C:C2    | 79:S2:1318:G:C8    | 3.07                     | 0.42              |
| 79:S2:1428:G:N2    | 79:S2:1585:U:H5'   | 2.35                     | 0.42              |
| 79:S2:1702:G:H2'   | 79:S2:1703:C:O4'   | 2.19                     | 0.42              |
| 79:S2:1726:G:H2'   | 79:S2:1727:G:C8    | 2.54                     | 0.42              |
| 82:PE:27:U:H2'     | 82:PE:28:C:H6      | 1.81                     | 0.42              |
| 82:PE:67:U:H2'     | 82:PE:68:C:O4'     | 2.19                     | 0.42              |
| 83:Ls:27:CYS:N     | 83:Ls:193:PHE:O    | 2.48                     | 0.42              |
| 2:sE:18:TRP:NE1    | 2:sE:42:LEU:HA     | 2.31                     | 0.42              |
| 2:sE:208:VAL:O     | 2:sE:219:ALA:HA    | 2.20                     | 0.42              |
| 3:sI:25:ARG:HA     | 79:s2:448:A:H5''   | 2.02                     | 0.42              |
| 6:sG:63:MET:HB2    | 6:sG:63:MET:HE3    | 1.65                     | 0.42              |
| 6:sG:216:ARG:O     | 6:sG:217:MET:SD    | 2.77                     | 0.42              |
| 7:sJ:132:GLN:O     | 7:sJ:133:ARG:HG2   | 2.19                     | 0.42              |
| 11:sB:127:VAL:HG22 | 11:sB:128:LYS:H    | 1.84                     | 0.42              |
| 15:sC:60:TRP:CZ3   | 15:sC:96:PHE:CE2   | 2.99                     | 0.42              |
| 15:sC:174:ILE:HG13 | 15:sC:175:GLY:N    | 2.33                     | 0.42              |
| 15:sC:264:SER:HB3  | 15:sC:267:GLN:HE22 | 1.85                     | 0.42              |
| 17:sO:103:ASN:O    | 17:sO:142:ARG:HD3  | 2.19                     | 0.42              |
| 20:l7:27:G:N2      | 20:l7:54:A:N6      | 2.68                     | 0.42              |
| 20:l7:39:C:H1'     | 31:lJ:46:GLN:NE2   | 2.27                     | 0.42              |
| 23:lB:145:GLN:HA   | 23:lB:148:LYS:CE   | 2.50                     | 0.42              |
| 24:lC:309:ILE:HG21 | 24:lC:311:ARG:HH21 | 1.83                     | 0.42              |
| 25:lD:106:ALA:O    | 25:lD:110:LEU:HD23 | 2.19                     | 0.42              |
| 25:lD:153:THR:O    | 25:lD:153:THR:OG1  | 2.34                     | 0.42              |
| 27:lF:69:ILE:CG2   | 27:lF:73:ARG:HH21  | 2.32                     | 0.42              |
| 29:lH:61:TRP:CH2   | 39:lS:152:PHE:CD2  | 3.08                     | 0.42              |
| 30:lI:142:LEU:HD23 | 30:lI:142:LEU:HA   | 1.78                     | 0.42              |
| 30:lI:179:ASP:OD1  | 30:lI:180:GLU:N    | 2.53                     | 0.42              |
| 33:lM:93:LYS:HE2   | 33:lM:93:LYS:HB3   | 1.64                     | 0.42              |
| 35:lO:18:ARG:NH2   | 35:lO:128:ARG:HH21 | 2.07                     | 0.42              |
| 35:lO:187:LYS:H    | 35:lO:187:LYS:HG3  | 1.66                     | 0.42              |
| 36:lP:19:GLY:N     | 36:lP:146:ILE:O    | 2.43                     | 0.42              |
| 36:lP:40:HIS:CE1   | 36:lP:42:ARG:H     | 2.38                     | 0.42              |
| 36:lP:96:LYS:HA    | 36:lP:99:GLU:OE1   | 2.19                     | 0.42              |
| 36:lP:128:ARG:HG3  | 36:lP:136:ILE:HG23 | 2.02                     | 0.42              |
| 37:lQ:175:GLU:HG3  | 46:la:50:PRO:O     | 2.20                     | 0.42              |
| 41:lU:74:SER:OG    | 41:lU:76:VAL:HG22  | 2.20                     | 0.42              |
| 43:lX:139:ARG:HD3  | 43:lX:140:LEU:N    | 2.35                     | 0.42              |
| 44:lY:43:ASN:O     | 44:lY:126:ARG:HD2  | 2.19                     | 0.42              |
| 45:lZ:72:VAL:HG23  | 45:lZ:101:PHE:HE1  | 1.84                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 49:ld:70:LYS:NZ    | 85:l5:2389:A:H5'   | 2.34                     | 0.42              |
| 51:lf:13:GLY:HA2   | 51:lf:97:ILE:HD11  | 2.02                     | 0.42              |
| 55:lj:74:PHE:HB2   | 55:lj:78:PHE:CZ    | 2.55                     | 0.42              |
| 64:sR:8:THR:HG1    | 79:s2:1371:U:P     | 2.43                     | 0.42              |
| 65:sD:103:GLU:OE2  | 65:sD:173:ARG:HD2  | 2.20                     | 0.42              |
| 69:sQ:113:ILE:HD13 | 69:sQ:120:LEU:HD23 | 2.02                     | 0.42              |
| 75:sg:17:TRP:N     | 75:sg:36:ARG:HB2   | 2.24                     | 0.42              |
| 75:sg:189:ILE:HG22 | 75:sg:190:GLY:N    | 2.31                     | 0.42              |
| 79:s2:28:U:H2'     | 79:s2:29:G:C8      | 2.55                     | 0.42              |
| 79:s2:149:A:C8     | 79:s2:168:C:N4     | 2.88                     | 0.42              |
| 79:s2:155:G:H2'    | 79:s2:156:G:C8     | 2.55                     | 0.42              |
| 79:s2:183:G:C2     | 79:s2:184:G:C8     | 3.08                     | 0.42              |
| 79:s2:558:G:HO2'   | 79:s2:559:G:H8     | 1.64                     | 0.42              |
| 79:s2:874:G:N3     | 79:s2:875:A:C8     | 2.87                     | 0.42              |
| 79:s2:1270:G:O2'   | 79:s2:1299:A:N6    | 2.36                     | 0.42              |
| 79:s2:1343:U:H2'   | 79:s2:1344:A:O4'   | 2.20                     | 0.42              |
| 79:s2:1487:A:H2'   | 79:s2:1488:C:C6    | 2.54                     | 0.42              |
| 79:s2:1538:C:H2'   | 79:s2:1539:U:H6    | 1.85                     | 0.42              |
| 79:s2:1777:G:H2'   | 79:s2:1778:C:C6    | 2.55                     | 0.42              |
| 80:cB:14:ASP:HB3   | 80:cB:465:PRO:HG2  | 2.00                     | 0.42              |
| 80:cB:304:ILE:HD12 | 80:cB:304:ILE:HA   | 1.86                     | 0.42              |
| 80:cB:802:SER:HA   | 85:l5:4605:A:N7    | 2.35                     | 0.42              |
| 81:aP:37:A:H2'     | 81:aP:38:C:O4'     | 2.20                     | 0.42              |
| 83:ls:112:ARG:NH1  | 85:l5:1969:G:OP1   | 2.52                     | 0.42              |
| 85:l5:381:U:H2'    | 85:l5:382:G:O4'    | 2.19                     | 0.42              |
| 85:l5:1178:G:OP1   | 85:l5:1178:G:N2    | 2.28                     | 0.42              |
| 85:l5:1632:A:O2'   | 85:l5:1634:A:OP1   | 2.36                     | 0.42              |
| 85:l5:1972:G:C6    | 85:l5:1973:G:C6    | 3.08                     | 0.42              |
| 85:l5:2839:U:O4    | 85:l5:2840:A:N6    | 2.53                     | 0.42              |
| 85:l5:2868:G:C2    | 85:l5:2883:G:C6    | 3.08                     | 0.42              |
| 85:l5:3614:G:O2'   | 85:l5:3615:G:OP1   | 2.37                     | 0.42              |
| 85:l5:3848:U:O2'   | 85:l5:4634:U:O4    | 2.23                     | 0.42              |
| 85:l5:4196:G:C4    | 85:l5:4197:G:C8    | 3.08                     | 0.42              |
| 85:l5:4594:U:H2'   | 85:l5:4595:G:H8    | 1.85                     | 0.42              |
| 85:l5:4919:G:H2'   | 85:l5:4920:C:C6    | 2.55                     | 0.42              |
| 80:CB:553:HIS:HA   | 80:CB:556:ILE:HG12 | 2.02                     | 0.42              |
| 2:SE:137:PRO:HD2   | 2:SE:149:TYR:CD2   | 2.54                     | 0.42              |
| 4:SL:65:ASN:OD1    | 4:SL:65:ASN:N      | 2.50                     | 0.42              |
| 6:SG:95:LYS:HA     | 6:SG:95:LYS:HD2    | 1.68                     | 0.42              |
| 6:SG:192:ILE:HA    | 6:SG:195:LYS:HG3   | 2.01                     | 0.42              |
| 10:SA:126:ASP:OD1  | 10:SA:128:ARG:HB3  | 2.20                     | 0.42              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 11:SB:162:ARG:HA  | 11:SB:162:ARG:HD2  | 1.89                     | 0.42              |
| 11:SB:168:MET:O   | 11:SB:172:MET:HG2  | 2.20                     | 0.42              |
| 12:SH:76:GLN:NE2  | 12:SH:77:VAL:H     | 2.18                     | 0.42              |
| 12:SH:147:LYS:C   | 12:SH:149:ASP:H    | 2.28                     | 0.42              |
| 16:SN:106:ARG:HA  | 16:SN:106:ARG:HH11 | 1.84                     | 0.42              |
| 17:SO:57:THR:N    | 17:SO:60:MET:HG2   | 2.30                     | 0.42              |
| 18:SW:28:ARG:NH2  | 79:S2:1093:A:H5''  | 2.35                     | 0.42              |
| 19:Sb:69:GLY:HA3  | 79:S2:1105:G:O3'   | 2.19                     | 0.42              |
| 85:L5:28:C:P      | 34:LN:193:ARG:HH22 | 2.43                     | 0.42              |
| 85:L5:33:A:C6     | 85:L5:34:A:C6      | 3.07                     | 0.42              |
| 85:L5:363:A:N1    | 85:L5:376:A:H5''   | 2.34                     | 0.42              |
| 85:L5:509:A:C4    | 46:La:82:VAL:HG12  | 2.55                     | 0.42              |
| 85:L5:1176:C:H2'  | 85:L5:1177:U:C6    | 2.54                     | 0.42              |
| 85:L5:1306:C:H2'  | 85:L5:1307:A:C8    | 2.54                     | 0.42              |
| 85:L5:1420:A:H5'  | 37:LQ:68:ARG:NH2   | 2.34                     | 0.42              |
| 85:L5:1497:A:N6   | 37:LQ:176:ARG:HD3  | 2.35                     | 0.42              |
| 85:L5:1520:C:C2   | 85:L5:1521:C:C5    | 3.08                     | 0.42              |
| 85:L5:1709:C:N4   | 85:L5:1716:G:N2    | 2.27                     | 0.42              |
| 85:L5:1991:A:H2'  | 85:L5:1991:A:N3    | 2.35                     | 0.42              |
| 85:L5:2020:U:H2'  | 85:L5:2021:G:H8    | 1.84                     | 0.42              |
| 85:L5:2066:C:H5'' | 51:Lf:36:ARG:NH2   | 2.35                     | 0.42              |
| 85:L5:2090:U:OP1  | 85:L5:2266:C:N4    | 2.45                     | 0.42              |
| 85:L5:2714:G:H2'  | 85:L5:2715:G:H8    | 1.83                     | 0.42              |
| 85:L5:3891:A:H2'  | 85:L5:3892:U:O4'   | 2.20                     | 0.42              |
| 85:L5:3926:C:H2'  | 85:L5:3927:U:C6    | 2.55                     | 0.42              |
| 85:L5:4110:C:H4'  | 85:L5:4112:C:H4'   | 2.02                     | 0.42              |
| 85:L5:4123:C:N4   | 85:L5:4124:G:O6    | 2.53                     | 0.42              |
| 85:L5:4129:G:C6   | 85:L5:4156:G:N2    | 2.88                     | 0.42              |
| 85:L5:4276:G:C6   | 85:L5:4277:G:C5    | 3.08                     | 0.42              |
| 85:L5:5025:C:H5   | 85:L5:5026:U:C2    | 2.38                     | 0.42              |
| 20:L7:57:C:C2     | 20:L7:58:A:N7      | 2.88                     | 0.42              |
| 21:L8:59:A:H5''   | 21:L8:61:A:C8      | 2.54                     | 0.42              |
| 23:LB:21:ARG:HB3  | 23:LB:274:TYR:HD2  | 1.83                     | 0.42              |
| 24:LC:207:PRO:HB3 | 24:LC:249:PHE:CD2  | 2.55                     | 0.42              |
| 24:LC:259:LYS:HD3 | 24:LC:262:GLU:OE2  | 2.20                     | 0.42              |
| 25:LD:157:ASN:H   | 25:LD:160:PHE:HD2  | 1.67                     | 0.42              |
| 26:LE:166:LYS:HZ3 | 26:LE:167:GLN:C    | 2.23                     | 0.42              |
| 26:LE:166:LYS:NZ  | 26:LE:167:GLN:O    | 2.38                     | 0.42              |
| 26:LE:192:LYS:HG2 | 51:Lf:107:PRO:CB   | 2.50                     | 0.42              |
| 27:LF:116:GLN:HB3 | 27:LF:119:ASN:HB2  | 2.01                     | 0.42              |
| 27:LF:179:LEU:HB3 | 27:LF:184:ILE:HB   | 2.02                     | 0.42              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 32:LL:115:GLN:O   | 32:LL:119:GLU:HG2  | 2.20                     | 0.42              |
| 34:LN:58:GLY:O    | 34:LN:135:ILE:HD12 | 2.20                     | 0.42              |
| 39:LS:99:ASP:OD1  | 39:LS:100:LEU:N    | 2.48                     | 0.42              |
| 41:LU:48:LYS:HG2  | 41:LU:53:ALA:N     | 2.35                     | 0.42              |
| 41:LU:111:GLU:OE1 | 41:LU:111:GLU:N    | 2.52                     | 0.42              |
| 42:LV:91:LYS:HD3  | 42:LV:91:LYS:HA    | 1.81                     | 0.42              |
| 48:Lc:81:LEU:HD23 | 48:Lc:91:VAL:HG23  | 2.02                     | 0.42              |
| 49:Ld:51:LYS:O    | 49:Ld:55:LYS:HG2   | 2.20                     | 0.42              |
| 51:Lf:43:LEU:HD12 | 51:Lf:44:GLY:N     | 2.35                     | 0.42              |
| 64:SR:39:ALA:HA   | 65:SD:209:SER:O    | 2.19                     | 0.42              |
| 66:SF:67:PRO:O    | 66:SF:70:GLU:HB3   | 2.20                     | 0.42              |
| 68:SP:52:LYS:HG2  | 68:SP:53:GLN:N     | 2.34                     | 0.42              |
| 70:SS:7:GLU:CD    | 70:SS:7:GLU:N      | 2.74                     | 0.42              |
| 71:ST:125:PRO:HA  | 71:ST:128:GLN:HG3  | 2.02                     | 0.42              |
| 72:SU:51:LYS:HB3  | 72:SU:90:ASP:O     | 2.20                     | 0.42              |
| 73:Sc:33:GLU:CD   | 73:Sc:35:MET:H     | 2.28                     | 0.42              |
| 75:Sg:296:GLN:NE2 | 75:Sg:297:THR:HB   | 2.35                     | 0.42              |
| 77:SZ:69:THR:OG1  | 77:SZ:70:PRO:HD2   | 2.19                     | 0.42              |
| 77:SZ:70:PRO:O    | 77:SZ:74:SER:OG    | 2.20                     | 0.42              |
| 77:SZ:98:LYS:HE3  | 77:SZ:113:THR:HG22 | 2.01                     | 0.42              |
| 78:Sf:135:HIS:CE1 | 79:S2:1307:U:HO2'  | 2.34                     | 0.42              |
| 79:S2:194:C:H2'   | 79:S2:195:C:C6     | 2.55                     | 0.42              |
| 79:S2:291:G:O2'   | 79:S2:292:A:OP1    | 2.38                     | 0.42              |
| 79:S2:811:A:H2'   | 79:S2:812:A:C8     | 2.55                     | 0.42              |
| 79:S2:1134:G:H2'  | 79:S2:1135:C:H6    | 1.83                     | 0.42              |
| 79:S2:1235:G:C6   | 79:S2:1236:G:C5    | 3.08                     | 0.42              |
| 79:S2:1349:G:H2'  | 79:S2:1350:U:C6    | 2.55                     | 0.42              |
| 79:S2:1386:A:H2'  | 79:S2:1387:G:O4'   | 2.20                     | 0.42              |
| 79:S2:1577:G:H1'  | 79:S2:1582:C:C2    | 2.55                     | 0.42              |
| 81:AP:25:C:C2     | 81:AP:26:G:C8      | 3.08                     | 0.42              |
| 81:AP:27:U:H2'    | 81:AP:28:U:C6      | 2.54                     | 0.42              |
| 83:Ls:78:LEU:O    | 83:Ls:82:ILE:HG12  | 2.20                     | 0.42              |
| 84:Lt:61:LYS:HD3  | 84:Lt:72:GLU:HG3   | 2.02                     | 0.42              |
| 2:sE:132:GLY:HA3  | 2:sE:138:HIS:HE2   | 1.85                     | 0.42              |
| 3:sI:128:LYS:HE3  | 3:sI:128:LYS:HB2   | 1.90                     | 0.42              |
| 4:sL:94:HIS:N     | 4:sL:103:GLU:O     | 2.49                     | 0.42              |
| 6:sG:3:LEU:HD23   | 6:sG:18:VAL:HG22   | 2.02                     | 0.42              |
| 6:sG:22:ARG:H     | 6:sG:22:ARG:CD     | 2.30                     | 0.42              |
| 6:sG:39:ASP:HB3   | 6:sG:46:LYS:NZ     | 2.34                     | 0.42              |
| 6:sG:132:ARG:NH1  | 79:s2:168:C:C2     | 2.88                     | 0.42              |
| 6:sG:222:GLU:O    | 6:sG:225:GLN:HG2   | 2.20                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:sA:186:ARG:O    | 13:sV:45:ARG:NH1   | 2.53                     | 0.42              |
| 11:sB:33:VAL:HG13  | 11:sB:44:ILE:HB    | 2.00                     | 0.42              |
| 12:sH:11:PRO:HG2   | 12:sH:44:ASN:HB2   | 2.02                     | 0.42              |
| 15:sC:184:VAL:HG11 | 15:sC:243:ALA:O    | 2.20                     | 0.42              |
| 15:sC:272:HIS:O    | 15:sC:275:LYS:HG3  | 2.20                     | 0.42              |
| 16:sN:34:LYS:HA    | 16:sN:37:ILE:HD12  | 2.02                     | 0.42              |
| 19:sb:50:ALA:O     | 19:sb:71:ALA:HB2   | 2.19                     | 0.42              |
| 20:l7:33:U:H2'     | 20:l7:34:C:C6      | 2.55                     | 0.42              |
| 20:l7:116:G:H4'    | 25:lD:79:TYR:HE2   | 1.84                     | 0.42              |
| 21:l8:75:G:C1'     | 57:ll:29:MET:HE1   | 2.50                     | 0.42              |
| 22:lA:9:ARG:HH12   | 85:l5:1628:C:H3'   | 1.85                     | 0.42              |
| 22:lA:186:TYR:HB2  | 22:lA:196:TRP:CZ3  | 2.54                     | 0.42              |
| 24:lC:167:ALA:HB1  | 24:lC:221:PHE:CE1  | 2.55                     | 0.42              |
| 24:lC:331:TYR:CZ   | 24:lC:335:MET:HE2  | 2.55                     | 0.42              |
| 24:lC:331:TYR:CE1  | 24:lC:335:MET:HG2  | 2.54                     | 0.42              |
| 25:lD:44:TYR:HB3   | 40:lT:33:ILE:HG23  | 2.01                     | 0.42              |
| 25:lD:108:ARG:HB3  | 25:lD:251:PRO:HB2  | 2.01                     | 0.42              |
| 25:lD:272:SER:OG   | 25:lD:273:LEU:N    | 2.53                     | 0.42              |
| 27:lF:68:GLU:OE2   | 27:lF:68:GLU:HA    | 2.20                     | 0.42              |
| 27:lF:75:ALA:HB2   | 40:lT:140:PHE:CE2  | 2.55                     | 0.42              |
| 27:lF:155:TYR:CZ   | 27:lF:187:MET:HE2  | 2.55                     | 0.42              |
| 27:lF:232:ASP:HB3  | 27:lF:236:ARG:NH2  | 2.30                     | 0.42              |
| 29:lH:60:TRP:HB2   | 85:l5:4764:A:C6    | 2.54                     | 0.42              |
| 29:lH:78:GLN:O     | 29:lH:82:LYS:HG2   | 2.20                     | 0.42              |
| 30:lI:150:GLU:O    | 30:lI:154:ARG:HG2  | 2.20                     | 0.42              |
| 32:lL:165:LYS:HZ2  | 85:l5:511:C:H3'    | 1.84                     | 0.42              |
| 34:lN:30:TYR:N     | 34:lN:30:TYR:CD1   | 2.88                     | 0.42              |
| 34:lN:195:ARG:NH1  | 85:l5:98:A:OP1     | 2.51                     | 0.42              |
| 35:lO:138:LEU:HA   | 35:lO:138:LEU:HD12 | 1.75                     | 0.42              |
| 39:lS:11:LYS:HZ3   | 39:lS:67:VAL:HG22  | 1.85                     | 0.42              |
| 44:lY:48:PRO:O     | 44:lY:115:ARG:NH2  | 2.50                     | 0.42              |
| 45:lZ:76:ASN:HB3   | 45:lZ:79:HIS:ND1   | 2.33                     | 0.42              |
| 46:la:105:ARG:NH1  | 85:l5:509:A:N7     | 2.67                     | 0.42              |
| 51:lf:75:THR:HG22  | 51:lf:76:ARG:HG2   | 2.02                     | 0.42              |
| 52:lg:105:LYS:HA   | 52:lg:105:LYS:HD2  | 1.84                     | 0.42              |
| 53:lh:79:LYS:H     | 53:lh:84:ARG:NH2   | 2.17                     | 0.42              |
| 56:lk:17:ARG:NH2   | 85:l5:2772:C:O3'   | 2.53                     | 0.42              |
| 56:lk:49:ASP:H     | 56:lk:52:LYS:HZ2   | 1.66                     | 0.42              |
| 63:lz:2:SER:OG     | 63:lz:3:SER:N      | 2.52                     | 0.42              |
| 64:sR:25:GLY:HA3   | 64:sR:27:ASP:OD2   | 2.19                     | 0.42              |
| 64:sR:28:PHE:N     | 79:s2:1455:A:H3'   | 2.28                     | 0.42              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 64:sR:116:ASN:OD1 | 64:sR:117:LEU:N    | 2.47                     | 0.42              |
| 65:sD:75:LYS:HZ1  | 67:sK:22:VAL:HG23  | 1.85                     | 0.42              |
| 65:sD:170:THR:OG1 | 65:sD:187:LYS:HG2  | 2.20                     | 0.42              |
| 67:sK:47:LYS:O    | 67:sK:50:GLN:HG3   | 2.20                     | 0.42              |
| 67:sK:51:SER:HA   | 79:s2:1276:A:O2'   | 2.19                     | 0.42              |
| 69:sQ:119:LEU:O   | 69:sQ:120:LEU:HD13 | 2.20                     | 0.42              |
| 69:sQ:146:ARG:HE  | 82:pE:33:U:H5      | 1.65                     | 0.42              |
| 70:sS:39:ARG:NH2  | 70:sS:83:PHE:HZ    | 2.18                     | 0.42              |
| 70:sS:73:ASN:OD1  | 70:sS:73:ASN:N     | 2.52                     | 0.42              |
| 75:sg:165:ILE:HB  | 75:sg:177:TRP:HB2  | 2.00                     | 0.42              |
| 75:sg:178:ASN:C   | 75:sg:179:LEU:HD22 | 2.45                     | 0.42              |
| 77:sZ:46:ASN:O    | 77:sZ:78:LYS:HG3   | 2.20                     | 0.42              |
| 79:s2:16:G:H5'    | 79:s2:669:A:N1     | 2.35                     | 0.42              |
| 79:s2:152:U:C2    | 79:s2:153:G:C8     | 3.08                     | 0.42              |
| 79:s2:601:G:N1    | 79:s2:622:C:N3     | 2.67                     | 0.42              |
| 79:s2:991:G:C6    | 79:s2:1134:G:H4'   | 2.55                     | 0.42              |
| 79:s2:1224:G:C4   | 79:s2:1225:U:C5    | 3.08                     | 0.42              |
| 79:s2:1227:G:C2   | 79:s2:1228:A:C8    | 3.08                     | 0.42              |
| 79:s2:1281:G:H2'  | 79:s2:1282:A:C8    | 2.55                     | 0.42              |
| 79:s2:1443:C:H5'' | 79:s2:1444:U:OP2   | 2.19                     | 0.42              |
| 79:s2:1589:A:H2'  | 79:s2:1590:C:O4'   | 2.19                     | 0.42              |
| 79:s2:1642:U:H2'  | 79:s2:1643:U:H6    | 1.85                     | 0.42              |
| 79:s2:1855:G:C4   | 79:s2:1856:C:C5    | 3.08                     | 0.42              |
| 80:cB:426:LYS:HE2 | 80:cB:444:LEU:HB3  | 2.01                     | 0.42              |
| 80:cB:626:GLN:HB3 | 80:cB:631:ARG:HE   | 1.85                     | 0.42              |
| 80:cB:701:ARG:NE  | 80:cB:703:ASP:OD2  | 2.47                     | 0.42              |
| 80:cB:820:LEU:HG  | 80:cB:830:ARG:HE   | 1.84                     | 0.42              |
| 85:l5:66:A:O2'    | 85:l5:326:C:O2'    | 2.37                     | 0.42              |
| 85:l5:94:A:H8     | 85:l5:94:A:O5'     | 2.02                     | 0.42              |
| 85:l5:299:C:H2'   | 85:l5:300:A:C8     | 2.55                     | 0.42              |
| 85:l5:993:G:C6    | 85:l5:1050:C:C4    | 3.08                     | 0.42              |
| 85:l5:2326:G:C4   | 85:l5:2327:G:C8    | 3.07                     | 0.42              |
| 85:l5:2528:G:H4'  | 85:l5:2783:A:H4'   | 2.01                     | 0.42              |
| 85:l5:2752:G:H2'  | 85:l5:2753:G:C8    | 2.55                     | 0.42              |
| 85:l5:2812:A:H2'  | 85:l5:2813:A:C8    | 2.54                     | 0.42              |
| 85:l5:4299:U:H2'  | 85:l5:4300:U:C6    | 2.55                     | 0.42              |
| 85:l5:4579:U:H2'  | 85:l5:4580:U:O4'   | 2.19                     | 0.42              |
| 85:l5:4691:A:H2'  | 85:l5:4692:A:O4'   | 2.19                     | 0.42              |
| 85:l5:4886:C:H2'  | 85:l5:4887:C:H6    | 1.85                     | 0.42              |
| 85:l5:4930:C:H2'  | 85:l5:4931:G:O4'   | 2.20                     | 0.42              |
| 85:l5:4998:G:H2'  | 85:l5:4999:G:H8    | 1.83                     | 0.42              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 80:CB:330:LYS:HD3 | 80:CB:331:GLU:N    | 2.35                     | 0.42              |
| 2:SE:45:ILE:HG23  | 2:SE:46:ILE:H      | 1.85                     | 0.42              |
| 2:SE:160:ILE:HG21 | 2:SE:169:ILE:HG12  | 2.02                     | 0.42              |
| 2:SE:166:THR:C    | 2:SE:168:LYS:HD2   | 2.44                     | 0.42              |
| 6:SG:92:ARG:NH2   | 79:S2:1738:C:OP1   | 2.32                     | 0.42              |
| 7:SJ:173:VAL:HG12 | 79:S2:561:A:OP2    | 2.19                     | 0.42              |
| 10:SA:168:ALA:HA  | 10:SA:171:VAL:HG22 | 2.01                     | 0.42              |
| 11:SB:39:PHE:HE1  | 11:SB:189:ILE:HD11 | 1.84                     | 0.42              |
| 15:SC:84:PHE:CE2  | 15:SC:264:SER:HA   | 2.55                     | 0.42              |
| 85:L5:35:U:H2'    | 85:L5:36:U:H5'     | 2.01                     | 0.42              |
| 85:L5:48:G:P      | 34:LN:192:TRP:HE1  | 2.43                     | 0.42              |
| 85:L5:278:G:C6    | 85:L5:330:G:N7     | 2.88                     | 0.42              |
| 85:L5:294:G:H3'   | 85:L5:294:G:N3     | 2.35                     | 0.42              |
| 85:L5:953:C:H2'   | 85:L5:954:C:C6     | 2.54                     | 0.42              |
| 85:L5:959:G:H4'   | 85:L5:960:A:H5''   | 2.02                     | 0.42              |
| 85:L5:983:C:H2'   | 85:L5:984:C:O4'    | 2.20                     | 0.42              |
| 85:L5:1190:C:H2'  | 85:L5:1191:C:C6    | 2.55                     | 0.42              |
| 85:L5:1306:C:H2'  | 85:L5:1307:A:H8    | 1.85                     | 0.42              |
| 85:L5:1308:C:H2'  | 85:L5:1309:C:H6    | 1.84                     | 0.42              |
| 85:L5:1508:A:H2'  | 85:L5:1509:C:C6    | 2.55                     | 0.42              |
| 85:L5:1816:C:C4   | 85:L5:1817:U:C4    | 3.08                     | 0.42              |
| 85:L5:2574:G:OP1  | 45:LZ:67:LYS:HD3   | 2.19                     | 0.42              |
| 85:L5:2611:A:H2'  | 85:L5:2612:G:H8    | 1.85                     | 0.42              |
| 85:L5:2638:G:H4'  | 52:Lg:24:ARG:HH12  | 1.83                     | 0.42              |
| 85:L5:2844:A:N6   | 85:L5:3839:G:O2'   | 2.53                     | 0.42              |
| 85:L5:2887:U:O2'  | 38:LR:79:GLY:HA3   | 2.20                     | 0.42              |
| 85:L5:2897:G:C2   | 85:L5:3603:G:C2    | 3.08                     | 0.42              |
| 85:L5:3692:A:H2   | 61:Lp:19:GLY:HA2   | 1.85                     | 0.42              |
| 85:L5:3752:C:O2'  | 85:L5:3776:G:H1'   | 2.20                     | 0.42              |
| 85:L5:3868:G:H22  | 85:L5:3900:G:H1'   | 1.85                     | 0.42              |
| 85:L5:4046:A:O2'  | 85:L5:4047:A:H5'   | 2.19                     | 0.42              |
| 85:L5:4100:C:C2   | 85:L5:4108:G:N7    | 2.87                     | 0.42              |
| 85:L5:4223:C:H2'  | 85:L5:4224:A:C8    | 2.54                     | 0.42              |
| 85:L5:4587:G:N1   | 85:L5:4716:C:N3    | 2.68                     | 0.42              |
| 85:L5:4595:G:H2'  | 85:L5:4596:C:C6    | 2.55                     | 0.42              |
| 85:L5:4691:A:OP1  | 29:LH:75:SER:OG    | 2.29                     | 0.42              |
| 85:L5:4924:C:H2'  | 85:L5:4925:U:N1    | 2.35                     | 0.42              |
| 85:L5:5027:C:O2'  | 85:L5:5028:G:H5''  | 2.20                     | 0.42              |
| 20:L7:58:A:C4     | 20:L7:59:G:C8      | 3.07                     | 0.42              |
| 21:L8:14:U:H5''   | 36:LP:123:PRO:HG3  | 2.02                     | 0.42              |
| 21:L8:106:G:H5''  | 21:L8:137:A:H5'    | 2.02                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 26:LE:181:LEU:HD21 | 26:LE:268:GLN:HB2  | 2.02                     | 0.42              |
| 29:LH:78:GLN:HA    | 29:LH:81:ILE:HG12  | 2.02                     | 0.42              |
| 31:LJ:10:ASN:O     | 31:LJ:11:PRO:C     | 2.63                     | 0.42              |
| 31:LJ:16:ARG:N     | 31:LJ:135:GLY:O    | 2.41                     | 0.42              |
| 31:LJ:84:GLU:O     | 31:LJ:88:LYS:HG3   | 2.20                     | 0.42              |
| 31:LJ:109:ILE:HD12 | 31:LJ:128:LEU:H    | 1.85                     | 0.42              |
| 32:LL:42:LYS:O     | 32:LL:46:ILE:HG12  | 2.20                     | 0.42              |
| 32:LL:161:TYR:HD2  | 46:La:105:ARG:HH21 | 1.68                     | 0.42              |
| 33:LM:61:ILE:HD13  | 33:LM:61:ILE:HA    | 1.89                     | 0.42              |
| 34:LN:63:ARG:O     | 34:LN:64:ILE:HD13  | 2.20                     | 0.42              |
| 36:LP:105:LYS:HG2  | 36:LP:107:LEU:HD22 | 2.02                     | 0.42              |
| 37:LQ:80:ALA:HB3   | 37:LQ:100:VAL:HA   | 2.01                     | 0.42              |
| 39:LS:19:THR:C     | 39:LS:21:LYS:H     | 2.27                     | 0.42              |
| 41:LU:108:GLU:OE2  | 41:LU:109:SER:OG   | 2.38                     | 0.42              |
| 42:LV:85:ARG:HG2   | 42:LV:101:ASN:ND2  | 2.32                     | 0.42              |
| 46:La:42:ARG:O     | 46:La:46:ASP:OD1   | 2.37                     | 0.42              |
| 46:La:47:LYS:HG2   | 46:La:48:TYR:CE1   | 2.55                     | 0.42              |
| 48:Lc:78:ASN:HD21  | 61:Lp:43:GLY:HA3   | 1.85                     | 0.42              |
| 52:Lg:43:LYS:HE3   | 52:Lg:43:LYS:HB3   | 1.86                     | 0.42              |
| 59:Ln:9:ARG:HA     | 59:Ln:12:ARG:NH1   | 2.30                     | 0.42              |
| 60:Lo:21:HIS:HA    | 60:Lo:72:CYS:HA    | 2.01                     | 0.42              |
| 64:SR:24:LEU:HD12  | 64:SR:34:VAL:CG2   | 2.50                     | 0.42              |
| 64:SR:62:GLN:H     | 64:SR:62:GLN:HG3   | 1.68                     | 0.42              |
| 65:SD:85:GLU:N     | 65:SD:85:GLU:OE1   | 2.53                     | 0.42              |
| 66:SF:204:ARG:NE   | 73:Sc:63:ARG:HG3   | 2.35                     | 0.42              |
| 68:SP:38:SER:HA    | 70:SS:88:LYS:HZ2   | 1.84                     | 0.42              |
| 68:SP:107:ILE:HG23 | 68:SP:111:MET:SD   | 2.59                     | 0.42              |
| 70:SS:102:GLY:HA2  | 70:SS:105:ASN:OD1  | 2.20                     | 0.42              |
| 71:ST:42:HIS:HA    | 71:ST:83:GLN:NE2   | 2.35                     | 0.42              |
| 73:Sc:30:VAL:HG12  | 73:Sc:44:ARG:O     | 2.20                     | 0.42              |
| 75:Sg:23:THR:HB    | 75:Sg:31:ILE:HG22  | 2.01                     | 0.42              |
| 75:Sg:149:GLU:N    | 75:Sg:171:ASP:OD2  | 2.33                     | 0.42              |
| 75:Sg:165:ILE:HD11 | 75:Sg:179:LEU:CD2  | 2.48                     | 0.42              |
| 75:Sg:242:SER:HA   | 75:Sg:291:TRP:CD1  | 2.55                     | 0.42              |
| 77:SZ:45:ASN:O     | 77:SZ:45:ASN:ND2   | 2.53                     | 0.42              |
| 77:SZ:85:ARG:O     | 77:SZ:89:GLN:OE1   | 2.38                     | 0.42              |
| 79:S2:394:G:N3     | 79:S2:395:G:C8     | 2.88                     | 0.42              |
| 79:S2:878:G:C6     | 79:S2:909:G:C6     | 3.08                     | 0.42              |
| 79:S2:1175:G:C6    | 79:S2:1176:G:C5    | 3.08                     | 0.42              |
| 79:S2:1262:C:H2'   | 79:S2:1263:U:O4'   | 2.19                     | 0.42              |
| 79:S2:1551:U:H2'   | 79:S2:1578:U:O4    | 2.20                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 83:Ls:193:PHE:HA  | 83:Ls:197:SER:O   | 2.20                     | 0.42              |
| 84:Lt:66:ASN:O    | 84:Lt:67:ARG:HB3  | 2.20                     | 0.42              |
| 87:IW:113:LYS:HD3 | 87:IW:116:LYS:CE  | 2.48                     | 0.42              |
| 1:cH:99:ILE:HD11  | 1:cH:106:ILE:HD11 | 2.02                     | 0.41              |
| 4:sL:92:TYR:CE1   | 4:sL:105:ARG:HB2  | 2.55                     | 0.41              |
| 7:sJ:102:ILE:HG12 | 7:sJ:106:LEU:HD13 | 2.02                     | 0.41              |
| 7:sJ:126:ALA:O    | 7:sJ:130:ILE:HG12 | 2.20                     | 0.41              |
| 7:sJ:131:ARG:HA   | 7:sJ:131:ARG:HD2  | 1.78                     | 0.41              |
| 7:sJ:133:ARG:NH2  | 79:s2:563:G:O5'   | 2.48                     | 0.41              |
| 7:sJ:171:GLY:N    | 79:s2:561:A:OP1   | 2.35                     | 0.41              |
| 8:sY:109:GLU:HG3  | 8:sY:113:ARG:NH2  | 2.35                     | 0.41              |
| 10:sA:143:PRO:CD  | 13:sV:32:ILE:HD11 | 2.48                     | 0.41              |
| 12:sH:98:ARG:HH12 | 12:sH:128:ALA:HB3 | 1.84                     | 0.41              |
| 12:sH:145:ARG:HD2 | 18:sW:51:GLU:OE2  | 2.20                     | 0.41              |
| 13:sV:59:ILE:HA   | 13:sV:62:MET:HE3  | 2.02                     | 0.41              |
| 21:l8:50:C:H2'    | 57:l1:26:TRP:CZ3  | 2.55                     | 0.41              |
| 21:l8:75:G:H4'    | 57:l1:29:MET:HE1  | 2.02                     | 0.41              |
| 22:lA:34:PHE:HZ   | 85:l5:4087:G:H2'  | 1.84                     | 0.41              |
| 22:lA:181:LYS:HE2 | 85:l5:1577:G:C4   | 2.55                     | 0.41              |
| 22:lA:196:TRP:CH2 | 85:l5:1613:A:C2   | 3.08                     | 0.41              |
| 23:lB:17:LEU:HA   | 23:lB:19:ARG:HD3  | 2.02                     | 0.41              |
| 24:lC:85:HIS:O    | 24:lC:89:GLN:NE2  | 2.53                     | 0.41              |
| 24:lC:212:ASN:HB3 | 24:lC:213:GLU:OE2 | 2.20                     | 0.41              |
| 25:lD:225:GLN:HA  | 25:lD:228:LYS:HG2 | 2.02                     | 0.41              |
| 25:lD:239:MET:HE1 | 25:lD:240:TYR:CD1 | 2.54                     | 0.41              |
| 26:lE:70:LYS:NZ   | 85:l5:982:U:O2    | 2.29                     | 0.41              |
| 26:lE:146:PRO:HA  | 26:lE:164:PHE:CE2 | 2.54                     | 0.41              |
| 27:lF:31:LYS:HE3  | 85:l5:1438:U:O3'  | 2.20                     | 0.41              |
| 30:lI:140:THR:OG1 | 30:lI:141:LYS:N   | 2.53                     | 0.41              |
| 32:lL:47:ALA:HB3  | 32:lL:48:PRO:HD3  | 2.01                     | 0.41              |
| 35:lO:32:LYS:HE3  | 35:lO:32:LYS:HB2  | 1.82                     | 0.41              |
| 35:lO:62:MET:SD   | 85:l5:2045:G:N1   | 2.93                     | 0.41              |
| 41:lU:23:LEU:HD12 | 41:lU:24:ASP:N    | 2.35                     | 0.41              |
| 41:lU:24:ASP:HB2  | 41:lU:69:LYS:HZ3  | 1.85                     | 0.41              |
| 41:lU:67:LYS:HA   | 41:lU:67:LYS:HD3  | 1.88                     | 0.41              |
| 42:lV:113:LYS:HB2 | 42:lV:113:LYS:HE3 | 1.63                     | 0.41              |
| 43:lX:77:ILE:HG21 | 43:lX:116:LEU:CD2 | 2.50                     | 0.41              |
| 45:lZ:92:ASP:OD1  | 45:lZ:94:THR:HG23 | 2.19                     | 0.41              |
| 50:le:91:CYS:N    | 50:le:92:ASN:OD1  | 2.52                     | 0.41              |
| 55:lj:28:HIS:CE1  | 55:lj:31:LYS:HG3  | 2.54                     | 0.41              |
| 55:lj:28:HIS:HD1  | 55:lj:31:LYS:H    | 1.67                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 63:lz:109:ALA:HB1 | 63:lz:139:THR:HB   | 2.01                     | 0.41              |
| 64:sR:31:ASN:HA   | 64:sR:34:VAL:HG12  | 2.02                     | 0.41              |
| 66:sF:96:ALA:HA   | 66:sF:99:ILE:HD12  | 2.01                     | 0.41              |
| 67:sK:28:HIS:NE2  | 74:sd:7:TYR:CZ     | 2.77                     | 0.41              |
| 68:sP:89:MET:HE3  | 68:sP:89:MET:N     | 2.26                     | 0.41              |
| 73:sc:17:VAL:HG21 | 73:sc:50:VAL:HG11  | 2.02                     | 0.41              |
| 73:sc:26:GLN:H    | 73:sc:26:GLN:HG2   | 1.58                     | 0.41              |
| 75:sg:164:ILE:CD1 | 75:sg:176:VAL:HG13 | 2.40                     | 0.41              |
| 79:s2:87:U:N3     | 79:s2:88:G:N7      | 2.68                     | 0.41              |
| 79:s2:373:G:C6    | 79:s2:392:A:C6     | 3.07                     | 0.41              |
| 79:s2:944:A:H2'   | 79:s2:945:U:C6     | 2.55                     | 0.41              |
| 79:s2:1117:C:H2'  | 79:s2:1118:C:C6    | 2.55                     | 0.41              |
| 79:s2:1189:A:H2'  | 79:s2:1190:A:C8    | 2.55                     | 0.41              |
| 79:s2:1260:A:C6   | 79:s2:1619:A:C6    | 3.08                     | 0.41              |
| 79:s2:1355:C:O5'  | 79:s2:1355:C:H6    | 2.02                     | 0.41              |
| 79:s2:1774:C:C4   | 79:s2:1775:U:H1'   | 2.55                     | 0.41              |
| 79:s2:1782:G:C8   | 79:s2:1784:G:N7    | 2.88                     | 0.41              |
| 79:s2:1841:C:H2'  | 79:s2:1842:C:C6    | 2.54                     | 0.41              |
| 80:cB:83:GLU:H    | 80:cB:83:GLU:CD    | 2.28                     | 0.41              |
| 80:cB:293:ILE:HB  | 80:cB:294:LEU:HD12 | 2.02                     | 0.41              |
| 80:cB:687:THR:O   | 80:cB:696:ASN:HA   | 2.19                     | 0.41              |
| 83:ls:40:MET:SD   | 83:ls:40:MET:C     | 3.03                     | 0.41              |
| 85:l5:229:G:H2'   | 85:l5:230:G:C8     | 2.54                     | 0.41              |
| 85:l5:328:A:H2'   | 85:l5:329:A:C8     | 2.55                     | 0.41              |
| 85:l5:506:C:H2'   | 85:l5:507:G:C8     | 2.55                     | 0.41              |
| 85:l5:674:G:H2'   | 85:l5:675:C:C6     | 2.55                     | 0.41              |
| 85:l5:949:G:H2'   | 85:l5:950:G:H8     | 1.84                     | 0.41              |
| 85:l5:1183:C:H2'  | 85:l5:1184:A:H8    | 1.79                     | 0.41              |
| 85:l5:1377:G:H4'  | 85:l5:1378:C:H5''  | 2.01                     | 0.41              |
| 85:l5:1617:G:H1'  | 85:l5:2513:A:H61   | 1.84                     | 0.41              |
| 85:l5:1991:A:H2'  | 85:l5:1991:A:N3    | 2.35                     | 0.41              |
| 85:l5:3716:C:N4   | 85:l5:3735:G:O2'   | 2.51                     | 0.41              |
| 85:l5:3861:A:H2'  | 85:l5:3862:A:H8    | 1.84                     | 0.41              |
| 85:l5:4139:G:N2   | 85:l5:4140:C:H41   | 2.13                     | 0.41              |
| 85:l5:4195:G:O2'  | 85:l5:4442:U:OP1   | 2.28                     | 0.41              |
| 85:l5:4736:C:H2'  | 85:l5:4737:G:C8    | 2.52                     | 0.41              |
| 85:l5:4881:U:H4'  | 85:l5:4882:U:H5'   | 2.02                     | 0.41              |
| 85:l5:4884:G:C6   | 85:l5:4936:G:C6    | 3.08                     | 0.41              |
| 85:l5:5062:G:C2   | 85:l5:5063:G:C8    | 3.08                     | 0.41              |
| 80:CB:78:PHE:HD1  | 80:CB:79:TYR:N     | 2.18                     | 0.41              |
| 80:CB:519:LYS:HD3 | 80:CB:568:ILE:HB   | 2.02                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 80:CB:776:VAL:HG13 | 80:CB:778:GLY:H    | 1.84                     | 0.41              |
| 2:SE:178:GLY:O     | 2:SE:231:GLY:HA2   | 2.20                     | 0.41              |
| 3:SI:110:ARG:HH21  | 3:SI:122:GLY:HA3   | 1.85                     | 0.41              |
| 4:SL:94:HIS:CD2    | 79:S2:355:G:H5'    | 2.54                     | 0.41              |
| 4:SL:150:GLY:HA2   | 4:SL:153:LYS:NZ    | 2.35                     | 0.41              |
| 5:SX:115:ILE:HD13  | 5:SX:115:ILE:HA    | 1.91                     | 0.41              |
| 6:SG:183:ARG:HG2   | 6:SG:187:HIS:CE1   | 2.55                     | 0.41              |
| 7:SJ:8:VAL:HG21    | 79:S2:828:G:OP1    | 2.20                     | 0.41              |
| 7:SJ:113:GLN:HE21  | 7:SJ:149:VAL:CG2   | 2.33                     | 0.41              |
| 7:SJ:122:SER:O     | 7:SJ:124:HIS:N     | 2.53                     | 0.41              |
| 86:Se:44:ASN:OD1   | 86:Se:44:ASN:N     | 2.48                     | 0.41              |
| 10:SA:108:PHE:CE2  | 10:SA:119:PRO:HD2  | 2.54                     | 0.41              |
| 12:SH:78:ARG:NH1   | 12:SH:81:ARG:HH22  | 2.18                     | 0.41              |
| 12:SH:138:GLU:H    | 12:SH:159:ASP:HB2  | 1.84                     | 0.41              |
| 14:Sa:93:LYS:HE2   | 14:Sa:93:LYS:HB2   | 1.91                     | 0.41              |
| 85:L5:153:G:C2     | 85:L5:154:G:C8     | 3.07                     | 0.41              |
| 85:L5:250:C:H2'    | 85:L5:251:C:H6     | 1.85                     | 0.41              |
| 85:L5:443:G:H2'    | 85:L5:444:G:H8     | 1.85                     | 0.41              |
| 85:L5:480:C:H2'    | 85:L5:481:G:H8     | 1.84                     | 0.41              |
| 85:L5:720:G:C6     | 85:L5:949:G:C6     | 3.08                     | 0.41              |
| 85:L5:739:G:C2     | 85:L5:926:G:C4     | 3.08                     | 0.41              |
| 85:L5:976:G:C2     | 24:LC:323:ARG:NH2  | 2.88                     | 0.41              |
| 85:L5:1318:C:H42   | 85:L5:1322:A:H8    | 1.68                     | 0.41              |
| 85:L5:1338:G:H2'   | 46:La:17:HIS:CE1   | 2.48                     | 0.41              |
| 85:L5:2073:C:H5'   | 27:LF:213:LEU:O    | 2.20                     | 0.41              |
| 85:L5:2374:A:H2'   | 85:L5:2375:A:H8    | 1.84                     | 0.41              |
| 85:L5:2509:C:H2'   | 85:L5:2510:G:H8    | 1.85                     | 0.41              |
| 85:L5:2720:C:H2'   | 85:L5:2721:G:O4'   | 2.20                     | 0.41              |
| 85:L5:2805:C:H2'   | 85:L5:2806:A:C8    | 2.54                     | 0.41              |
| 85:L5:3833:C:H2'   | 85:L5:3834:C:C6    | 2.51                     | 0.41              |
| 85:L5:3963:A:H5'   | 85:L5:3965:A:H5'   | 2.01                     | 0.41              |
| 85:L5:4041:C:O2    | 63:Lz:103:LEU:HD13 | 2.20                     | 0.41              |
| 85:L5:4102:C:H1'   | 85:L5:4105:A:N3    | 2.33                     | 0.41              |
| 85:L5:4105:A:O4'   | 85:L5:4106:G:C8    | 2.73                     | 0.41              |
| 85:L5:4258:C:H2'   | 85:L5:4259:C:C6    | 2.54                     | 0.41              |
| 85:L5:4548:A:H5'   | 85:L5:4549:G:H5'   | 2.02                     | 0.41              |
| 85:L5:4739:C:H2'   | 85:L5:4740:G:H5'   | 2.01                     | 0.41              |
| 85:L5:4915:G:H2'   | 85:L5:4916:G:H8    | 1.84                     | 0.41              |
| 20:L7:60:G:N3      | 20:L7:61:G:C8      | 2.88                     | 0.41              |
| 22:LA:51:ASP:OD1   | 22:LA:58:LEU:HD21  | 2.20                     | 0.41              |
| 23:LB:153:MET:HB3  | 23:LB:194:LEU:HD11 | 2.01                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:LB:299:ILE:O    | 23:LB:302:ASN:ND2  | 2.35                     | 0.41              |
| 25:LD:200:MET:CE   | 25:LD:240:TYR:HD2  | 2.31                     | 0.41              |
| 27:LF:159:TYR:CE2  | 27:LF:168:ALA:HB2  | 2.54                     | 0.41              |
| 30:LI:72:ALA:O     | 30:LI:76:MET:HG2   | 2.20                     | 0.41              |
| 31:LJ:7:GLU:HA     | 31:LJ:10:ASN:OD1   | 2.20                     | 0.41              |
| 38:LR:41:ILE:O     | 38:LR:45:ILE:HG12  | 2.19                     | 0.41              |
| 40:LT:81:LYS:HB2   | 47:Lb:16:TRP:CZ3   | 2.55                     | 0.41              |
| 43:LX:74:TYR:CD1   | 53:Lh:25:LYS:HG3   | 2.52                     | 0.41              |
| 47:Lb:39:PHE:O     | 47:Lb:43:MET:SD    | 2.78                     | 0.41              |
| 62:Lr:89:THR:O     | 62:Lr:92:SER:OG    | 2.29                     | 0.41              |
| 63:Lz:116:LEU:HD13 | 63:Lz:120:ILE:HD11 | 2.00                     | 0.41              |
| 64:SR:104:GLU:O    | 64:SR:107:LYS:HB2  | 2.20                     | 0.41              |
| 65:SD:156:LEU:HD12 | 65:SD:157:MET:H    | 1.85                     | 0.41              |
| 69:SQ:116:ASP:O    | 69:SQ:119:LEU:HG   | 2.19                     | 0.41              |
| 70:SS:22:GLY:HA2   | 70:SS:56:ALA:HB3   | 2.02                     | 0.41              |
| 75:Sg:217:MET:SD   | 75:Sg:217:MET:C    | 3.02                     | 0.41              |
| 79:S2:1046:U:H2'   | 79:S2:1047:C:C6    | 2.55                     | 0.41              |
| 79:S2:1069:U:C2    | 79:S2:1070:A:C8    | 3.08                     | 0.41              |
| 79:S2:1075:C:H2'   | 79:S2:1076:G:H8    | 1.84                     | 0.41              |
| 79:S2:1140:G:H2'   | 79:S2:1141:G:C8    | 2.55                     | 0.41              |
| 79:S2:1240:A:H1'   | 79:S2:1267:C:O2'   | 2.19                     | 0.41              |
| 79:S2:1686:G:H2'   | 79:S2:1687:C:C6    | 2.54                     | 0.41              |
| 79:S2:1748:G:C6    | 79:S2:1787:G:C6    | 3.08                     | 0.41              |
| 79:S2:1794:C:C2    | 79:S2:1795:G:C8    | 3.07                     | 0.41              |
| 81:AP:18:G:C5      | 81:AP:58:A:C5      | 3.08                     | 0.41              |
| 84:Lt:133:LEU:HD23 | 84:Lt:133:LEU:HA   | 1.84                     | 0.41              |
| 87:IW:109:ILE:O    | 87:IW:113:LYS:HG2  | 2.19                     | 0.41              |
| 87:LW:9:SER:HB2    | 87:LW:11:TYR:CD1   | 2.55                     | 0.41              |
| 1:cH:75:LEU:O      | 1:cH:79:LYS:NZ     | 2.53                     | 0.41              |
| 2:sE:58:GLY:N      | 79:s2:495:U:OP1    | 2.53                     | 0.41              |
| 2:sE:94:LYS:HG2    | 8:sY:17:LEU:HG     | 2.02                     | 0.41              |
| 5:sX:67:ARG:NH2    | 79:s2:618:C:H41    | 2.18                     | 0.41              |
| 6:sG:160:LYS:NZ    | 6:sG:172:LYS:O     | 2.53                     | 0.41              |
| 7:sJ:136:ARG:HG2   | 7:sJ:137:VAL:O     | 2.21                     | 0.41              |
| 8:sY:27:VAL:HG11   | 8:sY:35:VAL:HG21   | 2.01                     | 0.41              |
| 9:se:11:LYS:HG3    | 9:se:12:VAL:N      | 2.35                     | 0.41              |
| 10:sA:16:LEU:HD11  | 64:sR:115:SER:HB2  | 2.02                     | 0.41              |
| 10:sA:18:PHE:HD1   | 10:sA:173:LEU:HD21 | 1.85                     | 0.41              |
| 11:sB:193:ILE:HD12 | 11:sB:193:ILE:HA   | 1.90                     | 0.41              |
| 11:sB:220:LYS:HE2  | 11:sB:220:LYS:HB2  | 1.85                     | 0.41              |
| 12:sH:46:THR:CG2   | 12:sH:65:PRO:HD3   | 2.35                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 15:sC:196:ILE:O    | 15:sC:223:TYR:N    | 2.52                     | 0.41              |
| 16:sN:123:HIS:HE2  | 16:sN:141:TYR:HD2  | 1.67                     | 0.41              |
| 21:l8:124:U:H5'    | 85:l5:2544:G:H22   | 1.85                     | 0.41              |
| 22:lA:39:GLY:HA2   | 22:lA:93:LYS:HG3   | 2.03                     | 0.41              |
| 22:lA:42:LYS:HE3   | 22:lA:87:PHE:CG    | 2.55                     | 0.41              |
| 24:lC:28:PHE:CD2   | 24:lC:132:ALA:HB2  | 2.45                     | 0.41              |
| 24:lC:104:PRO:HD2  | 85:l5:1517:G:H1    | 1.85                     | 0.41              |
| 25:lD:107:ARG:HD2  | 25:lD:107:ARG:HA   | 1.78                     | 0.41              |
| 25:lD:164:LYS:HA   | 25:lD:164:LYS:HD2  | 1.85                     | 0.41              |
| 25:lD:284:LYS:HA   | 25:lD:284:LYS:HE3  | 2.02                     | 0.41              |
| 26:lE:185:PRO:HD3  | 85:l5:4938:A:H4'   | 2.02                     | 0.41              |
| 27:lF:144:TYR:CE2  | 27:lF:237:GLU:HA   | 2.55                     | 0.41              |
| 29:lH:1:MET:SD     | 29:lH:1:MET:N      | 2.76                     | 0.41              |
| 29:lH:157:SER:O    | 29:lH:161:ILE:HG23 | 2.20                     | 0.41              |
| 31:lJ:40:LEU:O     | 31:lJ:44:THR:OG1   | 2.13                     | 0.41              |
| 31:lJ:81:GLU:OE2   | 31:lJ:82:ILE:HG12  | 2.20                     | 0.41              |
| 35:lO:71:TYR:OH    | 85:l5:3888:G:P     | 2.78                     | 0.41              |
| 35:lO:93:LYS:CE    | 85:l5:1308:C:O3'   | 2.68                     | 0.41              |
| 37:lQ:186:TYR:CE2  | 37:lQ:188:ASN:HB3  | 2.55                     | 0.41              |
| 38:lR:104:ARG:HA   | 38:lR:107:ARG:NH1  | 2.35                     | 0.41              |
| 40:lT:122:LYS:HB2  | 40:lT:122:LYS:HE3  | 1.62                     | 0.41              |
| 41:lU:95:ASN:O     | 41:lU:96:LEU:HD22  | 2.19                     | 0.41              |
| 41:lU:107:LYS:HZ3  | 85:l5:2717:G:H5'   | 1.85                     | 0.41              |
| 42:lV:32:THR:HG21  | 42:lV:113:LYS:HG3  | 2.01                     | 0.41              |
| 44:lY:41:LYS:HE2   | 44:lY:41:LYS:HB2   | 1.93                     | 0.41              |
| 44:lY:50:ARG:HB2   | 44:lY:115:ARG:NH1  | 2.35                     | 0.41              |
| 45:lZ:55:ALA:H     | 85:l5:4129:G:P     | 2.43                     | 0.41              |
| 46:la:22:ILE:O     | 46:la:24:LYS:HG3   | 2.20                     | 0.41              |
| 49:ld:24:GLU:OE1   | 49:ld:85:ARG:CZ    | 2.67                     | 0.41              |
| 49:ld:34:HIS:HA    | 85:l5:4636:U:OP1   | 2.19                     | 0.41              |
| 51:lf:68:ARG:NH2   | 85:l5:443:G:OP1    | 2.53                     | 0.41              |
| 52:lg:65:MET:HE1   | 85:l5:2748:C:O2'   | 2.20                     | 0.41              |
| 61:lp:8:VAL:O      | 61:lp:11:VAL:HG22  | 2.21                     | 0.41              |
| 62:lr:20:ARG:O     | 62:lr:22:LYS:N     | 2.53                     | 0.41              |
| 63:lz:1:MET:N      | 85:l5:4054:C:OP1   | 2.30                     | 0.41              |
| 66:sF:42:LYS:HD2   | 66:sF:42:LYS:HA    | 1.75                     | 0.41              |
| 66:sF:91:ARG:HD2   | 77:sZ:103:HIS:CE1  | 2.55                     | 0.41              |
| 66:sF:119:SER:HA   | 66:sF:193:LYS:HD3  | 2.02                     | 0.41              |
| 66:sF:173:LEU:HD23 | 66:sF:173:LEU:HA   | 1.94                     | 0.41              |
| 67:sK:16:PHE:O     | 67:sK:91:PRO:HA    | 2.20                     | 0.41              |
| 68:sP:41:GLN:HG2   | 68:sP:84:ILE:HG12  | 2.02                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 69:sQ:73:LYS:NZ    | 79:s2:1585:U:O2    | 2.53                     | 0.41              |
| 71:sT:40:ALA:CB    | 71:sT:95:GLY:HA2   | 2.49                     | 0.41              |
| 75:sg:30:MET:O     | 75:sg:31:ILE:HD13  | 2.20                     | 0.41              |
| 75:sg:45:LEU:HB3   | 75:sg:47:ARG:NH1   | 2.35                     | 0.41              |
| 75:sg:220:ASP:HB3  | 75:sg:225:LYS:H    | 1.86                     | 0.41              |
| 77:sZ:92:LEU:HD23  | 77:sZ:92:LEU:HA    | 1.90                     | 0.41              |
| 79:s2:943:U:H2'    | 79:s2:944:A:H8     | 1.85                     | 0.41              |
| 79:s2:1135:C:H2'   | 79:s2:1136:U:H6    | 1.85                     | 0.41              |
| 79:s2:1294:G:N3    | 79:s2:1294:G:H2'   | 2.35                     | 0.41              |
| 79:s2:1518:C:C5'   | 79:s2:1519:U:H5''  | 2.50                     | 0.41              |
| 79:s2:1590:C:H3'   | 79:s2:1591:C:C6    | 2.55                     | 0.41              |
| 80:cB:50:ARG:HG3   | 80:cB:56:PHE:CZ    | 2.55                     | 0.41              |
| 80:cB:135:VAL:HG23 | 80:cB:181:ILE:HD11 | 2.01                     | 0.41              |
| 80:cB:157:MET:SD   | 80:cB:157:MET:C    | 3.03                     | 0.41              |
| 80:cB:283:LYS:HD3  | 80:cB:284:LYS:H    | 1.85                     | 0.41              |
| 80:cB:433:ASN:OD1  | 80:cB:441:ASP:HB2  | 2.21                     | 0.41              |
| 80:cB:604:MET:HB3  | 80:cB:704:VAL:HG12 | 2.01                     | 0.41              |
| 80:cB:604:MET:CB   | 80:cB:704:VAL:HA   | 2.48                     | 0.41              |
| 81:aP:36:C:C2      | 81:aP:37:A:C8      | 3.08                     | 0.41              |
| 84:lt:76:SER:HB3   | 84:lt:117:ARG:HG3  | 2.01                     | 0.41              |
| 85:l5:106:A:H8     | 85:l5:106:A:O5'    | 2.03                     | 0.41              |
| 85:l5:450:G:C6     | 85:l5:1298:C:C4    | 3.09                     | 0.41              |
| 85:l5:1074:G:N3    | 85:l5:1074:G:H2'   | 2.33                     | 0.41              |
| 85:l5:1170:G:N1    | 85:l5:1192:C:C4    | 2.88                     | 0.41              |
| 85:l5:1190:C:H2'   | 85:l5:1191:C:C6    | 2.54                     | 0.41              |
| 85:l5:1520:C:H2'   | 85:l5:1521:C:H6    | 1.85                     | 0.41              |
| 85:l5:1621:A:H2'   | 85:l5:1622:U:H6    | 1.85                     | 0.41              |
| 85:l5:1681:G:H2'   | 85:l5:1682:A:C8    | 2.56                     | 0.41              |
| 85:l5:1873:A:H2'   | 85:l5:1874:A:H8    | 1.84                     | 0.41              |
| 85:l5:2074:C:C2    | 85:l5:2075:G:C8    | 3.07                     | 0.41              |
| 85:l5:3651:A:H2'   | 85:l5:3652:A:C8    | 2.55                     | 0.41              |
| 85:l5:3967:G:O6    | 85:l5:4055:U:C4    | 2.73                     | 0.41              |
| 85:l5:4238:G:C2    | 85:l5:4239:A:C5    | 3.08                     | 0.41              |
| 85:l5:4432:C:H2'   | 85:l5:4433:G:O4'   | 2.20                     | 0.41              |
| 85:l5:4602:A:H3'   | 85:l5:4603:C:C6    | 2.55                     | 0.41              |
| 85:l5:4742:G:H2'   | 85:l5:4743:G:C8    | 2.55                     | 0.41              |
| 80:CB:291:GLN:O    | 80:CB:295:ASP:HB2  | 2.20                     | 0.41              |
| 80:CB:426:LYS:HD3  | 80:CB:446:PRO:HB3  | 2.02                     | 0.41              |
| 80:CB:743:PRO:O    | 80:CB:790:VAL:HG23 | 2.20                     | 0.41              |
| 80:CB:758:GLY:O    | 80:CB:762:VAL:HG23 | 2.20                     | 0.41              |
| 80:CB:779:THR:HG23 | 83:Ls:133:GLU:OE1  | 2.21                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:SE:129:ILE:HD12  | 2:SE:129:ILE:HA    | 1.82                     | 0.41              |
| 3:SI:181:GLN:HE22  | 79:S2:379:C:P      | 2.43                     | 0.41              |
| 4:SL:23:VAL:HG22   | 4:SL:24:LEU:N      | 2.33                     | 0.41              |
| 6:SG:41:LEU:HB3    | 6:SG:45:TRP:CD1    | 2.56                     | 0.41              |
| 6:SG:203:LYS:O     | 6:SG:203:LYS:NZ    | 2.54                     | 0.41              |
| 6:SG:216:ARG:C     | 6:SG:218:LYS:N     | 2.78                     | 0.41              |
| 7:SJ:107:GLU:OE2   | 7:SJ:108:ARG:HD2   | 2.20                     | 0.41              |
| 10:SA:51:LEU:HD23  | 10:SA:51:LEU:HA    | 1.81                     | 0.41              |
| 11:SB:119:THR:OG1  | 11:SB:143:THR:OG1  | 2.31                     | 0.41              |
| 11:SB:134:LEU:HD21 | 11:SB:218:LEU:HB2  | 2.01                     | 0.41              |
| 12:SH:100:ILE:HA   | 12:SH:100:ILE:HD13 | 1.82                     | 0.41              |
| 14:Sa:22:ARG:H     | 14:Sa:22:ARG:HG2   | 1.54                     | 0.41              |
| 17:SO:14:VAL:N     | 17:SO:15:ILE:HA    | 2.28                     | 0.41              |
| 17:SO:66:ARG:HE    | 17:SO:66:ARG:HB2   | 1.69                     | 0.41              |
| 17:SO:83:GLN:CD    | 17:SO:87:GLU:OE2   | 2.61                     | 0.41              |
| 18:SW:71:LYS:HZ3   | 79:S2:1156:U:P     | 2.42                     | 0.41              |
| 18:SW:107:SER:HG   | 79:S2:860:G:N2     | 2.18                     | 0.41              |
| 85:L5:74:G:H5'     | 32:LL:60:ARG:O     | 2.20                     | 0.41              |
| 85:L5:138:G:C6     | 85:L5:139:G:C6     | 3.08                     | 0.41              |
| 85:L5:302:C:H2'    | 85:L5:303:C:C6     | 2.54                     | 0.41              |
| 85:L5:305:A:H5''   | 54:Li:53:TYR:CE2   | 2.55                     | 0.41              |
| 85:L5:460:C:C2     | 85:L5:461:G:C8     | 3.08                     | 0.41              |
| 85:L5:1353:G:C2    | 85:L5:1504:G:C6    | 3.08                     | 0.41              |
| 85:L5:1403:G:N2    | 85:L5:1415:G:C4    | 2.88                     | 0.41              |
| 85:L5:1458:C:OP1   | 37:LQ:69:LYS:NZ    | 2.53                     | 0.41              |
| 85:L5:1815:G:C5    | 47:Lb:45:PHE:CE2   | 3.08                     | 0.41              |
| 85:L5:1977:C:H4'   | 84:Lt:83:LYS:NZ    | 2.35                     | 0.41              |
| 85:L5:2309:G:O6    | 85:L5:2330:G:C2    | 2.73                     | 0.41              |
| 85:L5:2535:G:H2'   | 85:L5:2536:A:C8    | 2.56                     | 0.41              |
| 85:L5:3598:C:H2'   | 85:L5:3599:A:C8    | 2.56                     | 0.41              |
| 85:L5:3659:G:H2'   | 85:L5:3660:C:C6    | 2.55                     | 0.41              |
| 85:L5:3872:A:H2'   | 85:L5:3873:G:H8    | 1.85                     | 0.41              |
| 85:L5:3919:C:H4'   | 22:LA:207:VAL:HG12 | 2.01                     | 0.41              |
| 85:L5:3967:G:H5'   | 85:L5:3970:G:H22   | 1.85                     | 0.41              |
| 85:L5:4103:C:O3'   | 85:L5:4107:G:OP1   | 2.37                     | 0.41              |
| 85:L5:4212:A:H4'   | 85:L5:4213:A:N3    | 2.35                     | 0.41              |
| 85:L5:4356:G:C2    | 85:L5:4357:G:C8    | 3.08                     | 0.41              |
| 85:L5:4407:G:C4    | 85:L5:4408:G:C8    | 3.07                     | 0.41              |
| 85:L5:4590:A:H2'   | 85:L5:4591:U:C6    | 2.55                     | 0.41              |
| 23:LB:53:MET:CB    | 23:LB:77:THR:HA    | 2.51                     | 0.41              |
| 25:LD:44:TYR:O     | 40:LT:33:ILE:HD11  | 2.19                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:LD:239:MET:SD   | 25:LD:240:TYR:N    | 2.93                     | 0.41              |
| 26:LE:223:ARG:HH12 | 26:LE:237:LYS:HB3  | 1.85                     | 0.41              |
| 27:LF:194:ILE:HD13 | 27:LF:194:ILE:HA   | 1.92                     | 0.41              |
| 32:LL:18:TRP:H     | 32:LL:18:TRP:CD1   | 2.37                     | 0.41              |
| 34:LN:22:LEU:HB3   | 34:LN:26:ARG:NH1   | 2.35                     | 0.41              |
| 37:LQ:25:LEU:HA    | 37:LQ:28:LEU:CD2   | 2.50                     | 0.41              |
| 38:LR:62:ARG:O     | 38:LR:65:LYS:HG2   | 2.20                     | 0.41              |
| 39:LS:26:PRO:HB2   | 39:LS:28:TYR:HE2   | 1.85                     | 0.41              |
| 40:LT:11:THR:HA    | 40:LT:14:MET:HB3   | 2.01                     | 0.41              |
| 40:LT:94:GLU:OE2   | 40:LT:94:GLU:N     | 2.30                     | 0.41              |
| 41:LU:100:LEU:HD23 | 41:LU:100:LEU:HA   | 1.84                     | 0.41              |
| 42:LV:60:MET:HE2   | 42:LV:129:TRP:HH2  | 1.85                     | 0.41              |
| 43:LX:120:ASP:HB3  | 43:LX:144:TYR:CZ   | 2.56                     | 0.41              |
| 44:LY:4:ASN:HB2    | 44:LY:7:VAL:HG12   | 2.01                     | 0.41              |
| 48:Lc:57:LYS:HA    | 48:Lc:60:ILE:HG12  | 2.01                     | 0.41              |
| 63:Lz:105:LYS:HE2  | 63:Lz:105:LYS:HB2  | 1.81                     | 0.41              |
| 64:SR:16:ILE:HD12  | 64:SR:16:ILE:HA    | 1.82                     | 0.41              |
| 66:SF:173:LEU:O    | 66:SF:177:LEU:HD23 | 2.21                     | 0.41              |
| 68:SP:120:SER:O    | 68:SP:120:SER:OG   | 2.37                     | 0.41              |
| 69:SQ:36:GLY:O     | 71:ST:7:LYS:HD3    | 2.20                     | 0.41              |
| 69:SQ:85:ARG:O     | 69:SQ:88:ILE:HG13  | 2.19                     | 0.41              |
| 70:SS:88:LYS:HE2   | 79:S2:1612:G:O3'   | 2.20                     | 0.41              |
| 71:ST:52:TRP:CD1   | 71:ST:52:TRP:H     | 2.38                     | 0.41              |
| 71:ST:98:SER:HG    | 79:S2:1568:C:P     | 2.43                     | 0.41              |
| 75:Sg:20:GLN:HE22  | 75:Sg:69:VAL:HG12  | 1.85                     | 0.41              |
| 75:Sg:129:ILE:HB   | 75:Sg:142:VAL:CG1  | 2.50                     | 0.41              |
| 75:Sg:242:SER:HA   | 75:Sg:243:PRO:HD3  | 1.92                     | 0.41              |
| 77:SZ:97:ILE:HG23  | 77:SZ:97:ILE:HD12  | 1.87                     | 0.41              |
| 77:SZ:104:ARG:HG3  | 77:SZ:105:ALA:N    | 2.34                     | 0.41              |
| 78:Sf:118:ARG:HD3  | 78:Sf:132:MET:O    | 2.21                     | 0.41              |
| 79:S2:118:C:H2'    | 79:S2:119:U:O4'    | 2.20                     | 0.41              |
| 79:S2:319:C:H2'    | 79:S2:320:G:C8     | 2.55                     | 0.41              |
| 79:S2:610:G:C6     | 79:S2:634:A:N1     | 2.88                     | 0.41              |
| 79:S2:1101:U:C2    | 79:S2:1102:G:N7    | 2.88                     | 0.41              |
| 79:S2:1162:C:H2'   | 79:S2:1163:C:O4'   | 2.20                     | 0.41              |
| 79:S2:1269:G:H2'   | 79:S2:1270:G:C8    | 2.54                     | 0.41              |
| 79:S2:1862:G:O2'   | 79:S2:1864:U:OP2   | 2.35                     | 0.41              |
| 82:PE:19:G:N1      | 82:PE:57:A:N3      | 2.68                     | 0.41              |
| 87:IW:49:ILE:HD13  | 87:IW:49:ILE:HA    | 1.96                     | 0.41              |
| 87:IW:80:ARG:HB3   | 87:IW:80:ARG:NH1   | 2.33                     | 0.41              |
| 1:CH:130:LEU:HD12  | 1:CH:131:LYS:N     | 2.35                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:cH:28:ALA:HA     | 1:cH:31:ARG:HD2    | 2.02                     | 0.41              |
| 2:sE:59:ASP:HB2    | 79:s2:494:C:OP1    | 2.20                     | 0.41              |
| 3:sI:186:ASP:OD1   | 79:s2:220:U:H4'    | 2.20                     | 0.41              |
| 4:sL:27:GLU:C      | 4:sL:29:GLY:HA2    | 2.45                     | 0.41              |
| 4:sL:60:CYS:HA     | 4:sL:114:SER:HB2   | 2.02                     | 0.41              |
| 6:sG:2:LYS:HB2     | 6:sG:108:VAL:HG12  | 2.02                     | 0.41              |
| 6:sG:92:ARG:NH2    | 79:s2:441:C:O2'    | 2.42                     | 0.41              |
| 8:sY:7:ILE:HG12    | 8:sY:44:LEU:HD21   | 2.02                     | 0.41              |
| 8:sY:26:ASP:HB2    | 8:sY:68:LYS:HD2    | 2.01                     | 0.41              |
| 10:sA:41:ARG:HD2   | 10:sA:42:LYS:O     | 2.21                     | 0.41              |
| 11:sB:162:ARG:HD2  | 79:s2:1004:U:OP1   | 2.20                     | 0.41              |
| 12:sH:45:ILE:HA    | 12:sH:45:ILE:HD12  | 1.78                     | 0.41              |
| 13:sV:69:ILE:HD12  | 13:sV:70:LEU:N     | 2.35                     | 0.41              |
| 14:sa:72:HIS:C     | 14:sa:73:TYR:HD2   | 2.28                     | 0.41              |
| 17:sO:128:ARG:H    | 17:sO:128:ARG:HG2  | 1.70                     | 0.41              |
| 18:sW:15:ASN:OD1   | 18:sW:15:ASN:C     | 2.64                     | 0.41              |
| 18:sW:91:ASN:OD1   | 18:sW:92:ASN:N     | 2.54                     | 0.41              |
| 20:l7:60:G:H2'     | 20:l7:61:G:H8      | 1.84                     | 0.41              |
| 21:l8:24:G:C6      | 85:l5:352:G:N2     | 2.88                     | 0.41              |
| 21:l8:104:A:OP2    | 55:lj:42:LYS:NZ    | 2.49                     | 0.41              |
| 22:lA:14:SER:OG    | 22:lA:15:VAL:N     | 2.52                     | 0.41              |
| 22:lA:90:CYS:HA    | 22:lA:101:VAL:O    | 2.20                     | 0.41              |
| 22:lA:109:GLU:O    | 22:lA:109:GLU:HG2  | 2.20                     | 0.41              |
| 24:lC:235:LEU:O    | 85:l5:1373:A:O2'   | 2.38                     | 0.41              |
| 24:lC:322:LEU:HD22 | 85:l5:1280:C:C4    | 2.55                     | 0.41              |
| 26:lE:114:ARG:N    | 62:lr:87:ARG:HH21  | 2.19                     | 0.41              |
| 27:lF:113:ARG:NH1  | 27:lF:208:LEU:O    | 2.53                     | 0.41              |
| 29:lH:61:TRP:CG    | 33:lM:33:GLN:HE22  | 2.38                     | 0.41              |
| 29:lH:165:THR:HG21 | 29:lH:179:ILE:H    | 1.84                     | 0.41              |
| 31:lJ:160:GLU:HA   | 31:lJ:163:MET:HE1  | 2.02                     | 0.41              |
| 32:lL:36:ARG:NH1   | 85:l5:1364:U:OP2   | 2.50                     | 0.41              |
| 35:lO:17:GLY:HA3   | 85:l5:2053:C:H5'   | 2.03                     | 0.41              |
| 35:lO:194:GLU:C    | 35:lO:194:GLU:CD   | 2.88                     | 0.41              |
| 39:lS:97:TYR:CZ    | 39:lS:109:CYS:HA   | 2.55                     | 0.41              |
| 40:lT:2:THR:OG1    | 85:l5:4219:A:H3'   | 2.20                     | 0.41              |
| 43:lX:48:ARG:HG3   | 85:l5:2472:A:H1'   | 2.02                     | 0.41              |
| 45:lZ:35:ASP:OD1   | 45:lZ:35:ASP:N     | 2.52                     | 0.41              |
| 49:ld:51:LYS:HE3   | 49:ld:51:LYS:HB3   | 1.90                     | 0.41              |
| 54:li:70:LEU:HB2   | 54:li:87:ARG:NH2   | 2.29                     | 0.41              |
| 59:ln:2:ARG:HD2    | 79:s2:1841:C:OP1   | 2.21                     | 0.41              |
| 62:lr:106:LEU:H    | 62:lr:106:LEU:HD12 | 1.84                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 64:sR:37:GLU:N     | 64:sR:37:GLU:OE1   | 2.53                     | 0.41              |
| 65:sD:168:VAL:HA   | 65:sD:189:MET:HA   | 2.02                     | 0.41              |
| 65:sD:201:LYS:HG3  | 65:sD:202:LYS:N    | 2.34                     | 0.41              |
| 66:sF:55:ARG:NH2   | 79:s2:1648:G:OP2   | 2.53                     | 0.41              |
| 66:sF:87:LEU:HA    | 66:sF:90:VAL:CG1   | 2.50                     | 0.41              |
| 67:sK:55:ARG:HD2   | 79:s2:1277:C:H4'   | 2.02                     | 0.41              |
| 67:sK:58:VAL:CG2   | 67:sK:69:TRP:HB3   | 2.50                     | 0.41              |
| 68:sP:37:TYR:CZ    | 68:sP:112:ILE:O    | 2.73                     | 0.41              |
| 69:sQ:13:PHE:CE2   | 79:s2:1442:U:O3'   | 2.73                     | 0.41              |
| 71:sT:3:GLY:HA2    | 79:s2:1424:G:H21   | 1.85                     | 0.41              |
| 71:sT:77:LYS:CE    | 79:s2:1587:G:H21   | 2.34                     | 0.41              |
| 74:sd:12:ARG:HA    | 74:sd:12:ARG:HD3   | 1.65                     | 0.41              |
| 75:sg:40:ILE:O     | 75:sg:59:LEU:N     | 2.54                     | 0.41              |
| 75:sg:215:GLN:HA   | 75:sg:231:ASP:HA   | 2.01                     | 0.41              |
| 76:sM:52:LEU:HD22  | 76:sM:65:VAL:CG2   | 2.50                     | 0.41              |
| 79:s2:448:A:H4'    | 79:s2:449:A:C5'    | 2.50                     | 0.41              |
| 79:s2:572:U:H1'    | 79:s2:578:C:N4     | 2.36                     | 0.41              |
| 79:s2:934:G:C4     | 79:s2:935:G:C8     | 3.09                     | 0.41              |
| 79:s2:1006:C:H2'   | 79:s2:1007:C:H6    | 1.85                     | 0.41              |
| 79:s2:1050:A:H4'   | 79:s2:1846:G:O2'   | 2.20                     | 0.41              |
| 79:s2:1111:U:H2'   | 79:s2:1112:U:O4'   | 2.20                     | 0.41              |
| 79:s2:1173:A:H2'   | 79:s2:1174:U:O4'   | 2.20                     | 0.41              |
| 79:s2:1649:U:H2'   | 79:s2:1650:A:C8    | 2.55                     | 0.41              |
| 80:cB:8:GLN:NE2    | 80:cB:45:ILE:HD11  | 2.35                     | 0.41              |
| 80:cB:18:ASN:OD1   | 80:cB:98:PHE:HA    | 2.19                     | 0.41              |
| 83:ls:37:SER:OG    | 85:l5:1970:A:OP1   | 2.38                     | 0.41              |
| 84:lt:78:SER:O     | 84:lt:82:ILE:HG12  | 2.20                     | 0.41              |
| 85:l5:9:C:H2'      | 85:l5:10:A:H8      | 1.85                     | 0.41              |
| 85:l5:248:C:H2'    | 85:l5:249:C:C6     | 2.56                     | 0.41              |
| 85:l5:1633:G:H5'   | 85:l5:1634:A:OP1   | 2.21                     | 0.41              |
| 85:l5:1684:A:C4    | 85:l5:1685:G:C8    | 3.09                     | 0.41              |
| 85:l5:1977:C:O2'   | 85:l5:1978:C:OP1   | 2.36                     | 0.41              |
| 85:l5:2798:A:OP1   | 85:l5:2798:A:H8    | 2.02                     | 0.41              |
| 85:l5:3694:U:H2'   | 85:l5:3695:U:C6    | 2.55                     | 0.41              |
| 85:l5:3851:U:H2'   | 85:l5:3852:A:O4'   | 2.19                     | 0.41              |
| 85:l5:4348:A:N6    | 85:l5:4350:C:C4    | 2.88                     | 0.41              |
| 85:l5:4350:C:C2    | 85:l5:4351:U:C5    | 3.08                     | 0.41              |
| 80:CB:117:ALA:O    | 80:CB:121:VAL:HG23 | 2.21                     | 0.41              |
| 80:CB:524:LEU:HD22 | 80:CB:536:CYS:SG   | 2.60                     | 0.41              |
| 80:CB:604:MET:HE1  | 80:CB:704:VAL:HB   | 2.02                     | 0.41              |
| 2:SE:20:LEU:HD13   | 2:SE:20:LEU:HA     | 1.92                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:SE:187:ALA:H     | 79:S2:809:A:P      | 2.42                     | 0.41              |
| 3:SI:57:ALA:H      | 3:SI:180:GLY:HA2   | 1.85                     | 0.41              |
| 3:SI:143:LYS:HE3   | 3:SI:144:LYS:HE3   | 2.01                     | 0.41              |
| 5:SX:140:ARG:CZ    | 5:SX:140:ARG:HB3   | 2.50                     | 0.41              |
| 6:SG:5:ILE:HD12    | 6:SG:111:LEU:O     | 2.20                     | 0.41              |
| 6:SG:98:ARG:NH1    | 6:SG:99:GLY:O      | 2.50                     | 0.41              |
| 8:SY:19:GLN:NE2    | 8:SY:85:ASN:HD21   | 2.18                     | 0.41              |
| 10:SA:59:LEU:HD21  | 10:SA:63:ARG:HD2   | 2.02                     | 0.41              |
| 11:SB:144:LYS:HB2  | 11:SB:144:LYS:HE3  | 1.83                     | 0.41              |
| 15:SC:89:LYS:HD3   | 15:SC:89:LYS:HA    | 1.79                     | 0.41              |
| 16:SN:14:SER:OG    | 79:S2:1016:U:H5''  | 2.19                     | 0.41              |
| 16:SN:101:HIS:CD2  | 79:S2:1008:A:H1'   | 2.56                     | 0.41              |
| 19:Sb:59:CYS:HB2   | 19:Sb:61:THR:HG22  | 2.02                     | 0.41              |
| 85:L5:72:C:H5      | 32:LL:67:HIS:HD2   | 1.63                     | 0.41              |
| 85:L5:284:G:H2'    | 85:L5:285:G:H8     | 1.84                     | 0.41              |
| 85:L5:292:G:H2'    | 85:L5:293:G:C8     | 2.55                     | 0.41              |
| 85:L5:689:U:H2'    | 85:L5:690:C:H6     | 1.84                     | 0.41              |
| 85:L5:1070:G:OP2   | 26:LE:65:ARG:NH1   | 2.53                     | 0.41              |
| 85:L5:1368:A:H8    | 85:L5:1368:A:O5'   | 2.03                     | 0.41              |
| 85:L5:1633:G:C6    | 22:LA:207:VAL:HG11 | 2.55                     | 0.41              |
| 85:L5:1897:A:OP2   | 27:LF:98:ILE:HD12  | 2.21                     | 0.41              |
| 85:L5:2073:C:H2'   | 85:L5:2074:C:H6    | 1.85                     | 0.41              |
| 85:L5:2602:G:H2'   | 85:L5:2603:C:H6    | 1.86                     | 0.41              |
| 85:L5:3911:C:C2    | 85:L5:3912:U:C5    | 3.08                     | 0.41              |
| 85:L5:3949:A:N6    | 85:L5:4063:U:O4    | 2.52                     | 0.41              |
| 85:L5:4056:A:OP1   | 63:Lz:41:TYR:OH    | 2.34                     | 0.41              |
| 85:L5:4116:C:O5'   | 85:L5:4116:C:H6    | 2.03                     | 0.41              |
| 85:L5:4431:U:H2'   | 85:L5:4432:C:H6    | 1.85                     | 0.41              |
| 21:L8:100:U:H2'    | 21:L8:101:C:H6     | 1.85                     | 0.41              |
| 23:LB:113:GLU:HG3  | 23:LB:178:ALA:HB2  | 2.03                     | 0.41              |
| 24:LC:80:ARG:H     | 24:LC:80:ARG:HG2   | 1.67                     | 0.41              |
| 24:LC:290:SER:OG   | 24:LC:291:ARG:N    | 2.53                     | 0.41              |
| 25:LD:215:ASP:OD1  | 25:LD:218:ALA:N    | 2.45                     | 0.41              |
| 26:LE:151:ILE:HA   | 26:LE:160:LYS:O    | 2.20                     | 0.41              |
| 26:LE:241:GLU:OE1  | 26:LE:241:GLU:N    | 2.51                     | 0.41              |
| 27:LF:36:LYS:HA    | 27:LF:39:GLN:HG2   | 2.02                     | 0.41              |
| 28:LG:105:GLU:HB2  | 28:LG:109:GLU:CD   | 2.45                     | 0.41              |
| 28:LG:142:THR:O    | 28:LG:145:THR:OG1  | 2.31                     | 0.41              |
| 28:LG:174:CYS:O    | 28:LG:178:GLY:N    | 2.53                     | 0.41              |
| 32:LL:194:ILE:HG13 | 32:LL:198:ARG:CZ   | 2.50                     | 0.41              |
| 33:LM:33:GLN:HE21  | 33:LM:33:GLN:HB3   | 1.67                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 37:LQ:85:THR:HA    | 37:LQ:104:ARG:O    | 2.20                     | 0.41              |
| 38:LR:114:LYS:H    | 38:LR:114:LYS:HG2  | 1.69                     | 0.41              |
| 38:LR:163:ARG:O    | 38:LR:167:LYS:HG2  | 2.20                     | 0.41              |
| 40:LT:26:PRO:O     | 40:LT:29:THR:HG22  | 2.19                     | 0.41              |
| 46:La:92:LYS:HD2   | 46:La:92:LYS:HA    | 1.81                     | 0.41              |
| 49:Ld:59:THR:OG1   | 49:Ld:102:LEU:O    | 2.24                     | 0.41              |
| 51:Lf:65:ASN:HB3   | 51:Lf:67:THR:HG23  | 2.02                     | 0.41              |
| 52:Lg:70:THR:HA    | 52:Lg:73:HIS:HE1   | 1.85                     | 0.41              |
| 54:Li:4:ARG:HD2    | 54:Li:4:ARG:HA     | 1.70                     | 0.41              |
| 56:Lk:8:ILE:O      | 56:Lk:12:LEU:HG    | 2.20                     | 0.41              |
| 60:Lo:12:CYS:CB    | 60:Lo:15:CYS:SG    | 2.83                     | 0.41              |
| 61:Lp:31:ILE:HD13  | 61:Lp:31:ILE:HA    | 1.85                     | 0.41              |
| 62:Lr:53:PRO:HB3   | 62:Lr:117:ILE:HD11 | 2.02                     | 0.41              |
| 64:SR:7:LYS:HD3    | 79:S2:1373:C:P     | 2.60                     | 0.41              |
| 66:SF:144:LEU:HD12 | 66:SF:145:ARG:N    | 2.34                     | 0.41              |
| 70:SS:2:SER:HB3    | 77:SZ:49:LEU:HD11  | 2.02                     | 0.41              |
| 75:Sg:210:GLY:C    | 75:Sg:236:ILE:HD11 | 2.45                     | 0.41              |
| 75:Sg:266:ILE:HD13 | 75:Sg:266:ILE:HA   | 1.84                     | 0.41              |
| 78:Sf:121:CYS:SG   | 78:Sf:123:SER:HB3  | 2.60                     | 0.41              |
| 79:S2:62:G:O2'     | 79:S2:172:U:OP1    | 2.37                     | 0.41              |
| 79:S2:179:C:H3'    | 79:S2:180:G:C8     | 2.55                     | 0.41              |
| 79:S2:319:C:H2'    | 79:S2:320:G:H8     | 1.83                     | 0.41              |
| 79:S2:1094:C:H2'   | 79:S2:1095:C:H6    | 1.82                     | 0.41              |
| 79:S2:1456:G:H2'   | 79:S2:1457:U:C6    | 2.55                     | 0.41              |
| 79:S2:1510:G:H2'   | 79:S2:1511:U:O4'   | 2.19                     | 0.41              |
| 81:AP:9:A:O2'      | 81:AP:45:G:N3      | 2.51                     | 0.41              |
| 87:LW:86:SER:OG    | 87:LW:89:ASP:OD2   | 2.23                     | 0.41              |
| 1:cH:55:THR:HG23   | 1:cH:56:LYS:HD2    | 2.03                     | 0.41              |
| 2:sE:99:PHE:HE1    | 2:sE:112:HIS:H     | 1.67                     | 0.41              |
| 2:sE:126:VAL:HG23  | 2:sE:139:LEU:HG    | 2.02                     | 0.41              |
| 4:sL:95:TYR:CZ     | 4:sL:97:ARG:HA     | 2.55                     | 0.41              |
| 8:sY:15:ASN:OD1    | 8:sY:18:LEU:HB3    | 2.20                     | 0.41              |
| 9:se:41:ARG:NH1    | 79:s2:639:C:OP1    | 2.54                     | 0.41              |
| 10:sA:21:ALA:HB1   | 10:sA:169:HIS:HB3  | 2.02                     | 0.41              |
| 10:sA:174:MET:HE1  | 10:sA:175:TRP:CE2  | 2.56                     | 0.41              |
| 11:sB:77:ASP:H     | 11:sB:78:GLU:CD    | 2.27                     | 0.41              |
| 14:sa:46:GLU:OE1   | 17:sO:113:GLN:HG3  | 2.20                     | 0.41              |
| 14:sa:64:LEU:HD23  | 14:sa:64:LEU:H     | 1.85                     | 0.41              |
| 17:sO:31:CYS:HB2   | 17:sO:93:LEU:HD21  | 2.02                     | 0.41              |
| 21:l8:8:U:C2       | 21:l8:9:A:C8       | 3.08                     | 0.41              |
| 21:l8:16:G:C4      | 85:l5:417:G:N2     | 2.89                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 21:l8:75:G:C2      | 57:l1:26:TRP:CD1   | 3.08                     | 0.41              |
| 22:lA:194:ASN:ND2  | 22:lA:194:ASN:O    | 2.53                     | 0.41              |
| 23:lB:42:HIS:ND1   | 23:lB:43:LEU:O     | 2.53                     | 0.41              |
| 23:lB:295:ASP:CG   | 23:lB:296:GLY:H    | 2.28                     | 0.41              |
| 23:lB:381:THR:HB   | 23:lB:383:GLU:OE1  | 2.20                     | 0.41              |
| 24:lC:84:THR:HG23  | 24:lC:86:ARG:N     | 2.35                     | 0.41              |
| 25:lD:127:GLY:N    | 25:lD:196:ARG:HB3  | 2.36                     | 0.41              |
| 29:lH:86:LEU:O     | 29:lH:187:VAL:HG22 | 2.20                     | 0.41              |
| 32:lL:75:GLY:HA3   | 32:lL:97:SER:O     | 2.19                     | 0.41              |
| 33:lM:101:LYS:HB2  | 35:lO:200:GLY:HA3  | 2.03                     | 0.41              |
| 34:lN:22:LEU:HD13  | 34:lN:26:ARG:HH22  | 1.84                     | 0.41              |
| 34:lN:26:ARG:O     | 34:lN:30:TYR:CD1   | 2.74                     | 0.41              |
| 34:lN:116:LEU:HD23 | 34:lN:133:ILE:HD11 | 2.02                     | 0.41              |
| 35:lO:34:VAL:HG11  | 35:lO:112:TYR:CE2  | 2.55                     | 0.41              |
| 40:lT:5:LYS:HE2    | 85:l5:4302:U:H4'   | 2.01                     | 0.41              |
| 40:lT:17:ARG:HG2   | 85:l5:4277:G:H5''  | 2.03                     | 0.41              |
| 46:la:127:LYS:HB3  | 46:la:128:PHE:CE1  | 2.55                     | 0.41              |
| 48:lc:48:LEU:HD21  | 48:lc:60:ILE:HG21  | 2.02                     | 0.41              |
| 50:le:77:PHE:CG    | 50:le:88:LEU:HD21  | 2.55                     | 0.41              |
| 54:li:68:ARG:HH12  | 85:l5:3722:G:H3'   | 1.84                     | 0.41              |
| 61:lp:22:LEU:HD23  | 61:lp:22:LEU:HA    | 1.78                     | 0.41              |
| 62:lr:20:ARG:HB3   | 62:lr:20:ARG:NH1   | 2.35                     | 0.41              |
| 67:sK:24:LYS:HB3   | 67:sK:26:ASP:OD2   | 2.19                     | 0.41              |
| 68:sP:85:ILE:HD12  | 68:sP:85:ILE:HA    | 1.84                     | 0.41              |
| 68:sP:101:THR:HG23 | 68:sP:103:ASN:ND2  | 2.35                     | 0.41              |
| 69:sQ:72:VAL:HG11  | 69:sQ:80:GLN:HG2   | 2.03                     | 0.41              |
| 70:sS:68:ILE:O     | 70:sS:71:MET:HG2   | 2.20                     | 0.41              |
| 70:sS:82:TRP:CD2   | 79:s2:1567:G:C6    | 3.08                     | 0.41              |
| 73:sc:62:GLU:H     | 73:sc:62:GLU:HG3   | 1.74                     | 0.41              |
| 75:sg:178:ASN:HB3  | 75:sg:185:LYS:HD3  | 2.02                     | 0.41              |
| 75:sg:241:PHE:CD1  | 75:sg:248:LEU:HD13 | 2.54                     | 0.41              |
| 75:sg:297:THR:HB   | 75:sg:311:GLN:HG2  | 2.01                     | 0.41              |
| 79:s2:202:G:H5''   | 79:s2:203:G:C8     | 2.55                     | 0.41              |
| 79:s2:394:G:N3     | 79:s2:394:G:H2'    | 2.35                     | 0.41              |
| 79:s2:456:C:C2     | 79:s2:457:C:C5     | 3.08                     | 0.41              |
| 79:s2:935:G:H2'    | 79:s2:936:G:C8     | 2.55                     | 0.41              |
| 79:s2:1114:U:O2'   | 79:s2:1115:U:H2'   | 2.21                     | 0.41              |
| 79:s2:1134:G:C4    | 79:s2:1135:C:C5    | 3.07                     | 0.41              |
| 79:s2:1332:A:N1    | 79:s2:1500:G:C4    | 2.89                     | 0.41              |
| 79:s2:1670:C:H2'   | 79:s2:1671:G:O4'   | 2.20                     | 0.41              |
| 79:s2:1827:U:H2'   | 79:s2:1828:C:H6    | 1.83                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 80:cB:27:HIS:HB3   | 80:cB:30:HIS:CE1   | 2.56                     | 0.41              |
| 80:cB:61:LYS:O     | 80:cB:63:GLU:N     | 2.53                     | 0.41              |
| 80:cB:207:PRO:HA   | 80:cB:212:VAL:HB   | 2.02                     | 0.41              |
| 80:cB:596:PRO:HD2  | 80:cB:720:GLN:OE1  | 2.20                     | 0.41              |
| 80:cB:756:VAL:O    | 80:cB:759:ILE:HG13 | 2.20                     | 0.41              |
| 83:ls:145:THR:C    | 83:ls:146:LYS:HD3  | 2.46                     | 0.41              |
| 85:l5:247:G:H2'    | 85:l5:248:C:C6     | 2.53                     | 0.41              |
| 85:l5:347:A:H2'    | 85:l5:348:G:C8     | 2.55                     | 0.41              |
| 85:l5:1080:C:C2    | 85:l5:1220:G:C2    | 3.08                     | 0.41              |
| 85:l5:1174:G:C2    | 85:l5:1187:G:N7    | 2.88                     | 0.41              |
| 85:l5:1270:A:H8    | 85:l5:2106:G:H21   | 1.66                     | 0.41              |
| 85:l5:1291:G:H2'   | 85:l5:1292:C:H6    | 1.83                     | 0.41              |
| 85:l5:1564:A:H8    | 85:l5:1564:A:OP2   | 2.04                     | 0.41              |
| 85:l5:1762:C:H5''  | 85:l5:1764:G:H22   | 1.85                     | 0.41              |
| 85:l5:1848:C:H2'   | 85:l5:1849:U:O4'   | 2.20                     | 0.41              |
| 85:l5:1933:G:H8    | 85:l5:1933:G:O5'   | 2.03                     | 0.41              |
| 85:l5:2017:A:HO2'  | 85:l5:2018:C:H6    | 1.56                     | 0.41              |
| 85:l5:2021:G:C6    | 85:l5:2022:C:N4    | 2.89                     | 0.41              |
| 85:l5:2377:C:H2'   | 85:l5:2378:G:O4'   | 2.20                     | 0.41              |
| 85:l5:3932:U:H2'   | 85:l5:3933:G:C8    | 2.56                     | 0.41              |
| 85:l5:4400:G:C5    | 85:l5:4401:G:C8    | 3.09                     | 0.41              |
| 85:l5:4412:C:H2'   | 85:l5:4413:C:C6    | 2.56                     | 0.41              |
| 85:l5:4932:U:H2'   | 85:l5:4933:C:C6    | 2.55                     | 0.41              |
| 80:CB:186:ASN:O    | 80:CB:204:MET:HE1  | 2.20                     | 0.41              |
| 80:CB:275:LYS:H    | 80:CB:275:LYS:HG2  | 1.60                     | 0.41              |
| 80:CB:672:LEU:O    | 80:CB:676:LYS:HG3  | 2.19                     | 0.41              |
| 6:SG:32:MET:SD     | 6:SG:100:CYS:O     | 2.78                     | 0.41              |
| 7:SJ:63:LEU:HD23   | 7:SJ:70:ARG:HB2    | 2.03                     | 0.41              |
| 8:SY:87:PRO:HG2    | 8:SY:90:ARG:NE     | 2.35                     | 0.41              |
| 8:SY:87:PRO:O      | 8:SY:90:ARG:HG2    | 2.20                     | 0.41              |
| 10:SA:41:ARG:HH12  | 79:S2:1126:G:P     | 2.42                     | 0.41              |
| 10:SA:50:ASN:HD21  | 10:SA:52:LYS:HE3   | 1.86                     | 0.41              |
| 10:SA:51:LEU:H     | 64:SR:105:MET:CE   | 2.33                     | 0.41              |
| 11:SB:66:VAL:C     | 11:SB:67:PHE:HD1   | 2.28                     | 0.41              |
| 11:SB:138:PHE:CD2  | 11:SB:214:LYS:HG3  | 2.55                     | 0.41              |
| 12:SH:147:LYS:O    | 12:SH:147:LYS:CD   | 2.60                     | 0.41              |
| 14:Sa:12:LYS:HG3   | 14:Sa:15:ARG:HB2   | 2.02                     | 0.41              |
| 14:Sa:97:PRO:HA    | 14:Sa:98:PRO:HD3   | 1.96                     | 0.41              |
| 15:SC:180:VAL:HG13 | 15:SC:197:PRO:HG3  | 2.03                     | 0.41              |
| 18:SW:33:VAL:HG13  | 18:SW:34:ILE:HD13  | 2.01                     | 0.41              |
| 18:SW:71:LYS:HB3   | 18:SW:130:PHE:CZ   | 2.56                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 18:SW:107:SER:OG  | 79:S2:860:G:N2     | 2.54                     | 0.41              |
| 85:L5:67:C:N4     | 85:L5:325:U:O2'    | 2.51                     | 0.41              |
| 85:L5:263:G:C8    | 85:L5:264:C:N4     | 2.88                     | 0.41              |
| 85:L5:486:C:H2'   | 85:L5:487:G:C8     | 2.55                     | 0.41              |
| 85:L5:665:C:H1'   | 85:L5:666:G:N7     | 2.36                     | 0.41              |
| 85:L5:956:A:N6    | 85:L5:1283:G:H1'   | 2.35                     | 0.41              |
| 85:L5:1217:G:H2'  | 85:L5:1218:G:C8    | 2.55                     | 0.41              |
| 85:L5:1548:G:O2'  | 85:L5:2812:A:N3    | 2.50                     | 0.41              |
| 85:L5:1700:G:H5'  | 85:L5:1701:A:O5'   | 2.21                     | 0.41              |
| 85:L5:1814:C:H2'  | 85:L5:1816:C:H5    | 1.86                     | 0.41              |
| 85:L5:1891:A:C6   | 85:L5:1892:A:N1    | 2.89                     | 0.41              |
| 85:L5:1984:A:H2'  | 85:L5:2011:C:OP1   | 2.20                     | 0.41              |
| 85:L5:2437:C:O2'  | 43:LX:125:ASN:ND2  | 2.53                     | 0.41              |
| 85:L5:2532:C:C2   | 85:L5:2533:C:C5    | 3.08                     | 0.41              |
| 85:L5:2554:U:H1'  | 85:L5:2574:G:H21   | 1.85                     | 0.41              |
| 85:L5:2735:G:N3   | 85:L5:2736:G:C8    | 2.88                     | 0.41              |
| 85:L5:3790:U:H4'  | 85:L5:3791:C:H3'   | 2.02                     | 0.41              |
| 85:L5:3854:C:H2'  | 85:L5:3855:C:H6    | 1.85                     | 0.41              |
| 85:L5:4105:A:C4'  | 85:L5:4106:G:O4'   | 2.68                     | 0.41              |
| 85:L5:4279:A:H5'  | 85:L5:4281:A:H1'   | 2.02                     | 0.41              |
| 85:L5:4323:A:H4'  | 25:LD:176:SER:OG   | 2.20                     | 0.41              |
| 85:L5:4755:G:N1   | 85:L5:4879:C:N3    | 2.68                     | 0.41              |
| 22:LA:82:ILE:HD11 | 22:LA:98:ILE:HG12  | 2.02                     | 0.41              |
| 22:LA:116:LEU:CB  | 22:LA:126:LEU:HB2  | 2.48                     | 0.41              |
| 24:LC:297:GLU:HA  | 24:LC:300:ARG:CZ   | 2.50                     | 0.41              |
| 26:LE:270:TYR:CG  | 33:LM:107:PHE:HD1  | 2.38                     | 0.41              |
| 32:LL:55:ILE:HG23 | 32:LL:76:PHE:HE1   | 1.85                     | 0.41              |
| 32:LL:96:ILE:CG2  | 32:LL:98:VAL:HG23  | 2.49                     | 0.41              |
| 34:LN:120:TRP:HE1 | 34:LN:123:GLU:CB   | 2.32                     | 0.41              |
| 35:LO:151:ALA:O   | 35:LO:155:THR:HG22 | 2.20                     | 0.41              |
| 37:LQ:5:ILE:HB    | 37:LQ:7:HIS:CE1    | 2.56                     | 0.41              |
| 38:LR:136:ARG:O   | 38:LR:139:MET:HG3  | 2.20                     | 0.41              |
| 41:LU:68:SER:C    | 41:LU:69:LYS:HD3   | 2.44                     | 0.41              |
| 42:LV:39:ILE:HA   | 42:LV:63:ALA:HB2   | 2.02                     | 0.41              |
| 43:LX:90:ILE:HD13 | 43:LX:95:THR:O     | 2.20                     | 0.41              |
| 44:LY:100:HIS:CD2 | 44:LY:102:SER:H    | 2.22                     | 0.41              |
| 44:LY:103:LYS:HA  | 44:LY:103:LYS:HD3  | 1.89                     | 0.41              |
| 45:LZ:39:SER:HB2  | 45:LZ:77:TYR:CD2   | 2.55                     | 0.41              |
| 45:LZ:91:LEU:HD13 | 45:LZ:96:VAL:HG21  | 2.02                     | 0.41              |
| 56:Lk:13:LEU:HD12 | 56:Lk:14:THR:N     | 2.35                     | 0.41              |
| 64:SR:104:GLU:HA  | 64:SR:107:LYS:HD3  | 2.01                     | 0.41              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 67:SK:46:MET:HA    | 67:SK:49:MET:HG2  | 2.02                     | 0.41              |
| 69:SQ:42:ILE:HG12  | 69:SQ:51:LEU:HD21 | 2.03                     | 0.41              |
| 70:SS:132:ARG:HB3  | 79:S2:1623:A:N7   | 2.35                     | 0.41              |
| 71:ST:5:THR:O      | 71:ST:135:ALA:HB1 | 2.20                     | 0.41              |
| 72:SU:83:ARG:NH2   | 79:S2:1391:C:O3'  | 2.54                     | 0.41              |
| 73:Sc:14:VAL:HG22  | 73:Sc:54:ASP:O    | 2.20                     | 0.41              |
| 79:S2:372:U:N3     | 79:S2:373:G:N7    | 2.68                     | 0.41              |
| 79:S2:608:C:H2'    | 79:S2:609:U:C6    | 2.55                     | 0.41              |
| 79:S2:1177:U:H2'   | 79:S2:1178:U:C6   | 2.55                     | 0.41              |
| 79:S2:1473:G:N2    | 79:S2:1476:A:OP2  | 2.54                     | 0.41              |
| 83:Ls:57:LYS:N     | 83:Ls:60:MET:SD   | 2.86                     | 0.41              |
| 3:sI:202:ILE:HD13  | 3:sI:202:ILE:HA   | 1.87                     | 0.41              |
| 4:sL:92:TYR:OH     | 79:s2:355:G:OP1   | 2.36                     | 0.41              |
| 4:sL:133:PRO:O     | 4:sL:134:LEU:HD13 | 2.21                     | 0.41              |
| 6:sG:24:LEU:HA     | 6:sG:27:PHE:CE2   | 2.56                     | 0.41              |
| 6:sG:202:ASN:O     | 6:sG:205:GLU:HG2  | 2.20                     | 0.41              |
| 7:sJ:111:GLN:CD    | 7:sJ:127:ARG:HB2  | 2.45                     | 0.41              |
| 8:sY:110:ARG:O     | 8:sY:114:MET:HG2  | 2.20                     | 0.41              |
| 9:se:29:THR:OG1    | 9:se:30:GLY:N     | 2.53                     | 0.41              |
| 10:sA:5:LEU:HD23   | 13:sV:79:VAL:HG23 | 2.02                     | 0.41              |
| 10:sA:42:LYS:HB3   | 10:sA:48:ILE:HG12 | 2.02                     | 0.41              |
| 13:sV:60:ARG:HG3   | 13:sV:65:SER:HB3  | 2.01                     | 0.41              |
| 16:sN:87:ASP:OD2   | 79:s2:924:G:N2    | 2.54                     | 0.41              |
| 17:sO:53:ILE:N     | 17:sO:53:ILE:HD13 | 2.35                     | 0.41              |
| 18:sW:24:GLN:HE21  | 19:sb:7:LEU:H     | 1.66                     | 0.41              |
| 18:sW:70:ASN:OD1   | 18:sW:70:ASN:C    | 2.63                     | 0.41              |
| 23:lB:95:THR:HG22  | 23:lB:98:GLY:O    | 2.21                     | 0.41              |
| 23:lB:128:LYS:HB3  | 23:lB:128:LYS:HE2 | 1.90                     | 0.41              |
| 27:lF:29:LYS:HA    | 27:lF:29:LYS:HD2  | 1.63                     | 0.41              |
| 27:lF:147:LEU:HD22 | 85:l5:943:A:OP1   | 2.20                     | 0.41              |
| 28:lG:134:PRO:HB3  | 28:lG:206:GLN:NE2 | 2.36                     | 0.41              |
| 30:lI:44:ASP:OD2   | 30:lI:44:ASP:N    | 2.52                     | 0.41              |
| 32:lL:87:HIS:HB3   | 32:lL:90:VAL:HG12 | 2.02                     | 0.41              |
| 33:lM:10:GLY:O     | 33:lM:62:LEU:HB2  | 2.19                     | 0.41              |
| 33:lM:85:LYS:H     | 33:lM:85:LYS:HG3  | 1.69                     | 0.41              |
| 38:lR:86:ASN:HB3   | 85:l5:1550:G:OP1  | 2.20                     | 0.41              |
| 40:lT:116:LYS:NZ   | 85:l5:1834:U:H2'  | 2.35                     | 0.41              |
| 41:lU:84:LYS:HD3   | 41:lU:110:TYR:HE1 | 1.85                     | 0.41              |
| 52:lg:13:TYR:CD1   | 85:l5:2513:A:C4   | 3.09                     | 0.41              |
| 53:lh:47:ILE:HG13  | 53:lh:48:ARG:H    | 1.86                     | 0.41              |
| 53:lh:47:ILE:HG13  | 53:lh:48:ARG:N    | 2.34                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 56:lk:35:LYS:HZ2   | 85:l5:2696:A:H62   | 1.68                     | 0.41              |
| 61:lp:29:ILE:HD11  | 61:lp:69:TRP:HB2   | 1.99                     | 0.41              |
| 61:lp:85:ARG:CZ    | 79:s2:940:U:P      | 3.08                     | 0.41              |
| 62:lr:7:TRP:O      | 62:lr:11:ARG:HB3   | 2.20                     | 0.41              |
| 65:sD:90:LYS:HD3   | 65:sD:91:VAL:C     | 2.46                     | 0.41              |
| 66:sF:128:ILE:HD11 | 73:sc:22:GLY:O     | 2.20                     | 0.41              |
| 67:sK:28:HIS:ND1   | 74:sd:8:TRP:CZ2    | 2.89                     | 0.41              |
| 69:sQ:24:HIS:CE1   | 79:s2:1408:U:H4'   | 2.55                     | 0.41              |
| 69:sQ:117:ARG:NE   | 69:sQ:121:VAL:HG11 | 2.35                     | 0.41              |
| 71:sT:97:LYS:NZ    | 79:s2:1566:G:H1    | 2.18                     | 0.41              |
| 72:sU:88:LEU:C     | 72:sU:89:ILE:HD13  | 2.46                     | 0.41              |
| 75:sg:260:ASP:OD2  | 75:sg:262:GLU:OE1  | 2.38                     | 0.41              |
| 79:s2:72:C:H5'     | 79:s2:73:C:C4      | 2.56                     | 0.41              |
| 79:s2:316:G:H2'    | 79:s2:317:C:C6     | 2.55                     | 0.41              |
| 79:s2:464:A:O2'    | 79:s2:465:A:OP1    | 2.33                     | 0.41              |
| 79:s2:482:G:N2     | 79:s2:485:A:OP2    | 2.53                     | 0.41              |
| 79:s2:872:A:O2'    | 79:s2:874:G:H8     | 2.03                     | 0.41              |
| 79:s2:1358:U:H2'   | 79:s2:1359:U:O4'   | 2.20                     | 0.41              |
| 80:cB:228:PHE:N    | 80:cB:228:PHE:CD2  | 2.88                     | 0.41              |
| 80:cB:289:PHE:O    | 80:cB:293:ILE:HB   | 2.20                     | 0.41              |
| 80:cB:833:GLN:H    | 80:cB:833:GLN:HG3  | 1.71                     | 0.41              |
| 81:aP:38:C:H2'     | 81:aP:39:G:C8      | 2.56                     | 0.41              |
| 83:ls:66:ARG:HH12  | 83:ls:79:LEU:HD11  | 1.86                     | 0.41              |
| 85:l5:666:G:H2'    | 85:l5:668:C:OP1    | 2.21                     | 0.41              |
| 85:l5:674:G:H2'    | 85:l5:675:C:H6     | 1.85                     | 0.41              |
| 85:l5:1080:C:C2    | 85:l5:1220:G:N2    | 2.89                     | 0.41              |
| 85:l5:1094:G:C6    | 85:l5:1095:A:C6    | 3.07                     | 0.41              |
| 85:l5:1624:G:C6    | 85:l5:1643:A:C8    | 3.08                     | 0.41              |
| 85:l5:2064:G:C6    | 85:l5:2065:G:C5    | 3.08                     | 0.41              |
| 85:l5:2071:A:C4    | 85:l5:2072:C:C5    | 3.09                     | 0.41              |
| 85:l5:2288:G:C2    | 85:l5:2290:C:C5    | 3.09                     | 0.41              |
| 85:l5:2438:A:N6    | 85:l5:2531:C:C4    | 2.88                     | 0.41              |
| 85:l5:2498:C:C2    | 85:l5:2499:C:C5    | 3.08                     | 0.41              |
| 85:l5:2776:G:H2'   | 85:l5:2777:G:C8    | 2.55                     | 0.41              |
| 85:l5:2800:G:C6    | 85:l5:2801:U:C4    | 3.08                     | 0.41              |
| 85:l5:2845:A:H2'   | 85:l5:2845:A:N3    | 2.35                     | 0.41              |
| 85:l5:3665:G:H2'   | 85:l5:3666:C:H6    | 1.86                     | 0.41              |
| 85:l5:3801:U:H2'   | 85:l5:3803:A:N7    | 2.35                     | 0.41              |
| 85:l5:3900:G:H5''  | 85:l5:3901:A:H4'   | 2.01                     | 0.41              |
| 85:l5:3935:C:N4    | 85:l5:3936:A:H62   | 2.18                     | 0.41              |
| 85:l5:4356:G:N3    | 85:l5:4357:G:C8    | 2.88                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 85:L5:4405:G:C4   | 85:L5:4406:U:C6    | 3.08                     | 0.41              |
| 85:L5:4602:A:H1'  | 85:L5:4610:A:H61   | 1.84                     | 0.41              |
| 85:L5:4695:C:H2'  | 85:L5:4696:C:O4'   | 2.21                     | 0.41              |
| 85:L5:5058:A:H2'  | 85:L5:5059:C:H6    | 1.85                     | 0.41              |
| 80:CB:226:LYS:HD3 | 80:CB:352:GLN:OE1  | 2.21                     | 0.41              |
| 80:CB:400:LYS:HG2 | 80:CB:402:VAL:HG12 | 2.03                     | 0.41              |
| 3:SI:138:ASN:C    | 3:SI:140:LYS:H     | 2.28                     | 0.41              |
| 3:SI:155:ASN:OD1  | 3:SI:155:ASN:C     | 2.64                     | 0.41              |
| 7:SJ:177:ASN:HA   | 7:SJ:180:LYS:HE2   | 2.01                     | 0.41              |
| 8:SY:12:PHE:CZ    | 8:SY:23:MET:HE2    | 2.56                     | 0.41              |
| 14:Sa:22:ARG:NH2  | 17:SO:142:ARG:O    | 2.51                     | 0.41              |
| 14:Sa:38:LYS:HG2  | 14:Sa:39:PHE:O     | 2.20                     | 0.41              |
| 17:SO:13:GLN:HB3  | 17:SO:15:ILE:HG13  | 2.02                     | 0.41              |
| 18:SW:20:ARG:HD2  | 18:SW:20:ARG:HA    | 1.68                     | 0.41              |
| 85:L5:338:A:H2'   | 85:L5:339:C:H6     | 1.86                     | 0.41              |
| 85:L5:480:C:OP1   | 62:Lr:47:LYS:NZ    | 2.53                     | 0.41              |
| 85:L5:964:A:C3'   | 85:L5:965:G:H4'    | 2.50                     | 0.41              |
| 85:L5:993:G:C6    | 85:L5:1050:C:C4    | 3.08                     | 0.41              |
| 85:L5:1170:G:H2'  | 85:L5:1171:G:C8    | 2.55                     | 0.41              |
| 85:L5:1417:C:C2   | 85:L5:1418:C:C5    | 3.09                     | 0.41              |
| 85:L5:1655:C:OP1  | 85:L5:1679:A:O2'   | 2.30                     | 0.41              |
| 85:L5:2336:G:H2'  | 85:L5:2337:C:C6    | 2.55                     | 0.41              |
| 85:L5:2380:G:C5   | 85:L5:2425:U:C4    | 3.08                     | 0.41              |
| 85:L5:2500:U:H2'  | 85:L5:2501:C:H6    | 1.85                     | 0.41              |
| 85:L5:2752:G:C5   | 85:L5:2753:G:C5    | 3.09                     | 0.41              |
| 85:L5:2823:G:H2'  | 85:L5:2824:C:H6    | 1.85                     | 0.41              |
| 85:L5:3640:U:H3'  | 85:L5:3646:A:N6    | 2.35                     | 0.41              |
| 85:L5:4090:G:H2'  | 85:L5:4091:G:O4'   | 2.21                     | 0.41              |
| 85:L5:4093:G:C2'  | 85:L5:4094:G:H8    | 2.33                     | 0.41              |
| 85:L5:4228:G:C2   | 85:L5:4373:G:C4    | 3.08                     | 0.41              |
| 85:L5:4520:G:H2'  | 85:L5:4521:U:O4'   | 2.20                     | 0.41              |
| 85:L5:4532:U:H2'  | 85:L5:4533:A:O4'   | 2.20                     | 0.41              |
| 85:L5:4889:G:C6   | 85:L5:4931:G:C6    | 3.08                     | 0.41              |
| 85:L5:4952:G:C4   | 85:L5:4953:G:C8    | 3.09                     | 0.41              |
| 21:L8:42:G:OP1    | 55:Lj:62:GLY:N     | 2.54                     | 0.41              |
| 23:LB:114:CYS:HB2 | 23:LB:165:HIS:CE1  | 2.56                     | 0.41              |
| 23:LB:312:LYS:HD2 | 23:LB:370:THR:HG21 | 2.02                     | 0.41              |
| 24:LC:318:PRO:CB  | 24:LC:325:MET:HE3  | 2.49                     | 0.41              |
| 25:LD:146:LEU:CD2 | 25:LD:163:LEU:HD22 | 2.51                     | 0.41              |
| 25:LD:157:ASN:OD1 | 25:LD:158:LYS:N    | 2.53                     | 0.41              |
| 25:LD:203:ASN:OD1 | 25:LD:203:ASN:N    | 2.52                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 32:LL:17:ASP:O    | 32:LL:21:ARG:NH2   | 2.53                     | 0.41              |
| 35:LO:92:THR:HG23 | 35:LO:95:GLY:H     | 1.85                     | 0.41              |
| 35:LO:158:GLU:O   | 35:LO:162:GLU:HG2  | 2.21                     | 0.41              |
| 36:LP:61:ARG:NH2  | 36:LP:77:GLY:O     | 2.54                     | 0.41              |
| 36:LP:127:ARG:HB2 | 36:LP:139:TYR:O    | 2.20                     | 0.41              |
| 37:LQ:186:TYR:HE2 | 37:LQ:188:ASN:CB   | 2.33                     | 0.41              |
| 39:LS:69:GLU:CD   | 39:LS:102:THR:H    | 2.22                     | 0.41              |
| 42:LV:62:MET:HA   | 42:LV:78:PRO:HA    | 2.02                     | 0.41              |
| 46:La:69:PHE:CE1  | 46:La:71:PRO:HD3   | 2.55                     | 0.41              |
| 56:Lk:68:GLU:CD   | 56:Lk:70:LYS:H     | 2.29                     | 0.41              |
| 58:Lm:94:MET:HG2  | 58:Lm:105:PRO:CA   | 2.50                     | 0.41              |
| 63:Lz:3:SER:OG    | 63:Lz:211:GLY:O    | 2.25                     | 0.41              |
| 63:Lz:3:SER:OG    | 63:Lz:213:PRO:HD3  | 2.20                     | 0.41              |
| 71:ST:92:PHE:CD1  | 79:S2:1589:A:H5'   | 2.55                     | 0.41              |
| 79:S2:332:G:N3    | 79:S2:332:G:H2'    | 2.35                     | 0.41              |
| 79:S2:479:C:H2'   | 79:S2:480:G:C8     | 2.54                     | 0.41              |
| 79:S2:499:G:N1    | 79:S2:504:G:C6     | 2.89                     | 0.41              |
| 79:S2:687:C:H4'   | 79:S2:688:U:OP2    | 2.19                     | 0.41              |
| 79:S2:691:G:N1    | 79:S2:692:G:N3     | 2.65                     | 0.41              |
| 79:S2:938:A:C6    | 79:S2:939:U:C4     | 3.09                     | 0.41              |
| 79:S2:960:U:H2'   | 79:S2:962:A:OP2    | 2.21                     | 0.41              |
| 79:S2:1446:A:O2'  | 79:S2:1447:G:H8    | 2.03                     | 0.41              |
| 82:PE:9:A:H5'     | 82:PE:11:C:OP2     | 2.21                     | 0.41              |
| 83:Ls:20:LEU:HD11 | 83:Ls:52:VAL:HG21  | 2.02                     | 0.41              |
| 84:Lt:59:THR:N    | 84:Lt:80:LEU:HD11  | 2.35                     | 0.41              |
| 1:cH:85:ARG:NH2   | 1:cH:90:LEU:O      | 2.54                     | 0.41              |
| 3:sI:10:LYS:HD3   | 79:s2:387:C:OP1    | 2.21                     | 0.41              |
| 3:sI:69:SER:OG    | 4:sL:19:ASN:O      | 2.28                     | 0.41              |
| 4:sL:52:GLU:CD    | 4:sL:52:GLU:O      | 2.63                     | 0.41              |
| 6:sG:71:GLY:O     | 6:sG:99:GLY:N      | 2.42                     | 0.41              |
| 6:sG:139:SER:HA   | 6:sG:142:ARG:NE    | 2.27                     | 0.41              |
| 6:sG:170:ARG:HH11 | 79:s2:67:C:H41     | 1.68                     | 0.41              |
| 7:sJ:174:LYS:HD2  | 7:sJ:174:LYS:HA    | 1.76                     | 0.41              |
| 9:se:29:THR:HG22  | 79:s2:524:U:H2'    | 2.03                     | 0.41              |
| 10:sA:170:SER:O   | 10:sA:174:MET:HG3  | 2.20                     | 0.41              |
| 12:sH:63:PHE:HA   | 12:sH:95:ILE:HG23  | 2.02                     | 0.41              |
| 13:sV:8:PHE:CE2   | 13:sV:10:ASP:OD2   | 2.74                     | 0.41              |
| 13:sV:27:LYS:HE2  | 15:sC:163:VAL:HG23 | 2.01                     | 0.41              |
| 15:sC:60:TRP:NE1  | 15:sC:62:PRO:CA    | 2.83                     | 0.41              |
| 20:l7:25:G:H2'    | 20:l7:26:C:C6      | 2.55                     | 0.41              |
| 20:l7:41:G:N2     | 20:l7:45:U:C2      | 2.89                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 21:l8:30:U:H2'     | 21:l8:31:G:C8      | 2.55                     | 0.41              |
| 21:l8:42:G:H2'     | 21:l8:43:A:H8      | 1.85                     | 0.41              |
| 21:l8:44:A:H2'     | 21:l8:45:C:C6      | 2.56                     | 0.41              |
| 22:lA:57:PRO:HB3   | 61:lp:54:ILE:CD1   | 2.50                     | 0.41              |
| 23:lB:276:HIS:O    | 85:l5:4716:C:H5''  | 2.21                     | 0.41              |
| 23:lB:284:ILE:H    | 23:lB:284:ILE:HD12 | 1.85                     | 0.41              |
| 24:lC:334:THR:HG21 | 27:lF:51:TYR:OH    | 2.21                     | 0.41              |
| 25:lD:212:MET:HE1  | 25:lD:233:PRO:HG2  | 2.02                     | 0.41              |
| 26:lE:62:MET:HE1   | 26:lE:65:ARG:HE    | 1.86                     | 0.41              |
| 26:lE:141:ARG:NH2  | 51:lf:110:ILE:O    | 2.53                     | 0.41              |
| 26:lE:151:ILE:HA   | 26:lE:160:LYS:O    | 2.21                     | 0.41              |
| 27:lF:77:LYS:HE3   | 85:l5:730:G:O6     | 2.21                     | 0.41              |
| 29:lH:89:ARG:NH2   | 29:lH:187:VAL:HA   | 2.29                     | 0.41              |
| 29:lH:134:CYS:HA   | 29:lH:146:LEU:HA   | 2.02                     | 0.41              |
| 29:lH:147:GLU:OE2  | 29:lH:147:GLU:N    | 2.54                     | 0.41              |
| 31:lJ:97:ASN:OD1   | 31:lJ:97:ASN:N     | 2.52                     | 0.41              |
| 42:lV:18:LEU:HD12  | 42:lV:54:ALA:C     | 2.45                     | 0.41              |
| 42:lV:26:ILE:O     | 42:lV:37:LEU:N     | 2.54                     | 0.41              |
| 43:lX:99:ILE:HD11  | 43:lX:133:GLU:HB3  | 2.02                     | 0.41              |
| 48:lc:50:ASN:OD1   | 48:lc:76:GLY:O     | 2.38                     | 0.41              |
| 49:ld:64:ILE:HD11  | 85:l5:2373:C:C4'   | 2.37                     | 0.41              |
| 49:ld:71:ALA:HB2   | 49:ld:108:TYR:CD2  | 2.55                     | 0.41              |
| 50:le:36:ARG:HH12  | 85:l5:2322:G:P     | 2.44                     | 0.41              |
| 51:lf:81:SER:OG    | 85:l5:1918:U:OP1   | 2.35                     | 0.41              |
| 52:lg:48:VAL:O     | 61:lp:61:MET:HG3   | 2.20                     | 0.41              |
| 52:lg:63:VAL:HG23  | 52:lg:66:ARG:NH2   | 2.36                     | 0.41              |
| 52:lg:101:LYS:O    | 52:lg:104:VAL:HG22 | 2.21                     | 0.41              |
| 52:lg:102:ILE:N    | 52:lg:102:ILE:HD13 | 2.35                     | 0.41              |
| 55:lj:28:HIS:CD2   | 85:l5:1532:G:H5'   | 2.55                     | 0.41              |
| 56:lk:34:PHE:HB2   | 56:lk:45:LEU:HB3   | 2.03                     | 0.41              |
| 60:lo:104:ILE:O    | 60:lo:104:ILE:HG22 | 2.21                     | 0.41              |
| 64:sR:53:TYR:CZ    | 79:s2:1466:G:C5    | 3.09                     | 0.41              |
| 65:sD:127:MET:HE1  | 65:sD:131:ALA:O    | 2.21                     | 0.41              |
| 66:sF:34:SER:HB3   | 73:sc:11:LEU:HD11  | 2.03                     | 0.41              |
| 66:sF:156:THR:HA   | 66:sF:159:ARG:NH1  | 2.36                     | 0.41              |
| 67:sK:5:LYS:HZ3    | 79:s2:1313:A:P     | 2.43                     | 0.41              |
| 69:sQ:12:VAL:HG11  | 69:sQ:91:ALA:N     | 2.36                     | 0.41              |
| 69:sQ:86:GLN:O     | 69:sQ:89:SER:OG    | 2.38                     | 0.41              |
| 69:sQ:105:LYS:HA   | 69:sQ:108:ILE:CD1  | 2.51                     | 0.41              |
| 70:sS:2:SER:HB3    | 77:sZ:49:LEU:HD23  | 2.02                     | 0.41              |
| 73:sc:13:ARG:O     | 73:sc:32:VAL:HA    | 2.19                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 73:sc:34:PHE:C    | 73:sc:35:MET:SD   | 3.03                     | 0.41              |
| 75:sg:147:HIS:CE1 | 75:sg:169:GLY:HA3 | 2.56                     | 0.41              |
| 79:s2:149:A:C2    | 79:s2:150:A:H1'   | 2.55                     | 0.41              |
| 79:s2:839:C:N4    | 79:s2:841:G:C6    | 2.89                     | 0.41              |
| 79:s2:907:G:C2    | 79:s2:908:A:C5    | 3.08                     | 0.41              |
| 79:s2:920:A:N7    | 79:s2:1021:U:O4   | 2.54                     | 0.41              |
| 79:s2:1370:A:C2   | 79:s2:1372:U:C2   | 3.08                     | 0.41              |
| 79:s2:1527:C:H2'  | 79:s2:1528:G:O4'  | 2.21                     | 0.41              |
| 79:s2:1539:U:H2'  | 79:s2:1540:G:C8   | 2.56                     | 0.41              |
| 79:s2:1546:G:H21  | 79:s2:1670:C:H1'  | 1.85                     | 0.41              |
| 79:s2:1687:C:H2'  | 79:s2:1688:C:H6   | 1.85                     | 0.41              |
| 79:s2:1774:C:C5   | 79:s2:1775:U:H1'  | 2.55                     | 0.41              |
| 85:l5:1360:G:H2'  | 85:l5:1361:G:C8   | 2.56                     | 0.41              |
| 85:l5:1392:A:H2'  | 85:l5:1393:G:C8   | 2.55                     | 0.41              |
| 85:l5:1475:G:N2   | 85:l5:1490:G:C4   | 2.89                     | 0.41              |
| 85:l5:1505:C:H2'  | 85:l5:1506:G:C8   | 2.54                     | 0.41              |
| 85:l5:1541:C:O2'  | 85:l5:2448:G:N3   | 2.53                     | 0.41              |
| 85:l5:1627:G:C5   | 85:l5:1628:C:C4   | 3.09                     | 0.41              |
| 85:l5:2294:G:C6   | 85:l5:2341:A:C6   | 3.09                     | 0.41              |
| 85:l5:2423:A:H2'  | 85:l5:2424:G:C8   | 2.56                     | 0.41              |
| 85:l5:2459:G:H2'  | 85:l5:2461:G:OP2  | 2.20                     | 0.41              |
| 85:l5:2602:G:C5   | 85:l5:2742:G:C6   | 3.08                     | 0.41              |
| 85:l5:2684:C:H2'  | 85:l5:2685:C:H6   | 1.83                     | 0.41              |
| 85:l5:2776:G:H2'  | 85:l5:2777:G:H8   | 1.86                     | 0.41              |
| 85:l5:3598:C:C2'  | 85:l5:3599:A:H5'  | 2.50                     | 0.41              |
| 85:l5:3971:G:H2'  | 85:l5:3973:G:H4'  | 2.03                     | 0.41              |
| 85:l5:4205:A:H2'  | 85:l5:4206:C:O4'  | 2.20                     | 0.41              |
| 85:l5:4638:U:C4   | 85:l5:4639:G:N1   | 2.89                     | 0.41              |
| 85:l5:4683:U:C2   | 85:l5:4684:A:C8   | 3.09                     | 0.41              |
| 80:CB:61:LYS:C    | 80:CB:63:GLU:H    | 2.29                     | 0.41              |
| 80:CB:253:VAL:O   | 80:CB:257:MET:SD  | 2.78                     | 0.41              |
| 80:CB:415:ARG:HB3 | 80:CB:417:PHE:CZ  | 2.55                     | 0.41              |
| 80:CB:603:TYR:HD1 | 80:CB:706:ASP:O   | 2.04                     | 0.41              |
| 80:CB:746:LEU:HB2 | 80:CB:815:ASP:HB2 | 2.03                     | 0.41              |
| 3:SI:10:LYS:HD3   | 79:S2:387:C:P     | 2.60                     | 0.41              |
| 3:SI:193:LYS:HA   | 3:SI:193:LYS:HD2  | 1.91                     | 0.41              |
| 5:SX:49:GLY:N     | 5:SX:100:VAL:O    | 2.49                     | 0.41              |
| 5:SX:109:GLY:C    | 5:SX:119:ARG:HG2  | 2.45                     | 0.41              |
| 7:SJ:55:LYS:HE2   | 7:SJ:55:LYS:HB2   | 1.80                     | 0.41              |
| 8:SY:103:SER:HB3  | 8:SY:106:GLN:NE2  | 2.34                     | 0.41              |
| 8:SY:116:LYS:NZ   | 79:S2:161:U:OP1   | 2.53                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 10:SA:54:THR:HB   | 10:SA:163:CYS:SG   | 2.60                     | 0.41              |
| 10:SA:73:ASP:OD1  | 10:SA:120:ARG:HB2  | 2.20                     | 0.41              |
| 10:SA:110:ASN:OD1 | 10:SA:112:ILE:HG12 | 2.21                     | 0.41              |
| 11:SB:87:ILE:H    | 11:SB:101:HIS:HB2  | 1.85                     | 0.41              |
| 11:SB:136:ARG:CZ  | 79:S2:941:C:H5''   | 2.51                     | 0.41              |
| 12:SH:34:SER:O    | 12:SH:36:LEU:HD22  | 2.21                     | 0.41              |
| 14:Sa:43:ASN:ND2  | 14:Sa:66:LYS:HG2   | 2.36                     | 0.41              |
| 14:Sa:58:VAL:HG11 | 17:SO:28:PHE:HZ    | 1.86                     | 0.41              |
| 16:SN:66:VAL:HG13 | 16:SN:67:THR:HG23  | 2.03                     | 0.41              |
| 17:SO:147:ARG:HB2 | 17:SO:147:ARG:HE   | 1.71                     | 0.41              |
| 85:L5:81:C:C4     | 85:L5:82:U:C4      | 3.08                     | 0.41              |
| 85:L5:207:G:H2'   | 85:L5:208:A:C8     | 2.56                     | 0.41              |
| 85:L5:276:C:OP2   | 54:Li:34:THR:HG21  | 2.20                     | 0.41              |
| 85:L5:444:G:N3    | 85:L5:2313:A:H2    | 2.19                     | 0.41              |
| 85:L5:468:U:C5    | 85:L5:469:C:H5     | 2.38                     | 0.41              |
| 85:L5:732:A:H2'   | 85:L5:733:A:O4'    | 2.20                     | 0.41              |
| 85:L5:1345:A:H2'  | 85:L5:1346:C:H6    | 1.82                     | 0.41              |
| 85:L5:1420:A:H2   | 85:L5:1501:C:C6    | 2.39                     | 0.41              |
| 85:L5:1535:C:C5'  | 55:Lj:11:ARG:NH1   | 2.84                     | 0.41              |
| 85:L5:2059:C:H2'  | 85:L5:2060:G:C8    | 2.51                     | 0.41              |
| 85:L5:2319:C:N4   | 50:Le:58:ILE:HD13  | 2.36                     | 0.41              |
| 85:L5:2384:U:H2'  | 85:L5:2385:U:C6    | 2.54                     | 0.41              |
| 85:L5:2394:G:O4'  | 85:L5:2397:G:N2    | 2.51                     | 0.41              |
| 85:L5:2394:G:O2'  | 85:L5:2819:U:O4    | 2.36                     | 0.41              |
| 85:L5:2554:U:H1'  | 85:L5:2574:G:N2    | 2.35                     | 0.41              |
| 85:L5:2658:G:C8   | 48:Lc:33:GLN:NE2   | 2.88                     | 0.41              |
| 85:L5:2762:G:H2'  | 85:L5:2764:A:H5''  | 2.03                     | 0.41              |
| 85:L5:3703:G:H2'  | 85:L5:3704:U:C6    | 2.55                     | 0.41              |
| 85:L5:3806:G:C2   | 85:L5:3807:A:C8    | 3.09                     | 0.41              |
| 85:L5:4140:C:N3   | 85:L5:4145:C:O2'   | 2.47                     | 0.41              |
| 85:L5:4215:C:H2'  | 85:L5:4216:G:O4'   | 2.21                     | 0.41              |
| 85:L5:4281:A:N6   | 85:L5:4283:G:H1'   | 2.36                     | 0.41              |
| 85:L5:4313:A:O2'  | 40:LT:68:THR:HG21  | 2.19                     | 0.41              |
| 85:L5:4313:A:H2'  | 85:L5:4314:C:O4'   | 2.20                     | 0.41              |
| 85:L5:4313:A:H1'  | 40:LT:90:ASN:HD22  | 1.85                     | 0.41              |
| 85:L5:4467:A:N3   | 85:L5:4510:A:H2    | 2.19                     | 0.41              |
| 85:L5:4545:G:H2'  | 85:L5:4546:A:H8    | 1.86                     | 0.41              |
| 85:L5:4561:C:C2   | 85:L5:4562:C:C5    | 3.09                     | 0.41              |
| 85:L5:4683:U:H2'  | 85:L5:4684:A:O4'   | 2.19                     | 0.41              |
| 85:L5:4744:A:H2'  | 85:L5:4745:G:O4'   | 2.20                     | 0.41              |
| 20:L7:71:G:C5     | 20:L7:72:U:C4      | 3.09                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:LC:172:LYS:HG3  | 24:LC:177:TRP:CG   | 2.56                     | 0.41              |
| 28:LG:217:LYS:HE3  | 28:LG:217:LYS:HB2  | 1.80                     | 0.41              |
| 30:LI:45:GLU:H     | 30:LI:45:GLU:CD    | 2.28                     | 0.41              |
| 30:LI:52:MET:HB2   | 30:LI:136:MET:H    | 1.86                     | 0.41              |
| 34:LN:120:TRP:HA   | 34:LN:130:PHE:CD1  | 2.55                     | 0.41              |
| 34:LN:159:ARG:HB3  | 34:LN:164:LEU:HB2  | 2.02                     | 0.41              |
| 36:LP:41:ILE:N     | 36:LP:41:ILE:HD13  | 2.36                     | 0.41              |
| 37:LQ:149:TYR:CD1  | 37:LQ:152:PHE:CD2  | 3.09                     | 0.41              |
| 38:LR:106:LEU:HD23 | 38:LR:106:LEU:HA   | 1.80                     | 0.41              |
| 38:LR:123:LEU:O    | 38:LR:127:VAL:HG12 | 2.21                     | 0.41              |
| 38:LR:132:PHE:CE1  | 38:LR:138:LEU:HA   | 2.56                     | 0.41              |
| 41:LU:46:ARG:C     | 41:LU:47:ILE:HD12  | 2.45                     | 0.41              |
| 42:LV:131:ARG:HD2  | 42:LV:131:ARG:N    | 2.35                     | 0.41              |
| 46:La:8:THR:HA     | 46:La:11:LEU:HB2   | 2.01                     | 0.41              |
| 48:Lc:35:LEU:HA    | 48:Lc:38:ILE:HG13  | 2.02                     | 0.41              |
| 48:Lc:77:ASN:OD1   | 48:Lc:79:ILE:N     | 2.51                     | 0.41              |
| 48:Lc:82:GLY:HA2   | 48:Lc:91:VAL:HG22  | 2.03                     | 0.41              |
| 54:Li:61:LEU:HD13  | 54:Li:94:LEU:HD23  | 2.03                     | 0.41              |
| 61:Lp:6:LYS:HE3    | 61:Lp:6:LYS:HB3    | 1.90                     | 0.41              |
| 66:SF:38:TYR:CE1   | 66:SF:144:LEU:HB3  | 2.56                     | 0.41              |
| 66:SF:119:SER:HA   | 66:SF:193:LYS:HD3  | 2.01                     | 0.41              |
| 67:SK:47:LYS:HE3   | 79:S2:1274:G:H5''  | 2.02                     | 0.41              |
| 69:SQ:14:GLY:N     | 69:SQ:21:ALA:O     | 2.36                     | 0.41              |
| 79:S2:211:G:N3     | 79:S2:211:G:H2'    | 2.36                     | 0.41              |
| 79:S2:508:A:H3'    | 79:S2:509:G:C8     | 2.37                     | 0.41              |
| 79:S2:550:C:H6     | 79:S2:550:C:OP2    | 2.03                     | 0.41              |
| 79:S2:753:C:C5     | 79:S2:791:C:H4'    | 2.55                     | 0.41              |
| 79:S2:1104:G:C6    | 79:S2:1105:G:C5    | 3.08                     | 0.41              |
| 79:S2:1113:A:C6    | 79:S2:1121:G:C6    | 3.09                     | 0.41              |
| 79:S2:1259:A:H3'   | 79:S2:1259:A:N3    | 2.36                     | 0.41              |
| 79:S2:1305:C:H2'   | 79:S2:1306:U:C6    | 2.56                     | 0.41              |
| 79:S2:1560:U:C2    | 79:S2:1575:G:O6    | 2.73                     | 0.41              |
| 79:S2:1563:G:H2'   | 79:S2:1564:C:H6    | 1.86                     | 0.41              |
| 83:Ls:40:MET:SD    | 83:Ls:41:GLN:HG3   | 2.60                     | 0.41              |
| 84:Lt:123:ARG:HH21 | 84:Lt:126:SER:HA   | 1.86                     | 0.41              |
| 87:LW:1:MET:SD     | 87:LW:1:MET:C      | 3.04                     | 0.41              |
| 1:cH:94:ASP:O      | 1:cH:97:THR:OG1    | 2.35                     | 0.41              |
| 3:sI:124:LYS:HB2   | 3:sI:124:LYS:HE2   | 1.61                     | 0.41              |
| 3:sI:130:THR:N     | 3:sI:131:PRO:HD2   | 2.35                     | 0.41              |
| 4:sL:12:LYS:HD2    | 4:sL:13:GLN:O      | 2.21                     | 0.41              |
| 4:sL:93:LEU:HG     | 4:sL:102:PHE:CD2   | 2.55                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 6:sG:218:LYS:O     | 6:sG:218:LYS:NZ    | 2.38                     | 0.41              |
| 7:sJ:41:ARG:HA     | 7:sJ:44:TRP:HE3    | 1.85                     | 0.41              |
| 8:sY:99:LYS:HA     | 8:sY:99:LYS:HD2    | 1.60                     | 0.41              |
| 10:sA:85:ARG:O     | 10:sA:89:LYS:HG3   | 2.21                     | 0.41              |
| 11:sB:128:LYS:HA   | 11:sB:134:LEU:HA   | 2.02                     | 0.41              |
| 18:sW:46:TYR:HE2   | 18:sW:130:PHE:HA   | 1.85                     | 0.41              |
| 19:sb:20:LYS:HA    | 19:sb:23:ARG:CZ    | 2.50                     | 0.41              |
| 20:l7:7:G:H5"      | 25:lD:22:ARG:CD    | 2.50                     | 0.41              |
| 22:lA:94:ALA:O     | 22:lA:102:LEU:HD22 | 2.21                     | 0.41              |
| 24:lC:341:LEU:HD12 | 24:lC:345:ARG:HH12 | 1.85                     | 0.41              |
| 27:lF:67:THR:O     | 27:lF:71:MET:SD    | 2.78                     | 0.41              |
| 27:lF:109:LEU:HD23 | 27:lF:109:LEU:HA   | 1.89                     | 0.41              |
| 28:lG:39:PHE:CD1   | 28:lG:47:PRO:HD3   | 2.56                     | 0.41              |
| 29:lH:41:ILE:HG22  | 29:lH:43:VAL:HG13  | 2.01                     | 0.41              |
| 29:lH:48:LEU:HD23  | 29:lH:48:LEU:HA    | 1.92                     | 0.41              |
| 33:lM:60:PHE:CE1   | 33:lM:86:TRP:HB2   | 2.56                     | 0.41              |
| 34:lN:31:ARG:HG3   | 34:lN:129:PHE:CZ   | 2.55                     | 0.41              |
| 36:lP:54:GLN:HG2   | 36:lP:83:TRP:CG    | 2.56                     | 0.41              |
| 39:lS:29:ARG:HE    | 40:lT:150:LEU:CD2  | 2.32                     | 0.41              |
| 41:lU:101:ARG:HG2  | 41:lU:103:VAL:HG23 | 2.03                     | 0.41              |
| 42:lV:89:ARG:HH11  | 85:l5:4673:U:H5'   | 1.85                     | 0.41              |
| 43:lX:74:TYR:HB2   | 53:lh:25:LYS:HD3   | 2.02                     | 0.41              |
| 44:lY:11:ARG:NH1   | 85:l5:229:G:OP1    | 2.50                     | 0.41              |
| 44:lY:46:SER:OG    | 85:l5:239:C:H5"    | 2.21                     | 0.41              |
| 45:lZ:134:LEU:HD21 | 45:lZ:136:PHE:HB3  | 2.03                     | 0.41              |
| 46:la:43:ILE:HG23  | 85:l5:1682:A:O2'   | 2.21                     | 0.41              |
| 46:la:85:GLN:HE22  | 85:l5:508:G:H21    | 1.68                     | 0.41              |
| 47:lb:42:ASN:ND2   | 85:l5:1816:C:N1    | 2.69                     | 0.41              |
| 53:lh:33:VAL:O     | 53:lh:36:VAL:HG12  | 2.20                     | 0.41              |
| 55:lj:34:CYS:SG    | 55:lj:37:CYS:N     | 2.87                     | 0.41              |
| 55:lj:71:TYR:HD2   | 55:lj:71:TYR:H     | 1.67                     | 0.41              |
| 63:lz:68:LEU:HD13  | 63:lz:90:LEU:HB2   | 2.02                     | 0.41              |
| 63:lz:96:ASN:CG    | 63:lz:125:GLY:H    | 2.28                     | 0.41              |
| 64:sR:3:ARG:HH22   | 79:s2:1467:C:C1'   | 2.31                     | 0.41              |
| 65:sD:193:ASP:O    | 65:sD:195:THR:HG23 | 2.20                     | 0.41              |
| 66:sF:56:TYR:O     | 66:sF:62:ARG:HB2   | 2.21                     | 0.41              |
| 67:sK:26:ASP:OD2   | 67:sK:26:ASP:N     | 2.54                     | 0.41              |
| 67:sK:52:LEU:HB3   | 67:sK:57:TYR:HD1   | 1.86                     | 0.41              |
| 67:sK:55:ARG:HB2   | 67:sK:57:TYR:CE1   | 2.56                     | 0.41              |
| 69:sQ:17:LYS:HA    | 69:sQ:126:ARG:NH1  | 2.36                     | 0.41              |
| 69:sQ:109:LYS:HZ2  | 69:sQ:109:LYS:C    | 2.29                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 69:sQ:135:PRO:HD3 | 69:sQ:141:TYR:CD1  | 2.55                     | 0.41              |
| 71:sT:41:LYS:NZ   | 79:s2:1569:A:P     | 2.93                     | 0.41              |
| 74:sd:16:GLN:H    | 74:sd:16:GLN:CD    | 2.28                     | 0.41              |
| 75:sg:38:LYS:NZ   | 75:sg:64:HIS:HD2   | 2.18                     | 0.41              |
| 75:sg:297:THR:HA  | 75:sg:311:GLN:HA   | 2.01                     | 0.41              |
| 76:sM:44:LYS:C    | 76:sM:46:GLN:H     | 2.28                     | 0.41              |
| 79:s2:202:G:H5''  | 79:s2:203:G:H8     | 1.86                     | 0.41              |
| 79:s2:603:C:H1'   | 79:s2:604:A:N7     | 2.36                     | 0.41              |
| 79:s2:650:A:H2'   | 79:s2:651:U:O4'    | 2.21                     | 0.41              |
| 79:s2:880:G:H2'   | 79:s2:881:G:C8     | 2.55                     | 0.41              |
| 79:s2:884:C:H2'   | 79:s2:885:U:O4'    | 2.20                     | 0.41              |
| 79:s2:917:U:O2'   | 79:s2:918:U:H5'    | 2.21                     | 0.41              |
| 79:s2:1037:G:C2   | 79:s2:1038:U:C5    | 3.09                     | 0.41              |
| 79:s2:1345:G:OP2  | 79:s2:1371:U:H5''  | 2.20                     | 0.41              |
| 79:s2:1533:A:N3   | 79:s2:1533:A:H2'   | 2.35                     | 0.41              |
| 79:s2:1630:A:C6   | 79:s2:1631:U:C5    | 3.08                     | 0.41              |
| 79:s2:1778:C:H2'  | 79:s2:1779:G:C8    | 2.56                     | 0.41              |
| 80:cB:61:LYS:C    | 80:cB:63:GLU:N     | 2.79                     | 0.41              |
| 80:cB:710:HIS:NE2 | 80:cB:712:ASP:HB2  | 2.36                     | 0.41              |
| 81:aP:14:A:C6     | 81:aP:22:U:C4      | 3.08                     | 0.41              |
| 81:aP:38:C:H2'    | 81:aP:39:G:H8      | 1.86                     | 0.41              |
| 84:lt:53:TRP:CH2  | 84:lt:56:LEU:HD11  | 2.56                     | 0.41              |
| 85:l5:117:C:H2'   | 85:l5:118:C:C6     | 2.56                     | 0.41              |
| 85:l5:518:G:C8    | 85:l5:644:G:C2     | 3.08                     | 0.41              |
| 85:l5:739:G:O2'   | 85:l5:740:G:H5''   | 2.21                     | 0.41              |
| 85:l5:1349:G:C6   | 85:l5:1508:A:C6    | 3.09                     | 0.41              |
| 85:l5:1415:G:C4   | 85:l5:1416:G:C8    | 3.09                     | 0.41              |
| 85:l5:1512:G:H2'  | 85:l5:1513:U:C6    | 2.55                     | 0.41              |
| 85:l5:1986:U:O4   | 85:l5:2013:A:N6    | 2.54                     | 0.41              |
| 85:l5:2874:U:O2'  | 85:l5:2876:G:N7    | 2.52                     | 0.41              |
| 85:l5:3936:A:C6   | 85:l5:4175:G:C6    | 3.08                     | 0.41              |
| 85:l5:4301:U:H2'  | 85:l5:4302:U:C6    | 2.56                     | 0.41              |
| 85:l5:4347:G:C6   | 85:l5:4366:A:N1    | 2.89                     | 0.41              |
| 85:l5:5038:A:H2'  | 85:l5:5039:U:C6    | 2.56                     | 0.41              |
| 80:CB:11:ALA:O    | 80:CB:15:LYS:NZ    | 2.44                     | 0.41              |
| 80:CB:336:LEU:O   | 80:CB:339:VAL:HG12 | 2.20                     | 0.41              |
| 80:CB:428:ARG:HD2 | 80:CB:489:GLU:OE1  | 2.19                     | 0.41              |
| 80:CB:503:PRO:HG3 | 80:CB:535:GLN:NE2  | 2.35                     | 0.41              |
| 5:SX:84:PHE:C     | 5:SX:84:PHE:CD2    | 2.96                     | 0.41              |
| 6:SG:167:LYS:HD3  | 6:SG:167:LYS:HA    | 1.70                     | 0.41              |
| 6:SG:203:LYS:HD2  | 6:SG:203:LYS:HA    | 1.78                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 7:SJ:37:LEU:H     | 7:SJ:37:LEU:HD12   | 1.86                     | 0.41              |
| 7:SJ:150:ARG:HG3  | 79:S2:821:G:C6     | 2.56                     | 0.41              |
| 10:SA:10:MET:H    | 10:SA:10:MET:HE3   | 1.85                     | 0.41              |
| 10:SA:216:ALA:HA  | 10:SA:219:GLU:OE1  | 2.20                     | 0.41              |
| 11:SB:91:VAL:HG12 | 11:SB:96:CYS:SG    | 2.61                     | 0.41              |
| 11:SB:186:ASN:OD1 | 11:SB:187:LYS:N    | 2.53                     | 0.41              |
| 12:SH:60:ILE:O    | 12:SH:92:VAL:HA    | 2.21                     | 0.41              |
| 12:SH:135:PHE:CD2 | 12:SH:136:PRO:HD3  | 2.56                     | 0.41              |
| 12:SH:145:ARG:HA  | 12:SH:145:ARG:HH11 | 1.86                     | 0.41              |
| 16:SN:70:LYS:O    | 16:SN:73:ARG:N     | 2.49                     | 0.41              |
| 18:SW:102:ILE:H   | 18:SW:113:HIS:CD2  | 2.39                     | 0.41              |
| 18:SW:113:HIS:O   | 18:SW:117:ARG:HG2  | 2.21                     | 0.41              |
| 85:L5:52:G:OP1    | 55:Lj:48:ASN:N     | 2.37                     | 0.41              |
| 85:L5:83:C:H4'    | 46:La:65:ARG:HH22  | 1.86                     | 0.41              |
| 85:L5:160:G:H2'   | 85:L5:161:G:H8     | 1.86                     | 0.41              |
| 85:L5:261:G:C6    | 85:L5:262:G:C6     | 3.09                     | 0.41              |
| 85:L5:387:G:H1'   | 85:L5:411:G:H21    | 1.84                     | 0.41              |
| 85:L5:506:C:H2'   | 85:L5:507:G:H8     | 1.85                     | 0.41              |
| 85:L5:657:C:H2'   | 85:L5:658:C:C6     | 2.56                     | 0.41              |
| 85:L5:727:C:H5''  | 27:LF:73:ARG:NH1   | 2.36                     | 0.41              |
| 85:L5:1319:U:OP1  | 46:La:22:ILE:HD13  | 2.21                     | 0.41              |
| 85:L5:1497:A:O4'  | 37:LQ:164:LYS:HA   | 2.20                     | 0.41              |
| 85:L5:1508:A:H2'  | 85:L5:1509:C:H6    | 1.86                     | 0.41              |
| 85:L5:1900:C:H4'  | 50:Le:60:TYR:CZ    | 2.56                     | 0.41              |
| 85:L5:1924:C:H5'' | 33:LM:34:ASN:ND2   | 2.35                     | 0.41              |
| 85:L5:2066:C:C2   | 85:L5:2067:C:C5    | 3.08                     | 0.41              |
| 85:L5:2292:C:H2'  | 85:L5:2293:U:C6    | 2.55                     | 0.41              |
| 85:L5:2557:G:C2   | 85:L5:2571:C:C2    | 3.08                     | 0.41              |
| 85:L5:2673:G:OP1  | 61:Lp:44:LYS:NZ    | 2.43                     | 0.41              |
| 85:L5:2684:C:H2'  | 85:L5:2685:C:C6    | 2.56                     | 0.41              |
| 85:L5:2726:G:H2'  | 85:L5:2727:C:H6    | 1.86                     | 0.41              |
| 85:L5:2751:G:C2   | 85:L5:2752:G:C8    | 3.09                     | 0.41              |
| 85:L5:3832:U:H2'  | 85:L5:3833:C:C6    | 2.55                     | 0.41              |
| 85:L5:3870:C:C2   | 85:L5:3886:G:C2    | 3.09                     | 0.41              |
| 85:L5:4102:C:C6   | 85:L5:4106:G:N9    | 2.88                     | 0.41              |
| 85:L5:4102:C:H2'  | 85:L5:4106:G:C4'   | 2.51                     | 0.41              |
| 85:L5:4536:C:H2'  | 85:L5:4537:C:H6    | 1.86                     | 0.41              |
| 85:L5:4909:A:O4'  | 85:L5:4912:G:H1'   | 2.21                     | 0.41              |
| 85:L5:5005:G:H2'  | 87:LW:51:TRP:CZ3   | 2.51                     | 0.41              |
| 85:L5:5044:A:H2'  | 85:L5:5045:G:H8    | 1.86                     | 0.41              |
| 21:L8:42:G:P      | 55:Lj:64:MET:HE1   | 2.60                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:LC:38:ASN:O     | 24:LC:42:THR:HG22  | 2.20                     | 0.41              |
| 25:LD:8:LYS:HB3    | 25:LD:13:PHE:CE2   | 2.56                     | 0.41              |
| 25:LD:68:ARG:HD3   | 25:LD:68:ARG:HA    | 1.45                     | 0.41              |
| 26:LE:166:LYS:HE2  | 26:LE:166:LYS:HB2  | 1.88                     | 0.41              |
| 27:LF:196:THR:O    | 27:LF:196:THR:OG1  | 2.38                     | 0.41              |
| 28:LG:197:LYS:HB2  | 28:LG:197:LYS:HE3  | 1.72                     | 0.41              |
| 30:LI:208:LYS:O    | 30:LI:212:LEU:HG   | 2.21                     | 0.41              |
| 32:LL:57:PRO:HG3   | 32:LL:75:GLY:O     | 2.20                     | 0.41              |
| 32:LL:194:ILE:HG13 | 32:LL:198:ARG:NH2  | 2.36                     | 0.41              |
| 33:LM:29:ASP:OD2   | 33:LM:30:VAL:N     | 2.53                     | 0.41              |
| 39:LS:103:ALA:O    | 39:LS:107:THR:HG23 | 2.21                     | 0.41              |
| 44:LY:21:ALA:HB1   | 44:LY:25:ILE:HG13  | 2.02                     | 0.41              |
| 44:LY:52:ASP:CG    | 44:LY:69:LYS:NZ    | 2.79                     | 0.41              |
| 47:Lb:51:LYS:HA    | 47:Lb:51:LYS:HD2   | 1.93                     | 0.41              |
| 50:Le:68:HIS:NE2   | 62:Lr:22:LYS:HG3   | 2.36                     | 0.41              |
| 54:Li:25:ARG:CZ    | 54:Li:26:HIS:H     | 2.34                     | 0.41              |
| 62:Lr:28:GLU:H     | 62:Lr:28:GLU:CD    | 2.29                     | 0.41              |
| 63:Lz:39:LYS:HE3   | 63:Lz:202:ARG:HH22 | 1.86                     | 0.41              |
| 66:SF:49:LEU:O     | 69:SQ:50:LYS:NZ    | 2.50                     | 0.41              |
| 75:Sg:124:SER:HB2  | 75:Sg:126:ASP:OD1  | 2.20                     | 0.41              |
| 75:Sg:127:LYS:HD2  | 75:Sg:148:SER:O    | 2.21                     | 0.41              |
| 75:Sg:174:VAL:HB   | 75:Sg:219:TRP:HZ3  | 1.85                     | 0.41              |
| 79:S2:30:C:C4      | 79:S2:31:U:C4      | 3.09                     | 0.41              |
| 79:S2:845:G:N1     | 79:S2:846:G:C2     | 2.89                     | 0.41              |
| 79:S2:937:C:H2'    | 79:S2:938:A:C8     | 2.55                     | 0.41              |
| 79:S2:1053:C:H2'   | 79:S2:1054:G:H8    | 1.85                     | 0.41              |
| 79:S2:1269:G:H2'   | 79:S2:1270:G:H8    | 1.86                     | 0.41              |
| 79:S2:1589:A:N3    | 79:S2:1653:U:O2'   | 2.54                     | 0.41              |
| 79:S2:1616:U:H2'   | 79:S2:1617:G:O4'   | 2.20                     | 0.41              |
| 79:S2:1817:G:H2'   | 79:S2:1818:A:H8    | 1.84                     | 0.41              |
| 84:Lt:121:LEU:HD12 | 84:Lt:121:LEU:HA   | 1.78                     | 0.41              |
| 84:Lt:131:GLU:HB2  | 84:Lt:152:ILE:CG2  | 2.49                     | 0.41              |
| 87:LW:23:ARG:HG3   | 87:LW:29:PHE:CE2   | 2.56                     | 0.41              |
| 87:LW:78:PHE:O     | 87:LW:78:PHE:CG    | 2.74                     | 0.41              |
| 1:CH:77:VAL:H      | 1:CH:77:VAL:HG23   | 1.65                     | 0.41              |
| 1:cH:79:LYS:HG2    | 1:cH:79:LYS:H      | 1.69                     | 0.41              |
| 4:sL:37:TYR:CE1    | 4:sL:51:ILE:HG13   | 2.56                     | 0.41              |
| 4:sL:38:LYS:HG2    | 4:sL:62:PHE:O      | 2.21                     | 0.41              |
| 4:sL:90:ARG:HE     | 4:sL:109:MET:HE3   | 1.86                     | 0.41              |
| 6:sG:136:LYS:H     | 79:s2:170:A:P      | 2.44                     | 0.41              |
| 7:sJ:144:ILE:HG22  | 7:sJ:147:PHE:N     | 2.36                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:sJ:174:LYS:CD    | 79:s2:560:A:H5'    | 2.51                     | 0.41              |
| 10:sA:30:LEU:HD22  | 10:sA:47:TYR:CE1   | 2.56                     | 0.41              |
| 10:sA:113:GLN:HG3  | 79:s2:1380:C:O2'   | 2.21                     | 0.41              |
| 10:sA:143:PRO:HD3  | 13:sV:32:ILE:CG1   | 2.51                     | 0.41              |
| 10:sA:159:ILE:O    | 10:sA:159:ILE:HG22 | 2.21                     | 0.41              |
| 11:sB:129:THR:HG23 | 11:sB:131:ASP:H    | 1.86                     | 0.41              |
| 11:sB:161:VAL:O    | 11:sB:164:ILE:HG13 | 2.20                     | 0.41              |
| 15:sC:74:LYS:HE3   | 15:sC:74:LYS:HB2   | 1.91                     | 0.41              |
| 17:sO:34:PHE:CD1   | 17:sO:98:ARG:HG2   | 2.55                     | 0.41              |
| 17:sO:118:ALA:O    | 17:sO:122:SER:N    | 2.52                     | 0.41              |
| 21:l8:154:G:C6     | 21:l8:155:C:N4     | 2.88                     | 0.41              |
| 23:lB:293:ILE:HD13 | 23:lB:293:ILE:HA   | 1.92                     | 0.41              |
| 24:lC:63:SER:OG    | 85:l5:1646:A:OP1   | 2.37                     | 0.41              |
| 28:lG:247:VAL:O    | 28:lG:250:ILE:HG22 | 2.21                     | 0.41              |
| 29:lH:12:ILE:HG13  | 29:lH:53:LYS:O     | 2.20                     | 0.41              |
| 29:lH:141:LYS:NZ   | 29:lH:142:ASP:OD1  | 2.54                     | 0.41              |
| 29:lH:150:ASP:OD1  | 29:lH:150:ASP:C    | 2.64                     | 0.41              |
| 30:II:183:ASP:O    | 30:II:187:LYS:HE2  | 2.21                     | 0.41              |
| 32:lL:6:ASN:HB2    | 46:la:48:TYR:CE1   | 2.56                     | 0.41              |
| 32:lL:36:ARG:HH21  | 85:l5:1363:C:P     | 2.44                     | 0.41              |
| 32:lL:87:HIS:O     | 32:lL:90:VAL:HG12  | 2.21                     | 0.41              |
| 35:lO:81:TRP:NE1   | 35:lO:99:LEU:HD11  | 2.36                     | 0.41              |
| 35:lO:82:ARG:HH12  | 85:l5:3887:C:P     | 2.44                     | 0.41              |
| 36:lP:17:SER:OG    | 36:lP:94:MET:SD    | 2.75                     | 0.41              |
| 36:lP:32:THR:HG21  | 36:lP:87:SER:HB3   | 2.03                     | 0.41              |
| 37:lQ:115:ARG:HD3  | 37:lQ:115:ARG:HA   | 1.89                     | 0.41              |
| 41:lU:72:VAL:O     | 41:lU:72:VAL:HG23  | 2.21                     | 0.41              |
| 42:lV:99:GLU:CD    | 87:lW:23:ARG:HA    | 2.46                     | 0.41              |
| 47:lb:32:LEU:HD13  | 85:l5:1464:C:H5'   | 2.02                     | 0.41              |
| 47:lb:91:ARG:N     | 47:lb:91:ARG:HD2   | 2.35                     | 0.41              |
| 51:lf:54:LYS:HD3   | 51:lf:54:LYS:C     | 2.46                     | 0.41              |
| 52:lg:96:LEU:HD12  | 52:lg:96:LEU:HA    | 1.84                     | 0.41              |
| 57:ll:13:LEU:HD11  | 85:l5:2407:G:C2    | 2.56                     | 0.41              |
| 60:lo:30:LYS:HD3   | 60:lo:30:LYS:HA    | 1.87                     | 0.41              |
| 62:lr:59:GLY:H     | 62:lr:121:GLN:NE2  | 2.19                     | 0.41              |
| 64:sR:39:ALA:HA    | 65:sD:206:ASP:HA   | 2.03                     | 0.41              |
| 64:sR:79:GLU:O     | 64:sR:82:ASP:HB3   | 2.21                     | 0.41              |
| 64:sR:105:MET:HA   | 64:sR:108:LEU:CD2  | 2.50                     | 0.41              |
| 67:sK:28:HIS:ND1   | 74:sd:8:TRP:HZ2    | 2.18                     | 0.41              |
| 70:sS:112:GLU:O    | 70:sS:116:LYS:HG2  | 2.21                     | 0.41              |
| 75:sg:38:LYS:CA    | 75:sg:65:PHE:HA    | 2.49                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 76:sM:35:ILE:HG13 | 76:sM:36:ARG:N     | 2.35                     | 0.41              |
| 79:s2:114:G:C6    | 79:s2:383:G:C2     | 3.09                     | 0.41              |
| 79:s2:389:A:H2'   | 79:s2:390:C:C6     | 2.56                     | 0.41              |
| 79:s2:478:G:H4'   | 80:cB:409:ARG:HH22 | 1.86                     | 0.41              |
| 79:s2:518:G:C2    | 79:s2:519:A:C5     | 3.09                     | 0.41              |
| 79:s2:609:U:C2    | 79:s2:610:G:N7     | 2.89                     | 0.41              |
| 79:s2:635:G:C6    | 79:s2:636:C:C4     | 3.09                     | 0.41              |
| 79:s2:642:U:H4'   | 79:s2:644:G:H4'    | 2.03                     | 0.41              |
| 79:s2:880:G:H2'   | 79:s2:881:G:H8     | 1.86                     | 0.41              |
| 79:s2:1218:C:H2'  | 79:s2:1219:C:H6    | 1.85                     | 0.41              |
| 79:s2:1304:U:C4   | 79:s2:1305:C:N4    | 2.89                     | 0.41              |
| 79:s2:1323:U:H2'  | 79:s2:1324:G:C8    | 2.56                     | 0.41              |
| 79:s2:1391:C:H2'  | 79:s2:1392:U:O4'   | 2.21                     | 0.41              |
| 79:s2:1424:G:H5'' | 79:s2:1425:G:OP2   | 2.21                     | 0.41              |
| 79:s2:1452:A:H4'  | 79:s2:1453:C:O4'   | 2.21                     | 0.41              |
| 79:s2:1693:G:H4'  | 79:s2:1694:U:OP1   | 2.21                     | 0.41              |
| 79:s2:1819:A:O2'  | 79:s2:1820:G:H5'   | 2.21                     | 0.41              |
| 80:cB:200:MET:HE1 | 80:cB:366:LYS:HE3  | 2.03                     | 0.41              |
| 80:cB:400:LYS:HD3 | 80:cB:401:MET:N    | 2.36                     | 0.41              |
| 80:cB:682:GLY:HA2 | 80:cB:722:ILE:HG23 | 2.02                     | 0.41              |
| 84:lt:81:ILE:HD13 | 84:lt:113:ALA:HB1  | 2.03                     | 0.41              |
| 85:l5:50:C:C2     | 85:l5:51:A:C8      | 3.09                     | 0.41              |
| 85:l5:282:C:C4    | 85:l5:283:G:C5     | 3.09                     | 0.41              |
| 85:l5:324:A:C6    | 85:l5:325:U:C4     | 3.09                     | 0.41              |
| 85:l5:505:G:C6    | 85:l5:654:C:N3     | 2.89                     | 0.41              |
| 85:l5:694:C:O2'   | 85:l5:695:G:H5'    | 2.21                     | 0.41              |
| 85:l5:964:A:C2'   | 85:l5:965:G:H4'    | 2.51                     | 0.41              |
| 85:l5:989:U:C2    | 85:l5:1064:G:O6    | 2.74                     | 0.41              |
| 85:l5:1368:A:H8   | 85:l5:1368:A:O5'   | 2.03                     | 0.41              |
| 85:l5:1480:C:H1'  | 85:l5:1482:G:H22   | 1.86                     | 0.41              |
| 85:l5:1554:A:N6   | 85:l5:1573:G:H1'   | 2.36                     | 0.41              |
| 85:l5:2362:U:H2'  | 85:l5:2363:A:C8    | 2.56                     | 0.41              |
| 85:l5:2659:A:C2   | 85:l5:2676:A:C8    | 3.09                     | 0.41              |
| 85:l5:2772:C:C2   | 85:l5:2773:G:C8    | 3.08                     | 0.41              |
| 85:l5:3650:C:C2   | 85:l5:3651:A:C8    | 3.09                     | 0.41              |
| 85:l5:3877:A:O2'  | 85:l5:4400:G:N2    | 2.53                     | 0.41              |
| 85:l5:3943:A:H5'  | 85:l5:3944:G:OP2   | 2.21                     | 0.41              |
| 85:l5:4198:G:H2'  | 85:l5:4199:C:C6    | 2.56                     | 0.41              |
| 85:l5:4209:G:C6   | 85:l5:4224:A:C6    | 3.08                     | 0.41              |
| 85:l5:4465:U:C4   | 85:l5:4488:A:C5    | 3.08                     | 0.41              |
| 85:l5:4889:G:C4   | 85:l5:4890:G:C8    | 3.08                     | 0.41              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 80:CB:390:PRO:C    | 80:CB:391:LYS:HD3 | 2.46                     | 0.41              |
| 2:SE:94:LYS:NZ     | 2:SE:95:THR:HG23  | 2.36                     | 0.41              |
| 2:SE:251:GLU:O     | 2:SE:254:LYS:HG3  | 2.20                     | 0.41              |
| 3:SI:143:LYS:HZ3   | 79:S2:196:C:N4    | 2.19                     | 0.41              |
| 4:SL:131:CYS:SG    | 4:SL:141:ASN:HB2  | 2.61                     | 0.41              |
| 4:SL:150:GLY:C     | 4:SL:152:LYS:H    | 2.27                     | 0.41              |
| 5:SX:7:LEU:HD12    | 5:SX:7:LEU:HA     | 1.82                     | 0.41              |
| 6:SG:198:ARG:HG3   | 6:SG:199:THR:N    | 2.35                     | 0.41              |
| 10:SA:140:VAL:HG13 | 15:SC:87:PRO:HG3  | 2.03                     | 0.41              |
| 10:SA:143:PRO:CB   | 13:SV:34:MET:HE1  | 2.51                     | 0.41              |
| 10:SA:206:ASP:HA   | 10:SA:207:PRO:HD3 | 1.97                     | 0.41              |
| 11:SB:30:TRP:HA    | 11:SB:48:LEU:HA   | 2.02                     | 0.41              |
| 11:SB:82:ARG:NH2   | 11:SB:188:LEU:O   | 2.54                     | 0.41              |
| 11:SB:227:LYS:HD3  | 11:SB:230:GLU:OE2 | 2.21                     | 0.41              |
| 12:SH:76:GLN:NE2   | 12:SH:135:PHE:CE2 | 2.89                     | 0.41              |
| 17:SO:147:ARG:HH21 | 17:SO:150:ARG:CZ  | 2.34                     | 0.41              |
| 85:L5:100:C:H2'    | 85:L5:101:A:O4'   | 2.20                     | 0.41              |
| 85:L5:109:G:H5'    | 32:LL:92:ARG:NE   | 2.35                     | 0.41              |
| 85:L5:167:C:N3     | 85:L5:269:G:N1    | 2.69                     | 0.41              |
| 85:L5:169:G:C2     | 85:L5:267:G:C2    | 3.09                     | 0.41              |
| 85:L5:192:G:H2'    | 85:L5:193:G:H8    | 1.85                     | 0.41              |
| 85:L5:269:G:C4     | 85:L5:270:U:C5    | 3.09                     | 0.41              |
| 85:L5:395:A:C6     | 85:L5:2379:A:C2   | 3.09                     | 0.41              |
| 85:L5:437:G:C5     | 85:L5:1311:G:C2   | 3.09                     | 0.41              |
| 85:L5:447:C:H2'    | 85:L5:448:G:H8    | 1.86                     | 0.41              |
| 85:L5:725:G:C6     | 85:L5:942:G:C6    | 3.09                     | 0.41              |
| 85:L5:919:C:H2'    | 85:L5:920:C:H6    | 1.86                     | 0.41              |
| 85:L5:1179:U:HO2'  | 85:L5:1180:C:P    | 2.40                     | 0.41              |
| 85:L5:1328:G:C6    | 85:L5:1329:G:C6   | 3.08                     | 0.41              |
| 85:L5:1354:A:C8    | 85:L5:1503:A:C6   | 3.09                     | 0.41              |
| 85:L5:1472:C:C2    | 85:L5:1473:U:C5   | 3.09                     | 0.41              |
| 85:L5:1909:G:C6    | 85:L5:1910:G:C5   | 3.08                     | 0.41              |
| 85:L5:2033:A:C2    | 85:L5:2034:G:N7   | 2.89                     | 0.41              |
| 85:L5:2045:G:O2'   | 85:L5:2046:G:H5'' | 2.21                     | 0.41              |
| 85:L5:2352:U:H2'   | 85:L5:2353:U:C6   | 2.56                     | 0.41              |
| 85:L5:2602:G:O4'   | 85:L5:2742:G:H2'  | 2.21                     | 0.41              |
| 85:L5:2673:G:H5'   | 85:L5:2673:G:N3   | 2.36                     | 0.41              |
| 85:L5:2897:G:C2    | 85:L5:2898:G:C5   | 3.09                     | 0.41              |
| 85:L5:3724:A:C6    | 85:L5:3725:G:C6   | 3.09                     | 0.41              |
| 85:L5:3787:G:H1'   | 85:L5:3789:C:N4   | 2.36                     | 0.41              |
| 85:L5:4169:G:H4'   | 85:L5:4171:C:C2   | 2.55                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 85:L5:4316:G:OP1   | 47:Lb:38:LYS:HE3   | 2.19                     | 0.41              |
| 85:L5:4417:C:H2'   | 85:L5:4418:G:O4'   | 2.20                     | 0.41              |
| 85:L5:4459:U:H5''  | 23:LB:10:ARG:NH1   | 2.36                     | 0.41              |
| 85:L5:4708:A:C2    | 85:L5:4709:U:H5'   | 2.55                     | 0.41              |
| 20:L7:46:C:OP1     | 25:LD:158:LYS:HG3  | 2.21                     | 0.41              |
| 20:L7:59:G:O2'     | 25:LD:267:ASN:HB3  | 2.21                     | 0.41              |
| 21:L8:93:C:O2'     | 21:L8:94:G:H8      | 2.03                     | 0.41              |
| 22:LA:46:LYS:HB3   | 22:LA:60:LYS:HD2   | 2.02                     | 0.41              |
| 25:LD:200:MET:HB3  | 25:LD:202:GLN:OE1  | 2.20                     | 0.41              |
| 28:LG:130:THR:C    | 28:LG:131:LYS:HG3  | 2.46                     | 0.41              |
| 29:LH:37:ASP:OD1   | 29:LH:39:ASN:N     | 2.47                     | 0.41              |
| 29:LH:66:GLU:HA    | 29:LH:69:THR:HG23  | 2.02                     | 0.41              |
| 29:LH:92:MET:HA    | 29:LH:182:SER:H    | 1.84                     | 0.41              |
| 30:LI:52:MET:CE    | 30:LI:165:ILE:HA   | 2.43                     | 0.41              |
| 32:LL:8:MET:HE2    | 37:LQ:166:TYR:HB3  | 2.01                     | 0.41              |
| 32:LL:80:GLU:OE2   | 32:LL:102:ARG:NH2  | 2.53                     | 0.41              |
| 35:LO:23:VAL:HG23  | 35:LO:33:VAL:HG11  | 2.02                     | 0.41              |
| 38:LR:172:ARG:HH22 | 79:S2:909:G:P      | 2.41                     | 0.41              |
| 41:LU:22:THR:HA    | 41:LU:71:THR:HA    | 2.02                     | 0.41              |
| 43:LX:40:ILE:HD12  | 43:LX:40:ILE:HA    | 1.98                     | 0.41              |
| 45:LZ:88:ASP:O     | 45:LZ:121:ARG:NH2  | 2.43                     | 0.41              |
| 45:LZ:106:LEU:HA   | 45:LZ:109:LYS:HG2  | 2.02                     | 0.41              |
| 47:Lb:39:PHE:O     | 47:Lb:40:LEU:C     | 2.64                     | 0.41              |
| 49:Ld:108:TYR:CD1  | 49:Ld:108:TYR:C    | 2.98                     | 0.41              |
| 53:Lh:28:LEU:HD11  | 53:Lh:32:ARG:CZ    | 2.51                     | 0.41              |
| 55:Lj:36:LYS:HA    | 55:Lj:45:ARG:HH21  | 1.86                     | 0.41              |
| 56:Lk:11:PHE:HE1   | 56:Lk:56:LEU:HD21  | 1.86                     | 0.41              |
| 56:Lk:17:ARG:HG2   | 56:Lk:19:ASP:OD1   | 2.21                     | 0.41              |
| 56:Lk:18:LYS:HB2   | 56:Lk:18:LYS:HE2   | 1.80                     | 0.41              |
| 56:Lk:52:LYS:HG2   | 56:Lk:52:LYS:H     | 1.66                     | 0.41              |
| 56:Lk:61:PRO:HA    | 56:Lk:62:PRO:HD2   | 1.97                     | 0.41              |
| 58:Lm:79:GLU:CD    | 58:Lm:81:SER:H     | 2.29                     | 0.41              |
| 62:Lr:73:PRO:HA    | 62:Lr:76:SER:OG    | 2.21                     | 0.41              |
| 62:Lr:86:ALA:O     | 62:Lr:89:THR:N     | 2.54                     | 0.41              |
| 64:SR:100:PRO:O    | 64:SR:104:GLU:HG2  | 2.20                     | 0.41              |
| 66:SF:121:PRO:HD2  | 66:SF:149:GLN:HE22 | 1.86                     | 0.41              |
| 67:SK:7:ASN:HA     | 67:SK:10:ALA:HB3   | 2.03                     | 0.41              |
| 68:SP:22:LEU:HD23  | 68:SP:22:LEU:H     | 1.85                     | 0.41              |
| 69:SQ:42:ILE:HG21  | 69:SQ:51:LEU:HG    | 2.01                     | 0.41              |
| 75:Sg:25:PRO:HG3   | 75:Sg:293:ALA:CB   | 2.51                     | 0.41              |
| 79:S2:374:G:H2'    | 79:S2:375:U:H6     | 1.86                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 79:S2:807:G:H2'   | 79:S2:808:A:H8     | 1.86                     | 0.41              |
| 79:S2:1005:G:H2'  | 79:S2:1006:C:H6    | 1.85                     | 0.41              |
| 79:S2:1121:G:C5   | 79:S2:1122:A:N7    | 2.89                     | 0.41              |
| 79:S2:1416:C:N4   | 79:S2:1417:C:H41   | 2.17                     | 0.41              |
| 79:S2:1796:G:C6   | 79:S2:1797:U:C4    | 3.08                     | 0.41              |
| 81:AP:9:A:H4'     | 81:AP:10:G:OP2     | 2.17                     | 0.41              |
| 87:IW:6:CYS:HB3   | 87:IW:11:TYR:H     | 1.85                     | 0.41              |
| 87:IW:30:GLN:C    | 87:IW:30:GLN:OE1   | 2.64                     | 0.41              |
| 87:IW:47:ARG:HA   | 87:IW:55:TYR:HB2   | 2.03                     | 0.41              |
| 1:CH:37:ASP:OD1   | 86:Se:47:PRO:CD    | 2.56                     | 0.41              |
| 1:CH:42:LYS:HD3   | 86:Se:42:PHE:CE2   | 2.56                     | 0.41              |
| 1:cH:113:ARG:H    | 1:cH:113:ARG:HG3   | 1.60                     | 0.41              |
| 2:sE:15:PRO:CD    | 2:sE:18:TRP:CE3    | 3.04                     | 0.41              |
| 2:sE:106:LYS:NZ   | 79:s2:846:G:OP2    | 2.51                     | 0.41              |
| 4:sL:103:GLU:CD   | 5:sX:11:ARG:HB2    | 2.46                     | 0.41              |
| 5:sX:101:LEU:HB2  | 5:sX:124:LYS:HB2   | 2.02                     | 0.41              |
| 6:sG:131:ARG:HB3  | 87:IW:82:ILE:HA    | 2.03                     | 0.41              |
| 7:sJ:24:ARG:O     | 7:sJ:28:GLU:HG3    | 2.21                     | 0.41              |
| 7:sJ:55:LYS:HA    | 7:sJ:58:ARG:NH1    | 2.36                     | 0.41              |
| 7:sJ:60:LEU:HD23  | 7:sJ:60:LEU:HA     | 1.77                     | 0.41              |
| 8:sY:87:PRO:HG2   | 8:sY:90:ARG:NH1    | 2.36                     | 0.41              |
| 9:se:33:LYS:CA    | 9:se:36:MET:HE1    | 2.49                     | 0.41              |
| 10:sA:27:GLY:H    | 10:sA:46:ILE:HG22  | 1.85                     | 0.41              |
| 10:sA:33:GLN:NE2  | 13:sV:63:GLY:O     | 2.54                     | 0.41              |
| 10:sA:196:GLU:OE2 | 10:sA:196:GLU:N    | 2.54                     | 0.41              |
| 11:sB:143:THR:HA  | 11:sB:207:LEU:HA   | 2.02                     | 0.41              |
| 11:sB:198:GLU:OE2 | 11:sB:201:CYS:SG   | 2.78                     | 0.41              |
| 14:sa:98:PRO:HG2  | 79:s2:1868:U:O4    | 2.20                     | 0.41              |
| 15:sC:216:MET:SD  | 15:sC:217:ALA:N    | 2.94                     | 0.41              |
| 15:sC:240:THR:O   | 15:sC:244:ILE:HG12 | 2.20                     | 0.41              |
| 16:sN:35:GLU:OE2  | 16:sN:39:LYS:HD3   | 2.21                     | 0.41              |
| 17:sO:33:ILE:CG2  | 17:sO:97:LEU:HD22  | 2.51                     | 0.41              |
| 17:sO:143:LYS:CB  | 79:s2:1047:C:H5'   | 2.51                     | 0.41              |
| 18:sW:66:THR:HG23 | 18:sW:68:ARG:H     | 1.85                     | 0.41              |
| 18:sW:82:GLN:HB3  | 79:s2:805:U:OP1    | 2.20                     | 0.41              |
| 18:sW:105:THR:O   | 18:sW:123:GLY:HA3  | 2.21                     | 0.41              |
| 20:l7:16:A:H2'    | 20:l7:17:C:C6      | 2.56                     | 0.41              |
| 20:l7:55:A:H4'    | 31:lJ:155:HIS:HB2  | 2.03                     | 0.41              |
| 20:l7:70:G:C2     | 20:l7:71:G:C5      | 3.09                     | 0.41              |
| 20:l7:80:U:C2     | 20:l7:81:G:C8      | 3.09                     | 0.41              |
| 21:l8:9:A:H2'     | 21:l8:10:G:H8      | 1.84                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 21:l8:26:C:H2'     | 21:l8:27:U:C6      | 2.56                     | 0.41              |
| 21:l8:66:A:H2'     | 21:l8:67:U:C6      | 2.56                     | 0.41              |
| 21:l8:75:G:C4'     | 57:ll:29:MET:HE1   | 2.51                     | 0.41              |
| 22:lA:129:ALA:O    | 22:lA:169:VAL:HG11 | 2.21                     | 0.41              |
| 22:lA:131:GLY:N    | 22:lA:169:VAL:HG13 | 2.34                     | 0.41              |
| 23:lB:231:VAL:HG13 | 23:lB:269:ALA:HB2  | 2.02                     | 0.41              |
| 24:lC:144:ILE:HB   | 24:lC:147:VAL:CG1  | 2.50                     | 0.41              |
| 24:lC:265:GLY:O    | 24:lC:279:LEU:HG   | 2.20                     | 0.41              |
| 25:lD:29:ASP:HA    | 85:l5:4280:A:N1    | 2.35                     | 0.41              |
| 25:lD:54:ARG:HB2   | 25:lD:61:ILE:HB    | 2.02                     | 0.41              |
| 25:lD:74:ILE:HD11  | 25:lD:76:CYS:O     | 2.20                     | 0.41              |
| 25:lD:180:PHE:HB2  | 25:lD:190:PHE:CE1  | 2.56                     | 0.41              |
| 25:lD:218:ALA:O    | 25:lD:221:LYS:HG3  | 2.21                     | 0.41              |
| 26:lE:140:LEU:HD12 | 26:lE:141:ARG:N    | 2.36                     | 0.41              |
| 26:lE:224:LYS:NZ   | 26:lE:234:ASP:OD2  | 2.44                     | 0.41              |
| 27:lF:100:GLY:HA2  | 85:l5:1877:G:O3'   | 2.21                     | 0.41              |
| 27:lF:103:PRO:HD3  | 85:l5:1876:U:O3'   | 2.21                     | 0.41              |
| 27:lF:159:TYR:O    | 27:lF:209:TRP:N    | 2.48                     | 0.41              |
| 27:lF:187:MET:O    | 27:lF:191:ILE:HG12 | 2.21                     | 0.41              |
| 29:lH:92:MET:HE3   | 29:lH:161:ILE:CG1  | 2.51                     | 0.41              |
| 31:lJ:35:ARG:HE    | 31:lJ:35:ARG:HB2   | 1.49                     | 0.41              |
| 31:lJ:153:ALA:HA   | 31:lJ:156:ARG:NH1  | 2.36                     | 0.41              |
| 32:lL:127:PHE:CD2  | 53:lh:118:LYS:HG2  | 2.56                     | 0.41              |
| 32:lL:179:PHE:O    | 32:lL:183:ARG:HG2  | 2.21                     | 0.41              |
| 33:lM:108:ASP:HB3  | 35:lO:199:HIS:HD2  | 1.84                     | 0.41              |
| 34:lN:50:ARG:NH1   | 85:l5:278:G:O4'    | 2.49                     | 0.41              |
| 34:lN:146:PRO:HA   | 34:lN:149:GLN:NE2  | 2.36                     | 0.41              |
| 35:lO:182:GLU:HG3  | 35:lO:182:GLU:H    | 1.64                     | 0.41              |
| 36:lP:69:ARG:NH1   | 85:l5:4980:C:N3    | 2.69                     | 0.41              |
| 36:lP:117:ILE:HD13 | 36:lP:117:ILE:HG21 | 1.87                     | 0.41              |
| 37:lQ:2:GLY:N      | 85:l5:1897:A:OP1   | 2.53                     | 0.41              |
| 39:lS:7:LEU:HB2    | 39:lS:107:THR:CG2  | 2.50                     | 0.41              |
| 41:lU:56:LEU:HD12  | 41:lU:58:GLY:H     | 1.86                     | 0.41              |
| 41:lU:81:ARG:CZ    | 85:l5:2622:G:O6    | 2.69                     | 0.41              |
| 42:lV:65:VAL:HG11  | 42:lV:72:LEU:HG    | 2.02                     | 0.41              |
| 43:lX:79:PHE:O     | 43:lX:99:ILE:HG22  | 2.21                     | 0.41              |
| 44:lY:65:GLN:CD    | 44:lY:65:GLN:N     | 2.79                     | 0.41              |
| 44:lY:103:LYS:HA   | 44:lY:103:LYS:HD3  | 1.82                     | 0.41              |
| 46:la:92:LYS:N     | 46:la:92:LYS:HD2   | 2.35                     | 0.41              |
| 48:lc:44:LYS:HA    | 48:lc:44:LYS:HD3   | 1.96                     | 0.41              |
| 48:lc:56:ARG:NH2   | 85:l5:2674:A:O4'   | 2.54                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 48:lc:89:TYR:CZ    | 85:l5:2673:G:C6    | 3.09                     | 0.41              |
| 50:le:22:ARG:O     | 50:le:25:SER:HB3   | 2.21                     | 0.41              |
| 50:le:44:ARG:NH2   | 85:l5:1315:C:OP1   | 2.45                     | 0.41              |
| 50:le:105:SER:HA   | 50:le:128:ARG:HG3  | 2.03                     | 0.41              |
| 53:lh:94:ARG:HH21  | 85:l5:135:G:N2     | 2.18                     | 0.41              |
| 54:li:84:LYS:HB2   | 54:li:84:LYS:HE3   | 1.85                     | 0.41              |
| 56:lk:26:LYS:NZ    | 85:l5:2696:A:OP1   | 2.53                     | 0.41              |
| 56:lk:53:ALA:O     | 56:lk:57:LYS:HG3   | 2.21                     | 0.41              |
| 60:lo:61:LYS:NZ    | 85:l5:4373:G:N7    | 2.67                     | 0.41              |
| 64:sR:4:VAL:HG11   | 79:s2:1212:G:O3'   | 2.20                     | 0.41              |
| 64:sR:5:ARG:CD     | 64:sR:9:VAL:HG23   | 2.49                     | 0.41              |
| 64:sR:9:VAL:HB     | 64:sR:49:LYS:HZ1   | 1.85                     | 0.41              |
| 64:sR:132:ARG:HH11 | 64:sR:133:GLY:CA   | 2.34                     | 0.41              |
| 66:sF:122:ARG:HA   | 66:sF:141:VAL:HG22 | 2.02                     | 0.41              |
| 66:sF:123:GLU:OE2  | 73:sc:63:ARG:NH1   | 2.54                     | 0.41              |
| 66:sF:126:THR:HG21 | 73:sc:26:GLN:HB2   | 2.03                     | 0.41              |
| 66:sF:193:LYS:HE3  | 66:sF:193:LYS:HB3  | 1.91                     | 0.41              |
| 68:sP:39:ALA:N     | 79:s2:1613:G:OP2   | 2.50                     | 0.41              |
| 70:sS:107:LEU:HD23 | 70:sS:107:LEU:HA   | 1.91                     | 0.41              |
| 73:sc:20:ARG:NH2   | 79:s2:1679:A:H5''  | 2.36                     | 0.41              |
| 74:sd:13:LYS:HD2   | 79:s2:1556:A:C5    | 2.55                     | 0.41              |
| 74:sd:22:ARG:NH2   | 79:s2:1553:C:H41   | 2.19                     | 0.41              |
| 75:sg:17:TRP:CE3   | 75:sg:303:THR:HG22 | 2.55                     | 0.41              |
| 75:sg:22:ALA:C     | 75:sg:32:LEU:HD21  | 2.46                     | 0.41              |
| 75:sg:259:TRP:HA   | 75:sg:267:VAL:H    | 1.86                     | 0.41              |
| 76:sM:23:LYS:HA    | 76:sM:26:LEU:HG    | 2.02                     | 0.41              |
| 79:s2:89:C:C2      | 79:s2:90:G:C8      | 3.09                     | 0.41              |
| 79:s2:314:U:H2'    | 79:s2:315:C:H6     | 1.85                     | 0.41              |
| 79:s2:353:C:H2'    | 79:s2:354:U:C6     | 2.55                     | 0.41              |
| 79:s2:459:C:H3'    | 79:s2:460:A:H8     | 1.85                     | 0.41              |
| 79:s2:490:C:H2'    | 79:s2:491:C:C6     | 2.56                     | 0.41              |
| 79:s2:521:A:H2'    | 79:s2:522:A:O4'    | 2.21                     | 0.41              |
| 79:s2:845:G:H2'    | 79:s2:846:G:C8     | 2.56                     | 0.41              |
| 79:s2:860:G:H3'    | 79:s2:861:A:C8     | 2.56                     | 0.41              |
| 79:s2:1181:A:H2'   | 79:s2:1182:A:C8    | 2.56                     | 0.41              |
| 79:s2:1206:G:O6    | 79:s2:1208:A:N6    | 2.53                     | 0.41              |
| 79:s2:1280:G:H2'   | 79:s2:1281:G:C8    | 2.56                     | 0.41              |
| 79:s2:1364:U:H5    | 79:s2:1375:G:H21   | 1.67                     | 0.41              |
| 79:s2:1365:G:C2    | 79:s2:1366:G:C5    | 3.09                     | 0.41              |
| 79:s2:1368:U:C2    | 79:s2:1370:A:OP1   | 2.74                     | 0.41              |
| 79:s2:1395:C:C2    | 79:s2:1474:A:C6    | 3.09                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 79:s2:1403:C:OP2  | 79:s2:1405:A:N6    | 2.29                     | 0.41              |
| 79:s2:1424:G:C2   | 79:s2:1425:G:C4    | 3.09                     | 0.41              |
| 79:s2:1490:G:C2   | 79:s2:1491:G:C5    | 3.09                     | 0.41              |
| 79:s2:1571:G:O2'  | 79:s2:1572:C:H5'   | 2.21                     | 0.41              |
| 79:s2:1684:C:C4   | 79:s2:1685:U:C4    | 3.09                     | 0.41              |
| 79:s2:1688:C:H2'  | 79:s2:1689:C:H6    | 1.85                     | 0.41              |
| 79:s2:1854:U:O2   | 79:s2:1855:G:C8    | 2.74                     | 0.41              |
| 80:cB:266:PHE:HB2 | 80:cB:288:THR:HG22 | 2.03                     | 0.41              |
| 80:cB:377:PRO:HA  | 80:cB:382:ALA:HB1  | 2.03                     | 0.41              |
| 80:cB:693:CYS:HB2 | 80:cB:695:GLU:CG   | 2.50                     | 0.41              |
| 81:aP:52:G:N1     | 81:aP:53:G:C5      | 2.89                     | 0.41              |
| 82:pE:4:C:H2'     | 82:pE:5:G:H8       | 1.85                     | 0.41              |
| 82:pE:23:A:H2'    | 82:pE:24:G:C8      | 2.56                     | 0.41              |
| 82:pE:42:G:C2     | 82:pE:43:A:C5      | 3.09                     | 0.41              |
| 83:ls:97:GLU:O    | 83:ls:101:MET:HG3  | 2.20                     | 0.41              |
| 83:ls:127:ASN:HA  | 83:ls:153:GLU:HG2  | 2.03                     | 0.41              |
| 85:l5:62:A:H2'    | 85:l5:63:G:C8      | 2.55                     | 0.41              |
| 85:l5:74:G:H3'    | 85:l5:75:G:H8      | 1.85                     | 0.41              |
| 85:l5:267:G:C2    | 85:l5:268:G:C4     | 3.09                     | 0.41              |
| 85:l5:385:A:HO2'  | 85:l5:387:G:H8     | 1.67                     | 0.41              |
| 85:l5:453:G:N3    | 85:l5:453:G:H2'    | 2.35                     | 0.41              |
| 85:l5:467:U:C2    | 85:l5:468:U:H1'    | 2.55                     | 0.41              |
| 85:l5:663:G:C6    | 85:l5:664:G:C6     | 3.09                     | 0.41              |
| 85:l5:751:G:C2    | 85:l5:915:A:C4     | 3.09                     | 0.41              |
| 85:l5:1085:C:H2'  | 85:l5:1086:C:C6    | 2.55                     | 0.41              |
| 85:l5:1245:C:C2   | 85:l5:1246:G:C8    | 3.09                     | 0.41              |
| 85:l5:1315:C:H2'  | 85:l5:1316:G:C8    | 2.56                     | 0.41              |
| 85:l5:1326:A:H4'  | 85:l5:4446:U:H4'   | 2.03                     | 0.41              |
| 85:l5:1338:G:H4'  | 85:l5:1339:U:H6    | 1.86                     | 0.41              |
| 85:l5:1413:C:H2'  | 85:l5:1414:C:C1'   | 2.51                     | 0.41              |
| 85:l5:1460:C:C2   | 85:l5:1461:C:C5    | 3.09                     | 0.41              |
| 85:l5:1617:G:C4   | 85:l5:1618:G:C8    | 3.09                     | 0.41              |
| 85:l5:1628:C:H2'  | 85:l5:1629:G:H8    | 1.85                     | 0.41              |
| 85:l5:1743:A:N1   | 85:l5:1789:C:O2'   | 2.40                     | 0.41              |
| 85:l5:2072:C:H2'  | 85:l5:2073:C:H6    | 1.86                     | 0.41              |
| 85:l5:2276:A:H2'  | 85:l5:2277:C:C6    | 2.56                     | 0.41              |
| 85:l5:2641:A:H3'  | 85:l5:2642:A:H8    | 1.85                     | 0.41              |
| 85:l5:3867:A:H2'  | 85:l5:3868:G:C8    | 2.55                     | 0.41              |
| 85:l5:3902:A:C6   | 85:l5:4523:A:C5    | 3.08                     | 0.41              |
| 85:l5:3927:U:H2'  | 85:l5:3928:A:C8    | 2.56                     | 0.41              |
| 85:l5:3954:A:C2   | 85:l5:3955:G:C8    | 3.09                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 85:15:3960:A:O2'  | 85:15:3961:G:H2'   | 2.20                     | 0.41              |
| 85:15:4131:G:C6   | 85:15:4132:C:C4    | 3.09                     | 0.41              |
| 85:15:4212:A:H4'  | 85:15:4213:A:N3    | 2.36                     | 0.41              |
| 85:15:4266:G:H4'  | 85:15:4267:G:C4    | 2.56                     | 0.41              |
| 85:15:4335:C:H2'  | 85:15:4336:A:O4'   | 2.20                     | 0.41              |
| 85:15:4435:U:H2'  | 85:15:4436:U:C6    | 2.56                     | 0.41              |
| 85:15:4472:G:C6   | 85:15:4484:A:C6    | 3.09                     | 0.41              |
| 85:15:4513:A:H2'  | 85:15:4514:G:C8    | 2.56                     | 0.41              |
| 85:15:4532:U:H2'  | 85:15:4533:A:O4'   | 2.20                     | 0.41              |
| 85:15:4535:A:H2'  | 85:15:4536:C:H6    | 1.85                     | 0.41              |
| 85:15:4653:C:C2   | 85:15:4654:C:C5    | 3.09                     | 0.41              |
| 85:15:4774:C:O2'  | 85:15:4775:C:O2    | 2.34                     | 0.41              |
| 85:15:4886:C:H2'  | 85:15:4887:C:C6    | 2.56                     | 0.41              |
| 85:15:4891:G:H2'  | 85:15:4891:G:N3    | 2.35                     | 0.41              |
| 85:15:4926:C:H5'  | 85:15:4927:G:H21   | 1.86                     | 0.41              |
| 85:15:4953:G:H2'  | 85:15:4954:G:C8    | 2.54                     | 0.41              |
| 85:15:4963:G:C6   | 85:15:4964:C:N4    | 2.88                     | 0.41              |
| 85:15:5002:U:H2'  | 85:15:5003:U:H6    | 1.85                     | 0.41              |
| 80:CB:91:GLN:O    | 80:CB:93:LYS:NZ    | 2.47                     | 0.41              |
| 80:CB:170:GLU:HG2 | 80:CB:171:PRO:HD2  | 2.02                     | 0.41              |
| 80:CB:308:LYS:O   | 80:CB:312:THR:HG23 | 2.21                     | 0.41              |
| 80:CB:337:LYS:HB3 | 80:CB:337:LYS:HE2  | 1.96                     | 0.41              |
| 80:CB:583:VAL:O   | 80:CB:608:PRO:HB3  | 2.21                     | 0.41              |
| 2:SE:47:PHE:HD2   | 2:SE:48:LEU:HD23   | 1.86                     | 0.41              |
| 2:SE:54:TYR:HD1   | 8:SY:17:LEU:HD22   | 1.85                     | 0.41              |
| 2:SE:171:ASP:N    | 2:SE:171:ASP:OD1   | 2.52                     | 0.41              |
| 2:SE:236:ILE:HD12 | 2:SE:236:ILE:HA    | 1.94                     | 0.41              |
| 2:SE:242:LYS:HA   | 2:SE:242:LYS:HD3   | 1.95                     | 0.41              |
| 3:SI:143:LYS:HZ2  | 79:S2:203:G:H5'    | 1.85                     | 0.41              |
| 4:SL:38:LYS:HD2   | 79:S2:292:A:O3'    | 2.21                     | 0.41              |
| 4:SL:65:ASN:HB3   | 79:S2:294:U:N3     | 2.36                     | 0.41              |
| 4:SL:94:HIS:O     | 4:SL:103:GLU:N     | 2.54                     | 0.41              |
| 4:SL:132:ARG:HG3  | 79:S2:114:G:H8     | 1.85                     | 0.41              |
| 5:SX:26:GLN:HG2   | 5:SX:27:TYR:N      | 2.36                     | 0.41              |
| 6:SG:1:MET:HE1    | 6:SG:108:VAL:C     | 2.45                     | 0.41              |
| 6:SG:13:GLN:H     | 6:SG:13:GLN:HG3    | 1.75                     | 0.41              |
| 6:SG:136:LYS:HB2  | 79:S2:170:A:O5'    | 2.20                     | 0.41              |
| 6:SG:160:LYS:O    | 6:SG:172:LYS:N     | 2.54                     | 0.41              |
| 7:SJ:42:GLU:O     | 7:SJ:46:VAL:HG22   | 2.20                     | 0.41              |
| 7:SJ:121:LYS:C    | 7:SJ:122:SER:HG    | 2.25                     | 0.41              |
| 8:SY:14:THR:HA    | 8:SY:21:LYS:HG2    | 2.01                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 8:SY:109:GLU:O    | 8:SY:113:ARG:HG2   | 2.21                     | 0.41              |
| 86:Se:16:THR:O    | 86:Se:18:LYS:NZ    | 2.29                     | 0.41              |
| 12:SH:76:GLN:H    | 12:SH:76:GLN:HG3   | 1.62                     | 0.41              |
| 12:SH:164:ASN:N   | 12:SH:164:ASN:OD1  | 2.49                     | 0.41              |
| 13:SV:54:ALA:HB2  | 15:SC:261:PHE:HE1  | 1.86                     | 0.41              |
| 14:Sa:22:ARG:NH1  | 17:SO:141:ARG:HG3  | 2.35                     | 0.41              |
| 14:Sa:70:LYS:C    | 14:Sa:71:LEU:HD12  | 2.45                     | 0.41              |
| 15:SC:187:ARG:NH2 | 15:SC:190:SER:HA   | 2.36                     | 0.41              |
| 15:SC:273:LEU:HG  | 15:SC:277:HIS:HB3  | 2.03                     | 0.41              |
| 17:SO:63:LYS:HD2  | 17:SO:63:LYS:HA    | 1.74                     | 0.41              |
| 17:SO:83:GLN:O    | 17:SO:87:GLU:HG2   | 2.20                     | 0.41              |
| 18:SW:11:LEU:HD12 | 18:SW:74:VAL:HB    | 2.02                     | 0.41              |
| 18:SW:102:ILE:N   | 18:SW:102:ILE:HD13 | 2.35                     | 0.41              |
| 85:L5:113:A:OP2   | 85:L5:156:G:N1     | 2.42                     | 0.41              |
| 85:L5:119:G:H1    | 28:LG:133:PRO:HD2  | 1.86                     | 0.41              |
| 85:L5:280:G:H1    | 34:LN:15:GLN:HE22  | 1.68                     | 0.41              |
| 85:L5:344:A:H2'   | 85:L5:345:C:O4'    | 2.21                     | 0.41              |
| 85:L5:677:G:H2'   | 85:L5:678:C:H6     | 1.86                     | 0.41              |
| 85:L5:735:G:H4'   | 33:LM:74:ARG:NH2   | 2.34                     | 0.41              |
| 85:L5:1189:G:H2'  | 85:L5:1190:C:C6    | 2.56                     | 0.41              |
| 85:L5:1481:C:O2'  | 85:L5:1482:G:O5'   | 2.39                     | 0.41              |
| 85:L5:1588:U:C4   | 85:L5:1607:C:H1'   | 2.56                     | 0.41              |
| 85:L5:1597:G:N3   | 85:L5:1599:A:N6    | 2.69                     | 0.41              |
| 85:L5:1625:G:C6   | 85:L5:1642:A:C8    | 3.09                     | 0.41              |
| 85:L5:1748:U:O4   | 85:L5:1783:C:N4    | 2.54                     | 0.41              |
| 85:L5:1757:U:O2'  | 85:L5:1758:G:H5''  | 2.21                     | 0.41              |
| 85:L5:1814:C:O3'  | 85:L5:1815:G:H8    | 2.04                     | 0.41              |
| 85:L5:1825:A:O2'  | 47:Lb:43:MET:HE1   | 2.21                     | 0.41              |
| 85:L5:1845:U:H2'  | 85:L5:1846:G:H8    | 1.86                     | 0.41              |
| 85:L5:1919:G:N3   | 39:LS:163:HIS:HB3  | 2.35                     | 0.41              |
| 85:L5:2036:C:H2'  | 85:L5:2037:C:H6    | 1.85                     | 0.41              |
| 85:L5:2056:G:C4   | 85:L5:2058:G:N7    | 2.88                     | 0.41              |
| 85:L5:2397:G:C8   | 85:L5:2399:G:C8    | 3.09                     | 0.41              |
| 85:L5:2403:A:C6   | 85:L5:2404:A:C5    | 3.09                     | 0.41              |
| 85:L5:2442:G:H2'  | 85:L5:2443:G:C8    | 2.56                     | 0.41              |
| 85:L5:2458:C:H2'  | 85:L5:2459:G:C8    | 2.55                     | 0.41              |
| 85:L5:2650:G:H2'  | 85:L5:2651:C:C6    | 2.56                     | 0.41              |
| 85:L5:2659:A:C2   | 85:L5:2676:A:C8    | 3.09                     | 0.41              |
| 85:L5:2743:A:H2'  | 85:L5:2744:A:H8    | 1.86                     | 0.41              |
| 85:L5:2878:G:OP2  | 85:L5:2879:A:O2'   | 2.35                     | 0.41              |
| 85:L5:2902:G:N7   | 85:L5:3594:C:N3    | 2.69                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 85:L5:3806:G:C4    | 85:L5:3807:A:C8    | 3.08                     | 0.41              |
| 85:L5:3844:U:H2'   | 85:L5:3845:A:C8    | 2.55                     | 0.41              |
| 85:L5:3873:G:C6    | 85:L5:3874:G:C6    | 3.09                     | 0.41              |
| 85:L5:3893:C:H1'   | 36:LP:69:ARG:NH1   | 2.36                     | 0.41              |
| 85:L5:3960:A:O2'   | 85:L5:3961:G:H2'   | 2.21                     | 0.41              |
| 85:L5:4096:C:H5'   | 85:L5:4109:G:O2'   | 2.21                     | 0.41              |
| 85:L5:4102:C:C6    | 85:L5:4106:G:C5    | 3.07                     | 0.41              |
| 85:L5:4127:A:C4    | 85:L5:4128:A:N7    | 2.89                     | 0.41              |
| 85:L5:4128:A:H5'   | 45:LZ:54:THR:OG1   | 2.21                     | 0.41              |
| 85:L5:4252:C:H3'   | 85:L5:4253:A:H8    | 1.86                     | 0.41              |
| 85:L5:4254:G:O2'   | 85:L5:4256:A:H2    | 2.04                     | 0.41              |
| 85:L5:4280:A:OP2   | 25:LD:19:LYS:NZ    | 2.54                     | 0.41              |
| 85:L5:4348:A:C6    | 85:L5:4350:C:N3    | 2.89                     | 0.41              |
| 85:L5:4441:A:C6    | 85:L5:4442:U:C4    | 3.09                     | 0.41              |
| 85:L5:4472:G:O2'   | 58:Lm:100:TYR:O    | 2.39                     | 0.41              |
| 85:L5:4538:G:H2'   | 85:L5:4539:U:C6    | 2.55                     | 0.41              |
| 85:L5:4611:A:C2    | 29:LH:120:GLU:HB3  | 2.56                     | 0.41              |
| 85:L5:4618:G:C2    | 85:L5:4619:U:C5    | 3.09                     | 0.41              |
| 85:L5:4652:G:H2'   | 85:L5:4653:C:H6    | 1.85                     | 0.41              |
| 85:L5:4726:G:C6    | 85:L5:4727:A:C6    | 3.08                     | 0.41              |
| 85:L5:4737:G:C6    | 85:L5:4963:G:C6    | 3.08                     | 0.41              |
| 85:L5:4871:C:H41   | 39:LS:172:PRO:HA   | 1.85                     | 0.41              |
| 85:L5:4884:G:N1    | 85:L5:4936:G:C6    | 2.89                     | 0.41              |
| 85:L5:4910:G:C4    | 35:LO:156:LEU:HD23 | 2.56                     | 0.41              |
| 85:L5:4930:C:H2'   | 85:L5:4931:G:O4'   | 2.20                     | 0.41              |
| 85:L5:4953:G:H2'   | 85:L5:4954:G:C8    | 2.56                     | 0.41              |
| 85:L5:5046:U:H2'   | 85:L5:5050:C:H41   | 1.85                     | 0.41              |
| 20:L7:60:G:H2'     | 20:L7:61:G:H8      | 1.86                     | 0.41              |
| 21:L8:15:G:H2'     | 21:L8:16:G:C8      | 2.56                     | 0.41              |
| 21:L8:29:G:H2'     | 21:L8:30:U:H6      | 1.86                     | 0.41              |
| 21:L8:91:A:H2'     | 21:L8:92:U:C6      | 2.56                     | 0.41              |
| 21:L8:140:C:H2'    | 21:L8:141:C:C6     | 2.56                     | 0.41              |
| 22:LA:116:LEU:HD13 | 22:LA:164:ALA:HB2  | 2.02                     | 0.41              |
| 23:LB:140:GLU:H    | 23:LB:140:GLU:HG3  | 1.66                     | 0.41              |
| 23:LB:307:TYR:CD1  | 23:LB:366:LYS:HA   | 2.56                     | 0.41              |
| 24:LC:112:HIS:HB2  | 34:LN:202:ARG:O    | 2.21                     | 0.41              |
| 26:LE:51:VAL:HG12  | 26:LE:54:ILE:HB    | 2.02                     | 0.41              |
| 26:LE:198:SER:O    | 26:LE:198:SER:OG   | 2.30                     | 0.41              |
| 26:LE:245:GLN:O    | 26:LE:248:ILE:HG12 | 2.21                     | 0.41              |
| 27:LF:111:LEU:HD23 | 27:LF:111:LEU:HA   | 1.89                     | 0.41              |
| 27:LF:241:ASN:O    | 27:LF:245:ARG:NH1  | 2.52                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 28:LG:30:PRO:HD2   | 45:LZ:123:LYS:NZ   | 2.34                     | 0.41              |
| 29:LH:81:ILE:O     | 29:LH:85:THR:HG22  | 2.21                     | 0.41              |
| 29:LH:88:PHE:CE2   | 29:LH:151:ILE:HB   | 2.56                     | 0.41              |
| 33:LM:14:TYR:CE1   | 33:LM:22:GLY:HA2   | 2.56                     | 0.41              |
| 34:LN:96:ARG:NH1   | 34:LN:100:SER:OG   | 2.54                     | 0.41              |
| 35:LO:130:LYS:HB2  | 35:LO:133:ARG:HG3  | 2.03                     | 0.41              |
| 35:LO:140:ARG:HG3  | 35:LO:141:LEU:N    | 2.36                     | 0.41              |
| 36:LP:64:ASN:O     | 36:LP:67:VAL:HG12  | 2.21                     | 0.41              |
| 36:LP:112:LEU:HD23 | 36:LP:112:LEU:HA   | 1.84                     | 0.41              |
| 37:LQ:24:TYR:HA    | 37:LQ:27:LEU:HD13  | 2.02                     | 0.41              |
| 38:LR:116:ASP:CG   | 38:LR:119:MET:HG3  | 2.45                     | 0.41              |
| 39:LS:11:LYS:HG2   | 39:LS:63:TYR:HE2   | 1.86                     | 0.41              |
| 39:LS:133:ALA:HB3  | 39:LS:136:LYS:HG2  | 2.02                     | 0.41              |
| 40:LT:38:ASP:H     | 40:LT:64:VAL:HG12  | 1.84                     | 0.41              |
| 40:LT:72:VAL:HG13  | 40:LT:93:ILE:HD11  | 2.03                     | 0.41              |
| 44:LY:24:HIS:CE1   | 44:LY:25:ILE:HG23  | 2.56                     | 0.41              |
| 45:LZ:88:ASP:OD2   | 45:LZ:121:ARG:NH1  | 2.54                     | 0.41              |
| 48:Lc:37:MET:HE3   | 48:Lc:42:LYS:NZ    | 2.36                     | 0.41              |
| 48:Lc:74:TYR:CE2   | 48:Lc:81:LEU:HB2   | 2.56                     | 0.41              |
| 49:Ld:25:TYR:O     | 49:Ld:85:ARG:HD2   | 2.21                     | 0.41              |
| 50:Le:91:CYS:O     | 50:Le:93:LYS:N     | 2.53                     | 0.41              |
| 53:Lh:58:LEU:HD12  | 53:Lh:59:THR:N     | 2.36                     | 0.41              |
| 54:Li:55:ARG:CA    | 54:Li:58:MET:HG3   | 2.46                     | 0.41              |
| 55:Lj:27:TYR:HA    | 55:Lj:34:CYS:HA    | 2.03                     | 0.41              |
| 56:Lk:27:LYS:HA    | 56:Lk:27:LYS:HD2   | 1.87                     | 0.41              |
| 60:Lo:23:VAL:CG2   | 60:Lo:68:LEU:HB3   | 2.51                     | 0.41              |
| 63:Lz:92:LYS:HB3   | 63:Lz:92:LYS:HE2   | 1.89                     | 0.41              |
| 64:SR:17:ILE:HD13  | 64:SR:17:ILE:HA    | 1.89                     | 0.41              |
| 64:SR:68:GLY:HA3   | 64:SR:69:ILE:HA    | 1.86                     | 0.41              |
| 65:SD:101:GLN:CG   | 65:SD:126:ILE:HD11 | 2.51                     | 0.41              |
| 65:SD:121:GLY:HA2  | 65:SD:124:ARG:HG3  | 2.01                     | 0.41              |
| 66:SF:34:SER:HA    | 73:Sc:55:VAL:CG1   | 2.50                     | 0.41              |
| 67:SK:16:PHE:CE2   | 67:SK:83:LEU:HD11  | 2.56                     | 0.41              |
| 68:SP:18:ARG:NE    | 70:SS:88:LYS:HD2   | 2.36                     | 0.41              |
| 68:SP:121:ILE:HD12 | 70:SS:120:HIS:CD2  | 2.53                     | 0.41              |
| 71:ST:101:ARG:HD2  | 79:S2:1565:C:OP2   | 2.21                     | 0.41              |
| 72:SU:113:GLU:OE1  | 72:SU:113:GLU:N    | 2.54                     | 0.41              |
| 75:Sg:267:VAL:HG12 | 75:Sg:268:ASP:OD2  | 2.21                     | 0.41              |
| 76:SM:79:VAL:CG2   | 76:SM:88:TRP:HH2   | 2.34                     | 0.41              |
| 78:Sf:143:LYS:HB2  | 79:S2:1310:U:H4'   | 2.03                     | 0.41              |
| 79:S2:29:G:C6      | 79:S2:646:G:C6     | 3.08                     | 0.41              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 79:S2:66:G:H2'     | 79:S2:67:C:H4'    | 2.02                     | 0.41              |
| 79:S2:89:C:O2'     | 79:S2:499:G:H5''  | 2.20                     | 0.41              |
| 79:S2:323:C:C2     | 79:S2:327:G:N2    | 2.89                     | 0.41              |
| 79:S2:353:C:H2'    | 79:S2:354:U:C6    | 2.55                     | 0.41              |
| 79:S2:532:C:C2     | 79:S2:533:A:C8    | 3.09                     | 0.41              |
| 79:S2:538:U:H2'    | 79:S2:539:C:N1    | 2.36                     | 0.41              |
| 79:S2:557:U:H5'    | 79:S2:558:G:H2'   | 2.03                     | 0.41              |
| 79:S2:845:G:C6     | 79:S2:846:G:C6    | 3.09                     | 0.41              |
| 79:S2:865:A:C6     | 79:S2:866:U:C4    | 3.09                     | 0.41              |
| 79:S2:986:G:H3'    | 79:S2:987:A:H8    | 1.86                     | 0.41              |
| 79:S2:1006:C:C2    | 79:S2:1007:C:C5   | 3.09                     | 0.41              |
| 79:S2:1195:A:H2'   | 79:S2:1196:A:C8   | 2.56                     | 0.41              |
| 79:S2:1259:A:N6    | 79:S2:1519:U:O5'  | 2.54                     | 0.41              |
| 79:S2:1464:C:H2'   | 79:S2:1465:A:C8   | 2.56                     | 0.41              |
| 79:S2:1478:U:H2'   | 79:S2:1479:G:H8   | 1.84                     | 0.41              |
| 79:S2:1540:G:C6    | 79:S2:1594:A:C6   | 3.09                     | 0.41              |
| 79:S2:1745:A:OP2   | 79:S2:1745:A:H3'  | 2.20                     | 0.41              |
| 81:AP:8:U:H1'      | 81:AP:48:C:H1'    | 2.02                     | 0.41              |
| 83:Ls:25:PRO:HB2   | 83:Ls:195:ASN:OD1 | 2.21                     | 0.41              |
| 87:LW:42:SER:OG    | 87:LW:44:ARG:HG3  | 2.21                     | 0.41              |
| 1:cH:53:SER:OG     | 1:cH:119:GLN:HG2  | 2.21                     | 0.41              |
| 4:sL:22:ARG:HD2    | 4:sL:23:VAL:O     | 2.20                     | 0.41              |
| 7:sJ:39:ASN:HB2    | 79:s2:642:U:P     | 2.61                     | 0.41              |
| 7:sJ:40:LYS:HE3    | 79:s2:641:A:OP1   | 2.21                     | 0.41              |
| 8:sY:120:THR:HA    | 79:s2:151:C:OP1   | 2.21                     | 0.41              |
| 8:sY:122:LYS:HZ2   | 79:s2:151:C:P     | 2.43                     | 0.41              |
| 10:sA:108:PHE:HD2  | 10:sA:136:GLU:HB3 | 1.86                     | 0.41              |
| 11:sB:62:LEU:O     | 11:sB:65:ARG:HD2  | 2.21                     | 0.41              |
| 13:sV:8:PHE:HD2    | 13:sV:10:ASP:CG   | 2.28                     | 0.41              |
| 13:sV:55:ILE:HD13  | 13:sV:55:ILE:HA   | 1.98                     | 0.41              |
| 15:sC:82:TYR:CZ    | 15:sC:164:PRO:HD3 | 2.56                     | 0.41              |
| 17:sO:83:GLN:CD    | 17:sO:83:GLN:C    | 2.89                     | 0.41              |
| 19:sb:33:MET:HE1   | 19:sb:79:PHE:CB   | 2.42                     | 0.41              |
| 20:l7:75:G:C8      | 39:lS:53:LYS:HG3  | 2.55                     | 0.41              |
| 22:lA:180:LEU:HD11 | 61:lp:18:TYR:CD2  | 2.56                     | 0.41              |
| 23:lB:24:ARG:NE    | 23:lB:28:LYS:HD2  | 2.36                     | 0.41              |
| 23:lB:113:GLU:HG3  | 23:lB:165:HIS:HE1 | 1.86                     | 0.41              |
| 23:lB:145:GLN:CD   | 23:lB:148:LYS:HE2 | 2.46                     | 0.41              |
| 24:lC:239:LYS:O    | 24:lC:248:ARG:NH1 | 2.54                     | 0.41              |
| 27:lF:97:GLY:H     | 85:l5:1896:A:P    | 2.44                     | 0.41              |
| 31:lJ:41:GLU:CD    | 31:lJ:48:PRO:HD3  | 2.46                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 32:IL:77:SER:OG   | 32:IL:102:ARG:O    | 2.36                     | 0.41              |
| 33:IM:91:TRP:O    | 33:IM:95:ILE:HG23  | 2.21                     | 0.41              |
| 34:IN:14:LYS:HE2  | 34:IN:120:TRP:HZ3  | 1.85                     | 0.41              |
| 37:IQ:24:TYR:O    | 37:IQ:28:LEU:HD23  | 2.21                     | 0.41              |
| 37:IQ:97:LYS:HZ3  | 37:IQ:98:LEU:N     | 2.19                     | 0.41              |
| 37:IQ:166:TYR:CE1 | 85:l5:1345:A:H5''  | 2.55                     | 0.41              |
| 38:IR:45:ILE:HG12 | 38:IR:50:ILE:HB    | 2.02                     | 0.41              |
| 38:IR:163:ARG:HD2 | 79:s2:871:U:H3     | 1.86                     | 0.41              |
| 42:IV:48:ARG:HD3  | 42:IV:49:LEU:H     | 1.85                     | 0.41              |
| 43:IX:106:LYS:O   | 43:IX:109:ILE:HG22 | 2.20                     | 0.41              |
| 45:IZ:3:LYS:HD3   | 45:IZ:3:LYS:HA     | 1.78                     | 0.41              |
| 47:lb:22:LYS:HB3  | 47:lb:22:LYS:HE3   | 1.88                     | 0.41              |
| 48:lc:94:LEU:N    | 48:lc:94:LEU:HD23  | 2.36                     | 0.41              |
| 59:ln:14:LYS:NZ   | 79:s2:1173:A:OP1   | 2.42                     | 0.41              |
| 59:ln:17:ARG:NH2  | 79:s2:1172:U:O3'   | 2.53                     | 0.41              |
| 64:sR:105:MET:HA  | 64:sR:108:LEU:HD23 | 2.03                     | 0.41              |
| 65:sD:193:ASP:CG  | 65:sD:194:PRO:HD3  | 2.46                     | 0.41              |
| 72:sU:46:LYS:HA   | 72:sU:46:LYS:HD3   | 1.64                     | 0.41              |
| 76:sM:41:ALA:CA   | 76:sM:44:LYS:NZ    | 2.84                     | 0.41              |
| 76:sM:52:LEU:O    | 76:sM:79:VAL:HG22  | 2.20                     | 0.41              |
| 79:s2:96:C:O2     | 79:s2:473:A:O2'    | 2.35                     | 0.41              |
| 79:s2:144:U:H2'   | 79:s2:145:G:H8     | 1.86                     | 0.41              |
| 79:s2:339:A:H5'   | 79:s2:340:C:OP1    | 2.21                     | 0.41              |
| 79:s2:835:C:H2'   | 79:s2:837:A:C6     | 2.56                     | 0.41              |
| 79:s2:1013:U:H2'  | 79:s2:1014:G:C8    | 2.52                     | 0.41              |
| 79:s2:1068:G:H2'  | 79:s2:1069:U:C5    | 2.56                     | 0.41              |
| 79:s2:1534:C:H5'' | 79:s2:1536:G:O4'   | 2.21                     | 0.41              |
| 79:s2:1795:G:H2'  | 79:s2:1796:G:H8    | 1.86                     | 0.41              |
| 80:cB:35:LEU:HD23 | 80:cB:35:LEU:HA    | 1.88                     | 0.41              |
| 80:cB:225:LEU:HG  | 80:cB:260:LEU:HD23 | 2.03                     | 0.41              |
| 80:cB:228:PHE:O   | 80:cB:231:MET:SD   | 2.79                     | 0.41              |
| 80:cB:358:LEU:HA  | 80:cB:359:PRO:HD3  | 1.92                     | 0.41              |
| 80:cB:518:PRO:O   | 80:cB:521:VAL:HG12 | 2.21                     | 0.41              |
| 80:cB:838:THR:HA  | 80:cB:841:ARG:HG2  | 2.03                     | 0.41              |
| 83:ls:97:GLU:HA   | 83:ls:100:ASP:OD2  | 2.20                     | 0.41              |
| 85:l5:275:C:H2'   | 85:l5:276:C:C6     | 2.56                     | 0.41              |
| 85:l5:725:G:C6    | 85:l5:942:G:C6     | 3.09                     | 0.41              |
| 85:l5:1095:A:H8   | 85:l5:1095:A:O5'   | 2.04                     | 0.41              |
| 85:l5:1185:G:H2'  | 85:l5:1186:U:C6    | 2.56                     | 0.41              |
| 85:l5:1217:G:H2'  | 85:l5:1218:G:C8    | 2.56                     | 0.41              |
| 85:l5:2385:U:H2'  | 85:l5:2386:U:H6    | 1.84                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 85:L5:2387:G:C4   | 85:L5:2388:A:C8    | 3.08                     | 0.41              |
| 85:L5:2594:C:H2'  | 85:L5:2595:C:C6    | 2.56                     | 0.41              |
| 85:L5:2712:G:C6   | 85:L5:2713:C:C4    | 3.09                     | 0.41              |
| 85:L5:2857:A:C2   | 85:L5:3840:U:H5'   | 2.56                     | 0.41              |
| 85:L5:2893:U:H2'  | 85:L5:2894:A:C8    | 2.55                     | 0.41              |
| 85:L5:3851:U:H3'  | 85:L5:3852:A:H8    | 1.86                     | 0.41              |
| 85:L5:4236:G:H4'  | 85:L5:4328:G:O2'   | 2.21                     | 0.41              |
| 85:L5:4513:A:H2'  | 85:L5:4514:G:H8    | 1.86                     | 0.41              |
| 85:L5:4664:A:C6   | 85:L5:4665:A:C5    | 3.09                     | 0.41              |
| 85:L5:4742:G:H2'  | 85:L5:4743:G:H8    | 1.86                     | 0.41              |
| 85:L5:4746:C:C2   | 85:L5:4747:C:C5    | 3.09                     | 0.41              |
| 85:L5:4771:C:H6   | 85:L5:4771:C:O5'   | 2.04                     | 0.41              |
| 85:L5:4896:G:C6   | 85:L5:4897:G:C6    | 3.08                     | 0.41              |
| 80:CB:533:MET:C   | 80:CB:533:MET:SD   | 3.04                     | 0.41              |
| 80:CB:741:MET:HB3 | 80:CB:817:TRP:HE3  | 1.87                     | 0.41              |
| 4:SL:126:VAL:HG23 | 4:SL:145:VAL:HA    | 2.02                     | 0.41              |
| 10:SA:94:THR:HG22 | 10:SA:183:LEU:CD2  | 2.48                     | 0.41              |
| 10:SA:186:ARG:HB2 | 10:SA:186:ARG:HH11 | 1.86                     | 0.41              |
| 12:SH:20:GLU:OE2  | 12:SH:23:ILE:HD12  | 2.21                     | 0.41              |
| 12:SH:191:GLU:HG2 | 12:SH:192:PHE:N    | 2.35                     | 0.41              |
| 16:SN:32:ASP:O    | 16:SN:36:GLN:HG3   | 2.21                     | 0.41              |
| 17:SO:67:ASP:OD1  | 17:SO:67:ASP:N     | 2.38                     | 0.41              |
| 18:SW:52:ILE:HB   | 18:SW:61:ILE:HD13  | 2.03                     | 0.41              |
| 85:L5:50:C:C2     | 85:L5:51:A:C8      | 3.09                     | 0.41              |
| 85:L5:60:G:C4     | 85:L5:61:A:C8      | 3.09                     | 0.41              |
| 85:L5:135:G:H22   | 53:Lh:94:ARG:HG3   | 1.86                     | 0.41              |
| 85:L5:154:G:C3'   | 53:Lh:105:LYS:HZ1  | 2.32                     | 0.41              |
| 85:L5:208:A:N3    | 85:L5:232:G:O2'    | 2.53                     | 0.41              |
| 85:L5:287:U:H2'   | 85:L5:288:G:C8     | 2.55                     | 0.41              |
| 85:L5:298:G:H2'   | 85:L5:299:C:C6     | 2.55                     | 0.41              |
| 85:L5:307:A:H2'   | 85:L5:308:G:C4     | 2.55                     | 0.41              |
| 85:L5:319:A:H2'   | 85:L5:320:C:C6     | 2.56                     | 0.41              |
| 85:L5:337:U:P     | 32:LL:35:ARG:HH12  | 2.42                     | 0.41              |
| 85:L5:358:C:OP1   | 24:LC:61:GLN:NE2   | 2.55                     | 0.41              |
| 85:L5:395:A:H2'   | 85:L5:396:A:C8     | 2.55                     | 0.41              |
| 85:L5:487:G:C6    | 85:L5:670:G:C6     | 3.09                     | 0.41              |
| 85:L5:1296:G:H2'  | 85:L5:1297:U:C6    | 2.56                     | 0.41              |
| 85:L5:1297:U:H2'  | 85:L5:1298:C:H6    | 1.86                     | 0.41              |
| 85:L5:1385:G:H2'  | 85:L5:1386:C:C6    | 2.56                     | 0.41              |
| 85:L5:2009:A:H2'  | 85:L5:2010:A:O4'   | 2.21                     | 0.41              |
| 85:L5:2259:G:H5'  | 85:L5:2260:C:C4    | 2.56                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 85:L5:2422:C:H5'   | 85:L5:3857:G:H21   | 1.86                     | 0.41              |
| 85:L5:2486:G:N7    | 85:L5:2493:G:C2    | 2.86                     | 0.41              |
| 85:L5:2734:U:H2'   | 85:L5:2735:G:H8    | 1.86                     | 0.41              |
| 85:L5:2822:G:C8    | 38:LR:20:LYS:NZ    | 2.89                     | 0.41              |
| 85:L5:4108:G:N3    | 85:L5:4109:G:N7    | 2.69                     | 0.41              |
| 85:L5:4216:G:C4    | 85:L5:4217:G:C8    | 3.08                     | 0.41              |
| 85:L5:4228:G:H5''  | 85:L5:4229:U:O4'   | 2.20                     | 0.41              |
| 85:L5:4389:C:H2'   | 85:L5:4390:A:H8    | 1.85                     | 0.41              |
| 85:L5:4631:G:H2'   | 85:L5:4632:U:H6    | 1.85                     | 0.41              |
| 85:L5:4878:C:H2'   | 85:L5:4879:C:C6    | 2.56                     | 0.41              |
| 85:L5:5053:U:H3'   | 85:L5:5054:C:C6    | 2.55                     | 0.41              |
| 20:L7:31:G:C6      | 20:L7:47:G:C6      | 3.09                     | 0.41              |
| 20:L7:70:G:C6      | 20:L7:106:G:C6     | 3.09                     | 0.41              |
| 21:L8:121:G:H2'    | 21:L8:122:G:H8     | 1.86                     | 0.41              |
| 23:LB:369:ASP:OD1  | 23:LB:370:THR:N    | 2.54                     | 0.41              |
| 28:LG:29:ASN:HB3   | 28:LG:32:PHE:CE2   | 2.56                     | 0.41              |
| 31:LJ:32:ARG:HH22  | 31:LJ:33:LEU:HB2   | 1.85                     | 0.41              |
| 33:LM:93:LYS:HB3   | 33:LM:93:LYS:HE2   | 1.71                     | 0.41              |
| 35:LO:174:LEU:HA   | 35:LO:177:LEU:CD1  | 2.48                     | 0.41              |
| 37:LQ:50:ARG:HA    | 37:LQ:53:MET:HG2   | 2.03                     | 0.41              |
| 38:LR:172:ARG:HH12 | 79:S2:909:G:P      | 2.44                     | 0.41              |
| 38:LR:181:LYS:HD3  | 38:LR:181:LYS:HA   | 1.71                     | 0.41              |
| 39:LS:13:VAL:HA    | 39:LS:28:TYR:O     | 2.20                     | 0.41              |
| 39:LS:91:HIS:HB2   | 39:LS:93:MET:CE    | 2.45                     | 0.41              |
| 39:LS:113:MET:HB3  | 39:LS:119:ALA:HB3  | 2.03                     | 0.41              |
| 53:Lh:16:GLU:OE1   | 53:Lh:16:GLU:N     | 2.44                     | 0.41              |
| 53:Lh:24:LEU:HB3   | 53:Lh:54:ILE:HD11  | 2.03                     | 0.41              |
| 53:Lh:105:LYS:O    | 53:Lh:109:ARG:HB2  | 2.21                     | 0.41              |
| 61:Lp:19:GLY:O     | 61:Lp:23:ARG:HG3   | 2.21                     | 0.41              |
| 63:Lz:30:GLU:OE2   | 63:Lz:208:SER:OG   | 2.39                     | 0.41              |
| 67:SK:15:LEU:HD21  | 67:SK:21:MET:CE    | 2.51                     | 0.41              |
| 75:Sg:257:LYS:HE2  | 75:Sg:266:ILE:HD11 | 2.02                     | 0.41              |
| 77:SZ:47:LEU:HB3   | 77:SZ:80:ARG:HD2   | 2.03                     | 0.41              |
| 79:S2:152:U:C2     | 79:S2:153:G:C8     | 3.09                     | 0.41              |
| 79:S2:158:A:H2'    | 79:S2:159:A:C8     | 2.56                     | 0.41              |
| 79:S2:845:G:H2'    | 79:S2:846:G:C8     | 2.55                     | 0.41              |
| 79:S2:951:C:H2'    | 79:S2:952:G:C8     | 2.56                     | 0.41              |
| 79:S2:977:C:H2'    | 79:S2:978:G:O4'    | 2.21                     | 0.41              |
| 79:S2:1035:A:H2'   | 79:S2:1036:A:C8    | 2.55                     | 0.41              |
| 79:S2:1067:C:H2'   | 79:S2:1068:G:O4'   | 2.20                     | 0.41              |
| 79:S2:1146:C:O2'   | 79:S2:1150:A:N1    | 2.49                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 79:S2:1630:A:C5   | 79:S2:1631:U:C5   | 3.08                     | 0.41              |
| 81:AP:48:C:C4     | 81:AP:59:A:C8     | 3.09                     | 0.41              |
| 82:PE:24:G:H2'    | 82:PE:25:C:C6     | 2.55                     | 0.41              |
| 2:sE:75:LYS:HD2   | 2:sE:77:ARG:NH2   | 2.35                     | 0.40              |
| 2:sE:99:PHE:CE1   | 2:sE:111:VAL:HA   | 2.56                     | 0.40              |
| 3:sI:65:PHE:HA    | 3:sI:187:GLY:O    | 2.21                     | 0.40              |
| 6:sG:12:CYS:SG    | 6:sG:128:THR:HA   | 2.62                     | 0.40              |
| 6:sG:28:TYR:HB3   | 6:sG:29:GLU:OE1   | 2.21                     | 0.40              |
| 6:sG:55:GLY:N     | 6:sG:63:MET:SD    | 2.94                     | 0.40              |
| 6:sG:135:PRO:O    | 6:sG:136:LYS:HD2  | 2.21                     | 0.40              |
| 7:sJ:129:LEU:HG   | 7:sJ:134:HIS:HB2  | 2.03                     | 0.40              |
| 11:sB:81:PHE:CD1  | 11:sB:109:LYS:HG2 | 2.56                     | 0.40              |
| 15:sC:84:PHE:CD2  | 15:sC:265:PRO:HD3 | 2.56                     | 0.40              |
| 17:sO:125:LYS:HA  | 17:sO:125:LYS:HD3 | 1.88                     | 0.40              |
| 18:sW:26:LEU:O    | 18:sW:27:ILE:HD13 | 2.21                     | 0.40              |
| 18:sW:49:GLU:HA   | 18:sW:49:GLU:OE2  | 2.21                     | 0.40              |
| 18:sW:57:ARG:NH2  | 19:sb:26:GLN:HE22 | 2.18                     | 0.40              |
| 21:l8:3:A:H4'     | 36:lP:61:ARG:HD3  | 2.03                     | 0.40              |
| 21:l8:154:G:H5'   | 28:lG:189:ARG:NH2 | 2.28                     | 0.40              |
| 23:lB:89:ILE:HD13 | 23:lB:89:ILE:HA   | 1.76                     | 0.40              |
| 24:lC:117:THR:HA  | 24:lC:120:LYS:HE2 | 2.03                     | 0.40              |
| 25:lD:67:ALA:O    | 25:lD:68:ARG:HD2  | 2.22                     | 0.40              |
| 25:lD:258:LYS:HE2 | 25:lD:258:LYS:HB3 | 1.96                     | 0.40              |
| 25:lD:291:GLN:N   | 25:lD:291:GLN:CD  | 2.79                     | 0.40              |
| 28:lG:133:PRO:HA  | 28:lG:134:PRO:HD3 | 1.90                     | 0.40              |
| 29:lH:49:GLY:O    | 29:lH:53:LYS:HD2  | 2.20                     | 0.40              |
| 29:lH:59:LYS:HA   | 29:lH:59:LYS:HD2  | 1.93                     | 0.40              |
| 29:lH:90:TYR:CE1  | 29:lH:184:LYS:HB3 | 2.56                     | 0.40              |
| 32:lL:63:THR:HG21 | 46:la:66:ASN:ND2  | 2.36                     | 0.40              |
| 34:lN:13:LYS:HA   | 34:lN:13:LYS:HD3  | 1.87                     | 0.40              |
| 34:lN:50:ARG:HH12 | 85:l5:278:G:C1'   | 2.35                     | 0.40              |
| 34:lN:96:ARG:HA   | 34:lN:171:SER:HB2 | 2.03                     | 0.40              |
| 36:lP:84:PRO:HB2  | 36:lP:87:SER:HB2  | 2.03                     | 0.40              |
| 38:lR:62:ARG:O    | 38:lR:66:ASN:OD1  | 2.38                     | 0.40              |
| 39:lS:99:ASP:OD1  | 39:lS:100:LEU:N   | 2.52                     | 0.40              |
| 39:lS:136:LYS:HE2 | 39:lS:136:LYS:HA  | 2.03                     | 0.40              |
| 39:lS:164:LYS:NZ  | 85:l5:1921:C:OP2  | 2.28                     | 0.40              |
| 40:lT:116:LYS:HZ3 | 85:l5:1834:U:H2'  | 1.86                     | 0.40              |
| 41:lU:56:LEU:HD11 | 41:lU:59:GLY:N    | 2.36                     | 0.40              |
| 43:lX:68:ARG:HH12 | 43:lX:70:LYS:NZ   | 2.19                     | 0.40              |
| 45:lZ:118:PHE:HB3 | 45:lZ:131:PHE:HZ  | 1.86                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 47:lb:37:PRO:HA    | 47:lb:40:LEU:HB3   | 2.03                     | 0.40              |
| 47:lb:95:ARG:HB2   | 85:l5:1266:G:N7    | 2.36                     | 0.40              |
| 48:lc:22:MET:C     | 48:lc:23:LYS:HG2   | 2.46                     | 0.40              |
| 49:ld:118:GLN:NE2  | 85:l5:5056:A:H1'   | 2.36                     | 0.40              |
| 53:lh:51:ARG:O     | 53:lh:54:ILE:HG12  | 2.22                     | 0.40              |
| 55:lj:58:THR:OG1   | 55:lj:59:THR:N     | 2.54                     | 0.40              |
| 60:lo:36:GLN:HA    | 60:lo:39:ARG:CZ    | 2.50                     | 0.40              |
| 62:lr:11:ARG:HG3   | 62:lr:12:ASN:N     | 2.34                     | 0.40              |
| 63:lz:172:VAL:HG12 | 63:lz:174:MET:H    | 1.85                     | 0.40              |
| 68:sP:91:GLY:N     | 68:sP:107:ILE:O    | 2.49                     | 0.40              |
| 70:sS:55:ARG:HH21  | 77:sZ:48:VAL:HG12  | 1.86                     | 0.40              |
| 70:sS:88:LYS:O     | 70:sS:88:LYS:CG    | 2.68                     | 0.40              |
| 70:sS:88:LYS:HB3   | 70:sS:95:TYR:HE1   | 1.86                     | 0.40              |
| 70:sS:113:ARG:HE   | 70:sS:114:LEU:HD12 | 1.85                     | 0.40              |
| 72:sU:24:LEU:HG    | 72:sU:87:ARG:O     | 2.21                     | 0.40              |
| 73:sc:20:ARG:HD3   | 73:sc:28:THR:OG1   | 2.20                     | 0.40              |
| 78:sf:88:PRO:HB2   | 78:sf:89:LYS:HD2   | 2.02                     | 0.40              |
| 78:sf:105:TYR:O    | 78:sf:117:LEU:HG   | 2.22                     | 0.40              |
| 79:s2:352:U:H2'    | 79:s2:353:C:H6     | 1.83                     | 0.40              |
| 79:s2:352:U:C4     | 79:s2:353:C:N4     | 2.90                     | 0.40              |
| 79:s2:387:C:H2'    | 79:s2:388:U:C6     | 2.56                     | 0.40              |
| 79:s2:693:A:O2'    | 79:s2:694:G:O4'    | 2.37                     | 0.40              |
| 79:s2:952:G:C5     | 79:s2:953:C:N3     | 2.90                     | 0.40              |
| 79:s2:1062:A:H2'   | 79:s2:1063:C:C6    | 2.56                     | 0.40              |
| 79:s2:1395:C:H2'   | 79:s2:1396:A:N3    | 2.35                     | 0.40              |
| 79:s2:1462:U:H2'   | 79:s2:1464:C:N4    | 2.35                     | 0.40              |
| 79:s2:1661:A:C6    | 79:s2:1662:U:C4    | 3.09                     | 0.40              |
| 79:s2:1672:U:C2    | 79:s2:1673:U:C5    | 3.09                     | 0.40              |
| 79:s2:1694:U:O3'   | 79:s2:1695:A:H8    | 2.04                     | 0.40              |
| 80:cB:81:LEU:HG    | 80:cB:85:ASP:HB2   | 2.03                     | 0.40              |
| 80:cB:119:LEU:HD23 | 80:cB:119:LEU:HA   | 1.90                     | 0.40              |
| 80:cB:381:ALA:O    | 80:cB:385:ILE:HG22 | 2.20                     | 0.40              |
| 80:cB:404:THR:HG23 | 80:cB:410:PHE:CA   | 2.51                     | 0.40              |
| 82:pE:15:G:C2      | 82:pE:59:G:C5      | 3.09                     | 0.40              |
| 82:pE:31:A:C5      | 82:pE:32:C:C4      | 3.09                     | 0.40              |
| 83:ls:65:ILE:O     | 83:ls:69:LEU:HB2   | 2.20                     | 0.40              |
| 85:l5:676:C:H2'    | 85:l5:677:G:C8     | 2.56                     | 0.40              |
| 85:l5:2503:G:O4'   | 85:l5:4084:G:N2    | 2.54                     | 0.40              |
| 85:l5:3593:C:H1'   | 85:l5:3595:U:O4    | 2.21                     | 0.40              |
| 85:l5:3700:C:H2'   | 85:l5:3746:A:H61   | 1.85                     | 0.40              |
| 85:l5:3839:G:C2    | 85:l5:3844:U:C4    | 3.09                     | 0.40              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 85:L5:3946:G:N2   | 85:L5:4067:U:O2    | 2.39                     | 0.40              |
| 85:L5:4055:U:H6   | 85:L5:4055:U:O5'   | 2.05                     | 0.40              |
| 85:L5:4095:G:H2'  | 85:L5:4096:C:C4    | 2.56                     | 0.40              |
| 85:L5:4669:A:C5   | 85:L5:4672:A:N7    | 2.89                     | 0.40              |
| 85:L5:4761:G:C2   | 85:L5:4762:A:C5    | 3.09                     | 0.40              |
| 85:L5:4884:G:C6   | 85:L5:4885:U:C4    | 3.09                     | 0.40              |
| 85:L5:4906:C:C2   | 85:L5:4916:G:C2    | 3.09                     | 0.40              |
| 5:SX:60:LYS:HG2   | 5:SX:114:ASP:O     | 2.21                     | 0.40              |
| 7:SJ:10:ARG:NH2   | 79:S2:827:A:OP2    | 2.54                     | 0.40              |
| 7:SJ:29:LEU:HA    | 7:SJ:32:ILE:HG22   | 2.03                     | 0.40              |
| 7:SJ:136:ARG:HA   | 7:SJ:141:VAL:HA    | 2.02                     | 0.40              |
| 11:SB:42:ARG:HA   | 11:SB:42:ARG:HD2   | 1.83                     | 0.40              |
| 11:SB:181:LEU:O   | 11:SB:185:VAL:HG12 | 2.20                     | 0.40              |
| 12:SH:65:PRO:HG2  | 12:SH:68:GLN:HG2   | 2.03                     | 0.40              |
| 14:Sa:10:ARG:HB2  | 14:Sa:33:ASP:CG    | 2.45                     | 0.40              |
| 15:SC:63:VAL:O    | 15:SC:63:VAL:HG13  | 2.22                     | 0.40              |
| 15:SC:88:ILE:O    | 15:SC:89:LYS:HD3   | 2.21                     | 0.40              |
| 15:SC:196:ILE:HB  | 15:SC:223:TYR:HB2  | 2.01                     | 0.40              |
| 16:SN:113:PHE:O   | 16:SN:116:ILE:HG12 | 2.21                     | 0.40              |
| 16:SN:129:TYR:HD2 | 16:SN:129:TYR:HA   | 1.80                     | 0.40              |
| 18:SW:90:GLN:O    | 18:SW:94:LEU:HD23  | 2.21                     | 0.40              |
| 85:L5:83:C:H4'    | 46:La:65:ARG:NH2   | 2.35                     | 0.40              |
| 85:L5:111:C:C2    | 85:L5:331:G:C2     | 3.09                     | 0.40              |
| 85:L5:151:G:O6    | 28:LG:139:GLY:HA3  | 2.21                     | 0.40              |
| 85:L5:306:A:H2'   | 85:L5:307:A:C8     | 2.55                     | 0.40              |
| 85:L5:715:G:H2'   | 85:L5:716:C:C6     | 2.56                     | 0.40              |
| 85:L5:949:G:H2'   | 85:L5:950:G:H8     | 1.86                     | 0.40              |
| 85:L5:1094:G:C2   | 85:L5:1095:A:C5    | 3.09                     | 0.40              |
| 85:L5:1242:G:C5   | 85:L5:1243:C:C5    | 3.09                     | 0.40              |
| 85:L5:1415:G:C4   | 85:L5:1416:G:C8    | 3.10                     | 0.40              |
| 85:L5:1463:C:H2'  | 85:L5:1464:C:C6    | 2.56                     | 0.40              |
| 85:L5:1510:G:OP1  | 46:La:2:PRO:HD2    | 2.21                     | 0.40              |
| 85:L5:1797:G:H2'  | 85:L5:1798:G:C8    | 2.56                     | 0.40              |
| 85:L5:2062:C:O5'  | 39:LS:4:SER:HB2    | 2.21                     | 0.40              |
| 85:L5:2285:A:H2'  | 85:L5:2286:G:C8    | 2.55                     | 0.40              |
| 85:L5:2590:G:N2   | 85:L5:2754:G:N3    | 2.69                     | 0.40              |
| 85:L5:2615:C:H2'  | 85:L5:2616:C:C6    | 2.55                     | 0.40              |
| 85:L5:2803:U:H2'  | 85:L5:2804:C:C6    | 2.56                     | 0.40              |
| 85:L5:3703:G:C4   | 85:L5:3704:U:C5    | 3.10                     | 0.40              |
| 85:L5:3952:A:H2   | 85:L5:4060:U:C4    | 2.38                     | 0.40              |
| 85:L5:4096:C:H2'  | 85:L5:4100:C:N3    | 2.36                     | 0.40              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 85:L5:4121:G:H5'' | 52:Lg:93:ARG:NH2   | 2.36                     | 0.40              |
| 85:L5:4281:A:C5   | 85:L5:4283:G:C8    | 3.09                     | 0.40              |
| 85:L5:4355:G:C2   | 85:L5:4356:G:C8    | 3.09                     | 0.40              |
| 85:L5:4645:C:H2'  | 85:L5:4646:U:C6    | 2.56                     | 0.40              |
| 85:L5:4906:C:C2   | 85:L5:4916:G:C2    | 3.09                     | 0.40              |
| 85:L5:5062:G:C2   | 85:L5:5063:G:C8    | 3.09                     | 0.40              |
| 22:LA:189:TYR:CB  | 22:LA:196:TRP:HB2  | 2.51                     | 0.40              |
| 23:LB:35:ASP:OD2  | 23:LB:193:LYS:NZ   | 2.53                     | 0.40              |
| 24:LC:51:PRO:HG3  | 32:LL:26:PHE:CE1   | 2.56                     | 0.40              |
| 24:LC:172:LYS:HA  | 24:LC:177:TRP:HB2  | 2.02                     | 0.40              |
| 26:LE:88:VAL:HA   | 26:LE:89:LEU:HA    | 1.77                     | 0.40              |
| 26:LE:239:LYS:HA  | 26:LE:239:LYS:HD2  | 1.86                     | 0.40              |
| 27:LF:157:ARG:HD3 | 27:LF:212:LYS:O    | 2.21                     | 0.40              |
| 29:LH:65:LYS:HD3  | 29:LH:65:LYS:HA    | 1.86                     | 0.40              |
| 30:LI:33:ILE:HB   | 30:LI:69:ARG:CZ    | 2.51                     | 0.40              |
| 34:LN:183:THR:O   | 34:LN:183:THR:OG1  | 2.34                     | 0.40              |
| 37:LQ:161:SER:O   | 37:LQ:162:HIS:ND1  | 2.54                     | 0.40              |
| 38:LR:81:ARG:HB3  | 38:LR:88:ARG:CZ    | 2.51                     | 0.40              |
| 43:LX:101:ASP:CG  | 43:LX:103:LYS:H    | 2.28                     | 0.40              |
| 57:Ll:44:TRP:CD1  | 57:Ll:44:TRP:H     | 2.40                     | 0.40              |
| 62:Lr:8:MET:HE2   | 62:Lr:8:MET:HB2    | 1.89                     | 0.40              |
| 64:SR:1:MET:HE2   | 79:S2:1468:C:C6    | 2.56                     | 0.40              |
| 66:SF:49:LEU:CB   | 69:SQ:50:LYS:HE2   | 2.51                     | 0.40              |
| 68:SP:107:ILE:C   | 68:SP:108:LYS:HD3  | 2.46                     | 0.40              |
| 71:ST:133:ARG:C   | 71:ST:137:GLN:HE22 | 2.29                     | 0.40              |
| 75:Sg:240:CYS:SG  | 75:Sg:298:LEU:HD11 | 2.61                     | 0.40              |
| 75:Sg:273:GLU:H   | 75:Sg:273:GLU:CD   | 2.28                     | 0.40              |
| 79:S2:412:G:O2'   | 79:S2:812:A:N6     | 2.54                     | 0.40              |
| 79:S2:674:C:O2'   | 79:S2:996:A:H1'    | 2.21                     | 0.40              |
| 79:S2:857:U:C2    | 79:S2:858:A:N7     | 2.89                     | 0.40              |
| 79:S2:1158:G:H2'  | 79:S2:1159:G:H8    | 1.87                     | 0.40              |
| 79:S2:1260:A:C2   | 79:S2:1620:A:C4    | 3.08                     | 0.40              |
| 79:S2:1389:C:C2   | 79:S2:1390:U:C5    | 3.09                     | 0.40              |
| 81:AP:34:A:H2'    | 81:AP:35:A:O4'     | 2.21                     | 0.40              |
| 83:Ls:51:ALA:HB1  | 83:Ls:90:PHE:O     | 2.21                     | 0.40              |
| 1:CH:27:LEU:HA    | 1:CH:30:ARG:HD2    | 2.02                     | 0.40              |
| 1:CH:121:LEU:C    | 1:CH:121:LEU:HD23  | 2.47                     | 0.40              |
| 3:sI:26:LYS:HE2   | 3:sI:26:LYS:HB2    | 1.89                     | 0.40              |
| 4:sL:10:TYR:CE2   | 4:sL:12:LYS:HB3    | 2.56                     | 0.40              |
| 5:sX:53:GLU:OE1   | 5:sX:55:VAL:CG2    | 2.69                     | 0.40              |
| 6:sG:131:ARG:NH1  | 79:s2:168:C:H4'    | 2.36                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:sJ:60:LEU:HD11   | 7:sJ:73:GLU:HB3    | 2.02                     | 0.40              |
| 8:sY:103:SER:HB3   | 8:sY:106:GLN:HE22  | 1.85                     | 0.40              |
| 11:sB:149:GLN:NE2  | 79:s2:1123:C:O2'   | 2.54                     | 0.40              |
| 12:sH:106:ARG:NH2  | 79:s2:861:A:H2'    | 2.36                     | 0.40              |
| 12:sH:160:LYS:HD3  | 12:sH:190:PRO:O    | 2.22                     | 0.40              |
| 13:sV:29:HIS:HE1   | 15:sC:86:LEU:O     | 2.03                     | 0.40              |
| 17:sO:56:VAL:HG21  | 17:sO:80:ASP:OD1   | 2.21                     | 0.40              |
| 17:sO:103:ASN:OD1  | 17:sO:103:ASN:N    | 2.49                     | 0.40              |
| 18:sW:112:ASP:N    | 18:sW:115:GLU:OE2  | 2.55                     | 0.40              |
| 21:l8:7:U:H2'      | 21:l8:8:U:H6       | 1.86                     | 0.40              |
| 23:lB:156:TYR:OH   | 85:l5:4912:G:N2    | 2.55                     | 0.40              |
| 23:lB:234:ARG:HG3  | 23:lB:272:LYS:HB2  | 2.03                     | 0.40              |
| 23:lB:385:LYS:NZ   | 85:l5:5001:U:OP1   | 2.52                     | 0.40              |
| 24:lC:5:ARG:HH12   | 24:lC:26:ALA:N     | 2.19                     | 0.40              |
| 24:lC:152:LEU:HD21 | 24:lC:174:LEU:HD13 | 2.03                     | 0.40              |
| 25:lD:86:TYR:HE2   | 25:lD:247:ILE:HG13 | 1.86                     | 0.40              |
| 28:lG:75:LYS:HD2   | 28:lG:240:ASN:ND2  | 2.35                     | 0.40              |
| 29:lH:71:ARG:NH1   | 85:l5:4691:A:OP1   | 2.52                     | 0.40              |
| 33:lM:108:ASP:HB3  | 35:lO:199:HIS:NE2  | 2.37                     | 0.40              |
| 35:lO:125:LYS:HG2  | 35:lO:129:LEU:HD12 | 2.03                     | 0.40              |
| 35:lO:190:ASP:OD1  | 35:lO:191:LYS:N    | 2.54                     | 0.40              |
| 40:lT:85:LEU:HD23  | 40:lT:85:LEU:HA    | 1.88                     | 0.40              |
| 43:lX:37:LYS:HA    | 43:lX:38:LYS:HA    | 1.64                     | 0.40              |
| 44:lY:55:VAL:O     | 44:lY:67:ILE:HD12  | 2.21                     | 0.40              |
| 47:lb:9:THR:HG22   | 85:l5:1874:A:OP1   | 2.21                     | 0.40              |
| 47:lb:103:LYS:HG2  | 47:lb:104:LEU:HD22 | 2.02                     | 0.40              |
| 51:lf:54:LYS:NZ    | 85:l5:4748:U:OP2   | 2.41                     | 0.40              |
| 53:lh:32:ARG:C     | 53:lh:32:ARG:CD    | 2.95                     | 0.40              |
| 54:li:66:ASP:OD2   | 54:li:87:ARG:CZ    | 2.70                     | 0.40              |
| 55:lj:8:PHE:HD1    | 55:lj:11:ARG:HH21  | 1.69                     | 0.40              |
| 55:lj:63:ARG:CD    | 55:lj:65:ARG:HG2   | 2.52                     | 0.40              |
| 60:lo:61:LYS:NZ    | 85:l5:4373:G:O6    | 2.31                     | 0.40              |
| 62:lr:92:SER:O     | 62:lr:95:HIS:HB2   | 2.22                     | 0.40              |
| 64:sR:40:ILE:C     | 64:sR:41:ILE:HG12  | 2.44                     | 0.40              |
| 66:sF:122:ARG:HG2  | 66:sF:197:GLU:OE1  | 2.21                     | 0.40              |
| 66:sF:164:ARG:HA   | 66:sF:164:ARG:HD2  | 1.82                     | 0.40              |
| 67:sK:48:ALA:O     | 67:sK:51:SER:OG    | 2.27                     | 0.40              |
| 70:sS:40:TYR:HA    | 70:sS:43:VAL:HG22  | 2.03                     | 0.40              |
| 70:sS:99:LEU:HD23  | 70:sS:99:LEU:N     | 2.37                     | 0.40              |
| 71:sT:67:ARG:NH1   | 79:s2:1587:G:C4    | 2.90                     | 0.40              |
| 71:sT:118:ASP:OD1  | 71:sT:118:ASP:N    | 2.53                     | 0.40              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 75:sg:34:ALA:HA    | 75:sg:40:ILE:CD1  | 2.51                     | 0.40              |
| 76:sM:23:LYS:NZ    | 76:sM:26:LEU:HD21 | 2.35                     | 0.40              |
| 76:sM:68:LEU:O     | 76:sM:71:GLU:HG2  | 2.22                     | 0.40              |
| 79:s2:92:A:N7      | 79:s2:447:A:C4    | 2.89                     | 0.40              |
| 79:s2:122:G:C6     | 79:s2:123:G:N7    | 2.89                     | 0.40              |
| 79:s2:141:A:N6     | 79:s2:177:G:O2'   | 2.54                     | 0.40              |
| 79:s2:398:A:H4'    | 79:s2:399:C:H5''  | 2.03                     | 0.40              |
| 79:s2:447:A:C6     | 79:s2:449:A:C6    | 3.09                     | 0.40              |
| 79:s2:602:G:OP2    | 79:s2:603:C:O2'   | 2.30                     | 0.40              |
| 79:s2:888:U:H1'    | 79:s2:889:U:H3'   | 2.04                     | 0.40              |
| 79:s2:1206:G:C6    | 79:s2:1693:G:N1   | 2.89                     | 0.40              |
| 79:s2:1370:A:N3    | 79:s2:1386:A:O2'  | 2.53                     | 0.40              |
| 79:s2:1452:A:C6    | 79:s2:1475:G:N7   | 2.89                     | 0.40              |
| 79:s2:1714:U:C2    | 79:s2:1820:G:N2   | 2.90                     | 0.40              |
| 80:cB:76:SER:C     | 80:cB:77:LEU:HD12 | 2.47                     | 0.40              |
| 80:cB:130:ASP:HB3  | 80:cB:133:SER:HB2 | 2.03                     | 0.40              |
| 80:cB:323:LEU:HD23 | 80:cB:323:LEU:HA  | 1.87                     | 0.40              |
| 80:cB:830:ARG:HB3  | 80:cB:831:PRO:HG3 | 2.03                     | 0.40              |
| 84:lt:117:ARG:HG2  | 84:lt:118:HIS:H   | 1.85                     | 0.40              |
| 85:l5:181:C:O2     | 85:l5:256:G:C2    | 2.74                     | 0.40              |
| 85:l5:201:C:C2     | 85:l5:202:C:C5    | 3.09                     | 0.40              |
| 85:l5:260:C:H2'    | 85:l5:261:G:C8    | 2.55                     | 0.40              |
| 85:l5:281:U:H2'    | 85:l5:282:C:C6    | 2.56                     | 0.40              |
| 85:l5:353:A:C6     | 85:l5:360:A:C8    | 3.08                     | 0.40              |
| 85:l5:431:G:C6     | 85:l5:3888:G:C6   | 3.10                     | 0.40              |
| 85:l5:464:G:H2'    | 85:l5:465:G:C8    | 2.54                     | 0.40              |
| 85:l5:468:U:C2     | 85:l5:686:A:N1    | 2.90                     | 0.40              |
| 85:l5:654:C:C4     | 85:l5:655:C:N4    | 2.89                     | 0.40              |
| 85:l5:946:C:H2'    | 85:l5:947:C:H6    | 1.85                     | 0.40              |
| 85:l5:1253:G:H2'   | 85:l5:1256:G:H5'  | 2.03                     | 0.40              |
| 85:l5:2609:G:H2'   | 85:l5:2610:G:H8   | 1.85                     | 0.40              |
| 85:l5:3806:G:C2    | 85:l5:3807:A:C8   | 3.10                     | 0.40              |
| 85:l5:4093:G:C8    | 85:l5:4095:G:C2   | 3.10                     | 0.40              |
| 85:l5:4152:G:H2'   | 85:l5:4153:C:C6   | 2.56                     | 0.40              |
| 85:l5:4236:G:H2'   | 85:l5:4237:C:C6   | 2.55                     | 0.40              |
| 85:l5:4273:A:H62   | 85:l5:4335:C:N4   | 2.18                     | 0.40              |
| 85:l5:4538:G:C4    | 85:l5:4539:U:C5   | 3.09                     | 0.40              |
| 85:l5:4620:U:OP2   | 85:l5:4670:C:N4   | 2.49                     | 0.40              |
| 85:l5:4681:A:H2'   | 85:l5:4682:U:O4'  | 2.21                     | 0.40              |
| 85:l5:4736:C:H4'   | 85:l5:5068:G:C4   | 2.57                     | 0.40              |
| 85:l5:4742:G:N2    | 85:l5:4959:U:H1'  | 2.36                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 85:L5:4748:U:H2'   | 85:L5:4749:C:C6    | 2.56                     | 0.40              |
| 85:L5:4768:G:H2'   | 85:L5:4769:G:C8    | 2.56                     | 0.40              |
| 80:CB:183:GLU:O    | 80:CB:187:VAL:HG12 | 2.21                     | 0.40              |
| 80:CB:425:LEU:O    | 80:CB:446:PRO:HA   | 2.21                     | 0.40              |
| 2:SE:183:VAL:HG23  | 2:SE:220:THR:HG21  | 2.02                     | 0.40              |
| 3:SI:26:LYS:NZ     | 79:S2:444:G:O6     | 2.54                     | 0.40              |
| 3:SI:139:LYS:HA    | 3:SI:139:LYS:HD2   | 1.77                     | 0.40              |
| 4:SL:29:GLY:HA3    | 4:SL:30:LYS:HA     | 1.34                     | 0.40              |
| 7:SJ:28:GLU:HG2    | 7:SJ:43:VAL:HG11   | 2.03                     | 0.40              |
| 7:SJ:137:VAL:CG2   | 7:SJ:138:ARG:H     | 2.35                     | 0.40              |
| 11:SB:110:MET:HA   | 11:SB:110:MET:HE2  | 2.04                     | 0.40              |
| 12:SH:47:ALA:HB3   | 12:SH:63:PHE:HB2   | 2.02                     | 0.40              |
| 12:SH:130:LEU:HB3  | 12:SH:177:TYR:CE2  | 2.56                     | 0.40              |
| 12:SH:144:ILE:HG13 | 18:SW:52:ILE:HG23  | 2.04                     | 0.40              |
| 13:SV:74:LYS:N     | 13:SV:74:LYS:HD2   | 2.36                     | 0.40              |
| 13:SV:74:LYS:HZ2   | 13:SV:78:ILE:HG22  | 1.85                     | 0.40              |
| 17:SO:72:TYR:CE1   | 66:SF:204:ARG:HD2  | 2.56                     | 0.40              |
| 17:SO:119:LEU:O    | 17:SO:124:MET:HB2  | 2.21                     | 0.40              |
| 18:SW:52:ILE:HD12  | 18:SW:60:LYS:O     | 2.20                     | 0.40              |
| 85:L5:81:C:H2'     | 85:L5:82:U:O4'     | 2.22                     | 0.40              |
| 85:L5:115:C:OP1    | 34:LN:2:GLY:N      | 2.54                     | 0.40              |
| 85:L5:191:G:N1     | 85:L5:251:C:N3     | 2.69                     | 0.40              |
| 85:L5:647:G:C4     | 85:L5:648:G:C8     | 3.09                     | 0.40              |
| 85:L5:1217:G:C6    | 85:L5:1218:G:C6    | 3.10                     | 0.40              |
| 85:L5:1258:G:H2'   | 85:L5:1259:G:H8    | 1.80                     | 0.40              |
| 85:L5:1359:G:OP1   | 24:LC:114:ARG:NH1  | 2.54                     | 0.40              |
| 85:L5:1608:G:H2'   | 85:L5:1609:U:C6    | 2.56                     | 0.40              |
| 85:L5:1688:G:H2'   | 85:L5:1689:G:H8    | 1.84                     | 0.40              |
| 85:L5:1759:G:H3'   | 85:L5:1760:G:C8    | 2.56                     | 0.40              |
| 85:L5:1815:G:C6    | 47:Lb:45:PHE:CE2   | 3.10                     | 0.40              |
| 85:L5:1912:G:C5    | 85:L5:2057:A:C4    | 3.09                     | 0.40              |
| 85:L5:2060:G:H2'   | 85:L5:2061:U:H6    | 1.87                     | 0.40              |
| 85:L5:2439:G:N7    | 85:L5:2777:G:C6    | 2.89                     | 0.40              |
| 85:L5:2448:G:C5    | 85:L5:2511:A:C6    | 3.09                     | 0.40              |
| 85:L5:2521:G:OP2   | 52:Lg:8:ARG:NH2    | 2.54                     | 0.40              |
| 85:L5:2609:G:H2'   | 85:L5:2610:G:H8    | 1.86                     | 0.40              |
| 85:L5:2638:G:H4'   | 52:Lg:24:ARG:NH1   | 2.36                     | 0.40              |
| 85:L5:2735:G:H2'   | 85:L5:2736:G:H8    | 1.84                     | 0.40              |
| 85:L5:3966:A:N6    | 85:L5:4057:C:C2    | 2.89                     | 0.40              |
| 85:L5:4097:G:O5'   | 85:L5:4111:U:O2    | 2.40                     | 0.40              |
| 85:L5:4112:C:H2'   | 85:L5:4115:G:H5''  | 2.03                     | 0.40              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 85:L5:4471:U:OP1  | 29:LH:168:LYS:NZ   | 2.34                     | 0.40              |
| 85:L5:4525:C:H2'  | 85:L5:4526:U:H6    | 1.86                     | 0.40              |
| 85:L5:4563:U:H2'  | 85:L5:4564:A:C8    | 2.54                     | 0.40              |
| 85:L5:4688:C:H2'  | 85:L5:4689:U:C6    | 2.56                     | 0.40              |
| 85:L5:4737:G:C6   | 85:L5:4738:C:C4    | 3.09                     | 0.40              |
| 85:L5:4872:G:C2   | 35:LO:203:VAL:HG23 | 2.56                     | 0.40              |
| 20:L7:110:G:H2'   | 20:L7:111:C:H6     | 1.87                     | 0.40              |
| 24:LC:304:ALA:HA  | 24:LC:305:PRO:HD3  | 1.97                     | 0.40              |
| 25:LD:205:ALA:HB1 | 25:LD:209:ARG:NH2  | 2.37                     | 0.40              |
| 29:LH:129:ARG:HD2 | 29:LH:156:ASN:HB3  | 2.03                     | 0.40              |
| 30:LI:52:MET:HE1  | 30:LI:165:ILE:HG23 | 2.03                     | 0.40              |
| 32:LL:70:VAL:N    | 32:LL:159:ASN:OD1  | 2.51                     | 0.40              |
| 32:LL:162:LYS:HE3 | 32:LL:162:LYS:HB2  | 1.88                     | 0.40              |
| 33:LM:53:LYS:H    | 33:LM:53:LYS:HG3   | 1.59                     | 0.40              |
| 38:LR:145:LEU:HA  | 38:LR:148:ASP:OD2  | 2.21                     | 0.40              |
| 38:LR:172:ARG:HG3 | 38:LR:172:ARG:H    | 1.70                     | 0.40              |
| 40:LT:49:GLN:N    | 40:LT:49:GLN:OE1   | 2.54                     | 0.40              |
| 44:LY:22:PRO:HG2  | 44:LY:24:HIS:CE1   | 2.56                     | 0.40              |
| 47:Lb:93:LEU:HD12 | 47:Lb:93:LEU:HA    | 1.84                     | 0.40              |
| 48:Lc:22:MET:N    | 48:Lc:22:MET:HE2   | 2.36                     | 0.40              |
| 50:Le:70:LEU:HB2  | 50:Le:74:PHE:O     | 2.21                     | 0.40              |
| 51:Lf:8:LYS:N     | 51:Lf:31:GLU:OE2   | 2.52                     | 0.40              |
| 60:Lo:2:VAL:N     | 60:Lo:90:HIS:O     | 2.54                     | 0.40              |
| 62:Lr:97:ILE:HD11 | 62:Lr:103:ARG:O    | 2.21                     | 0.40              |
| 66:SF:40:ALA:HB3  | 66:SF:68:ILE:H     | 1.85                     | 0.40              |
| 67:SK:16:PHE:CZ   | 67:SK:80:ARG:HA    | 2.56                     | 0.40              |
| 70:SS:12:ILE:C    | 70:SS:13:LEU:HD12  | 2.46                     | 0.40              |
| 70:SS:82:TRP:CG   | 79:S2:1567:G:C6    | 3.08                     | 0.40              |
| 70:SS:114:LEU:HB3 | 70:SS:122:GLY:HA3  | 2.03                     | 0.40              |
| 72:SU:28:ASN:HB2  | 72:SU:30:LYS:NZ    | 2.36                     | 0.40              |
| 75:Sg:64:HIS:CE1  | 75:Sg:65:PHE:CE2   | 3.09                     | 0.40              |
| 75:Sg:239:LEU:HA  | 75:Sg:250:ALA:HA   | 2.02                     | 0.40              |
| 78:Sf:92:LYS:O    | 78:Sf:94:LYS:HD3   | 2.21                     | 0.40              |
| 79:S2:160:U:O4    | 79:S2:468:A:H4'    | 2.21                     | 0.40              |
| 79:S2:176:U:H2'   | 79:S2:177:G:C8     | 2.56                     | 0.40              |
| 79:S2:187:G:C6    | 79:S2:213:G:N1     | 2.90                     | 0.40              |
| 79:S2:322:C:H2'   | 79:S2:323:C:C1'    | 2.51                     | 0.40              |
| 79:S2:493:A:H1'   | 79:S2:574:A:H5'    | 2.02                     | 0.40              |
| 79:S2:859:G:C6    | 79:S2:860:G:C6     | 3.09                     | 0.40              |
| 79:S2:936:G:H2'   | 79:S2:937:C:H6     | 1.85                     | 0.40              |
| 79:S2:937:C:C2    | 79:S2:938:A:C8     | 3.09                     | 0.40              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 79:S2:974:C:H2'    | 79:S2:975:G:H8    | 1.85                     | 0.40              |
| 79:S2:1390:U:H2'   | 79:S2:1391:C:C6   | 2.56                     | 0.40              |
| 79:S2:1404:U:O2'   | 79:S2:1580:A:H8   | 2.04                     | 0.40              |
| 79:S2:1713:C:H2'   | 79:S2:1714:U:H6   | 1.84                     | 0.40              |
| 79:S2:1738:C:H2'   | 79:S2:1739:C:C6   | 2.56                     | 0.40              |
| 79:S2:1795:G:H2'   | 79:S2:1796:G:C8   | 2.55                     | 0.40              |
| 81:AP:25:C:C2'     | 81:AP:26:G:H5'    | 2.51                     | 0.40              |
| 84:Lt:47:ALA:HB2   | 84:Lt:70:GLN:NE2  | 2.35                     | 0.40              |
| 87:IW:12:LYS:NZ    | 87:IW:14:TYR:CE2  | 2.68                     | 0.40              |
| 87:LW:90:ILE:HG13  | 87:LW:91:MET:N    | 2.34                     | 0.40              |
| 1:cH:52:HIS:ND1    | 1:cH:52:HIS:C     | 2.80                     | 0.40              |
| 2:sE:9:LEU:O       | 2:sE:28:ALA:N     | 2.50                     | 0.40              |
| 2:sE:94:LYS:O      | 8:sY:16:ARG:NH1   | 2.45                     | 0.40              |
| 7:sJ:65:GLU:O      | 7:sJ:66:LYS:HB3   | 2.22                     | 0.40              |
| 8:sY:105:LYS:H     | 8:sY:105:LYS:HG2  | 1.51                     | 0.40              |
| 9:se:18:LYS:N      | 9:se:18:LYS:HD2   | 2.36                     | 0.40              |
| 10:sA:142:LEU:CA   | 13:sV:32:ILE:HD11 | 2.50                     | 0.40              |
| 10:sA:155:ARG:NH2  | 79:s2:1137:U:O3'  | 2.55                     | 0.40              |
| 11:sB:97:LEU:H     | 11:sB:97:LEU:HD23 | 1.87                     | 0.40              |
| 12:sH:31:GLU:N     | 12:sH:31:GLU:OE1  | 2.54                     | 0.40              |
| 12:sH:145:ARG:CZ   | 18:sW:52:ILE:H    | 2.33                     | 0.40              |
| 14:sa:47:ALA:O     | 14:sa:50:VAL:HG12 | 2.21                     | 0.40              |
| 15:sC:81:ILE:HD12  | 15:sC:81:ILE:HA   | 1.90                     | 0.40              |
| 15:sC:264:SER:HB3  | 15:sC:267:GLN:NE2 | 2.36                     | 0.40              |
| 21:l8:31:G:C6      | 85:l5:344:A:N1    | 2.89                     | 0.40              |
| 27:lF:97:GLY:N     | 85:l5:1896:A:OP1  | 2.54                     | 0.40              |
| 28:lG:98:LEU:HA    | 28:lG:101:LYS:HE2 | 2.03                     | 0.40              |
| 32:lL:63:THR:HG22  | 32:lL:65:ARG:H    | 1.86                     | 0.40              |
| 33:lM:90:ARG:NH2   | 85:l5:4868:G:H5'' | 2.36                     | 0.40              |
| 34:lN:114:ARG:NH1  | 34:lN:151:ILE:O   | 2.54                     | 0.40              |
| 36:lP:27:LYS:HD3   | 36:lP:63:TYR:CG   | 2.56                     | 0.40              |
| 36:lP:101:ASN:ND2  | 85:l5:400:A:H4'   | 2.36                     | 0.40              |
| 38:lR:95:TRP:CE2   | 38:lR:99:MET:HE1  | 2.56                     | 0.40              |
| 39:lS:84:TYR:CE1   | 39:lS:93:MET:SD   | 3.14                     | 0.40              |
| 40:lT:39:ILE:C     | 40:lT:99:SER:HG   | 2.29                     | 0.40              |
| 42:lV:40:ILE:HD11  | 85:l5:3799:A:C4   | 2.52                     | 0.40              |
| 45:lZ:134:LEU:HD23 | 45:lZ:134:LEU:C   | 2.46                     | 0.40              |
| 48:lc:79:ILE:H     | 48:lc:79:ILE:HG13 | 1.68                     | 0.40              |
| 52:lg:37:LYS:HB2   | 52:lg:60:ARG:CZ   | 2.51                     | 0.40              |
| 53:lh:76:LYS:O     | 85:l5:136:C:N4    | 2.39                     | 0.40              |
| 56:lk:40:ARG:HG2   | 56:lk:41:TYR:CE2  | 2.56                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 60:lo:61:LYS:HA    | 60:lo:61:LYS:CE    | 2.40                     | 0.40              |
| 61:lp:44:LYS:HE3   | 61:lp:59:SER:HB2   | 2.03                     | 0.40              |
| 64:sR:29:HIS:C     | 64:sR:32:LYS:HB2   | 2.47                     | 0.40              |
| 64:sR:32:LYS:HG2   | 79:s2:1453:C:N1    | 2.37                     | 0.40              |
| 65:sD:65:ARG:O     | 65:sD:69:LEU:HD23  | 2.22                     | 0.40              |
| 65:sD:190:LEU:HB2  | 65:sD:200:PRO:CD   | 2.51                     | 0.40              |
| 67:sK:50:GLN:HA    | 67:sK:53:LYS:HB3   | 2.04                     | 0.40              |
| 68:sP:22:LEU:O     | 68:sP:26:LEU:HD22  | 2.22                     | 0.40              |
| 68:sP:94:VAL:O     | 68:sP:105:VAL:N    | 2.52                     | 0.40              |
| 70:sS:114:LEU:HB3  | 70:sS:122:GLY:HA3  | 2.04                     | 0.40              |
| 71:sT:39:LEU:HD23  | 71:sT:39:LEU:HA    | 1.68                     | 0.40              |
| 74:sd:40:ARG:HD3   | 79:s2:1256:G:C5    | 2.57                     | 0.40              |
| 75:sg:14:HIS:HB2   | 75:sg:37:ASP:OD2   | 2.20                     | 0.40              |
| 75:sg:61:GLY:O     | 75:sg:88:ARG:NH1   | 2.54                     | 0.40              |
| 77:sZ:66:LYS:HB3   | 77:sZ:111:ARG:NE   | 2.32                     | 0.40              |
| 77:sZ:85:ARG:NH2   | 79:s2:1598:G:N7    | 2.69                     | 0.40              |
| 77:sZ:94:LYS:CG    | 77:sZ:96:LEU:HD22  | 2.51                     | 0.40              |
| 79:s2:71:G:N2      | 79:s2:73:C:OP1     | 2.54                     | 0.40              |
| 79:s2:177:G:H1     | 79:s2:313:A:P      | 2.45                     | 0.40              |
| 79:s2:556:U:H3'    | 79:s2:557:U:C4'    | 2.51                     | 0.40              |
| 79:s2:1075:C:H2'   | 79:s2:1076:G:H8    | 1.87                     | 0.40              |
| 79:s2:1459:G:H2'   | 79:s2:1460:C:H6    | 1.85                     | 0.40              |
| 79:s2:1617:G:N2    | 79:s2:1619:A:H3'   | 2.37                     | 0.40              |
| 79:s2:1639:G:H8    | 79:s2:1639:G:OP2   | 2.04                     | 0.40              |
| 79:s2:1754:G:C6    | 79:s2:1779:G:C2    | 3.09                     | 0.40              |
| 79:s2:1804:U:H2'   | 79:s2:1805:G:C8    | 2.56                     | 0.40              |
| 80:cB:88:PHE:CD1   | 80:cB:226:LYS:HE2  | 2.57                     | 0.40              |
| 80:cB:434:TYR:HE1  | 80:cB:442:LEU:HD12 | 1.85                     | 0.40              |
| 80:cB:590:LEU:HD11 | 80:cB:705:HIS:HB2  | 2.02                     | 0.40              |
| 83:ls:29:ILE:HD13  | 83:ls:191:GLN:HB2  | 2.02                     | 0.40              |
| 84:lt:65:GLN:OE1   | 84:lt:66:ASN:N     | 2.54                     | 0.40              |
| 84:lt:142:ASN:HD22 | 84:lt:148:PRO:HB3  | 1.87                     | 0.40              |
| 85:l5:1242:G:C5    | 85:l5:1243:C:C5    | 3.10                     | 0.40              |
| 85:l5:1383:G:C4    | 85:l5:1384:C:C5    | 3.09                     | 0.40              |
| 85:l5:1416:G:C6    | 85:l5:1417:C:C4    | 3.09                     | 0.40              |
| 85:l5:1473:U:H2'   | 85:l5:1474:C:H6    | 1.86                     | 0.40              |
| 85:l5:2098:G:H2'   | 85:l5:2099:G:H8    | 1.80                     | 0.40              |
| 85:l5:2260:C:H4'   | 85:l5:2261:G:O4'   | 2.21                     | 0.40              |
| 85:l5:2500:U:H2'   | 85:l5:2501:C:C6    | 2.56                     | 0.40              |
| 85:l5:2629:C:C4    | 85:l5:2630:U:C4    | 3.09                     | 0.40              |
| 85:l5:2816:G:H2'   | 85:l5:2817:C:H6    | 1.86                     | 0.40              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 85:L5:3834:C:C2    | 85:L5:3835:C:C5   | 3.09                     | 0.40              |
| 85:L5:4308:C:C2    | 85:L5:4309:G:C8   | 3.09                     | 0.40              |
| 85:L5:4645:C:H2'   | 85:L5:4646:U:H6   | 1.86                     | 0.40              |
| 85:L5:4948:C:H3'   | 85:L5:4949:G:H2'  | 2.01                     | 0.40              |
| 80:CB:160:MET:HE2  | 80:CB:160:MET:HB3 | 2.00                     | 0.40              |
| 80:CB:227:GLN:H    | 80:CB:227:GLN:CD  | 2.27                     | 0.40              |
| 80:CB:412:ALA:HB3  | 80:CB:472:LEU:HB2 | 2.04                     | 0.40              |
| 80:CB:622:VAL:HG13 | 80:CB:631:ARG:HD3 | 2.03                     | 0.40              |
| 80:CB:820:LEU:HD12 | 80:CB:820:LEU:HA  | 1.88                     | 0.40              |
| 3:SI:6:ASP:O       | 79:S2:386:C:H4'   | 2.20                     | 0.40              |
| 3:SI:107:THR:OG1   | 3:SI:108:PRO:HD3  | 2.21                     | 0.40              |
| 3:SI:140:LYS:HD2   | 3:SI:140:LYS:O    | 2.22                     | 0.40              |
| 4:SL:21:LYS:HB3    | 4:SL:21:LYS:HE3   | 1.91                     | 0.40              |
| 5:SX:121:LYS:HE3   | 5:SX:121:LYS:HB2  | 1.83                     | 0.40              |
| 6:SG:105:ASN:OD1   | 6:SG:105:ASN:N    | 2.54                     | 0.40              |
| 6:SG:136:LYS:NZ    | 79:S2:65:C:OP1    | 2.49                     | 0.40              |
| 11:SB:180:ASP:CG   | 11:SB:181:LEU:N   | 2.79                     | 0.40              |
| 85:L5:86:U:H2'     | 85:L5:87:A:H8     | 1.85                     | 0.40              |
| 85:L5:132:G:H3'    | 85:L5:133:C:H4'   | 2.02                     | 0.40              |
| 85:L5:387:G:C5     | 85:L5:412:G:C5    | 3.09                     | 0.40              |
| 85:L5:490:C:H2'    | 85:L5:491:G:C8    | 2.56                     | 0.40              |
| 85:L5:518:G:N1     | 85:L5:643:C:O2    | 2.55                     | 0.40              |
| 85:L5:1317:U:H2'   | 85:L5:1318:C:H6   | 1.79                     | 0.40              |
| 85:L5:1577:G:P     | 22:LA:181:LYS:HZ1 | 2.42                     | 0.40              |
| 85:L5:1654:G:C6    | 85:L5:3914:U:H5'' | 2.57                     | 0.40              |
| 85:L5:2072:C:H2'   | 85:L5:2073:C:C6   | 2.57                     | 0.40              |
| 85:L5:2455:G:H1'   | 85:L5:2471:G:N7   | 2.36                     | 0.40              |
| 85:L5:2644:G:H2'   | 85:L5:2645:G:C8   | 2.56                     | 0.40              |
| 85:L5:2695:A:N3    | 85:L5:2697:A:C8   | 2.90                     | 0.40              |
| 85:L5:2728:U:H2'   | 85:L5:2729:C:C6   | 2.56                     | 0.40              |
| 85:L5:3685:C:H2'   | 85:L5:3686:G:O4'  | 2.22                     | 0.40              |
| 85:L5:3718:A:C4    | 85:L5:3719:A:C8   | 3.09                     | 0.40              |
| 85:L5:4340:U:H5'   | 37:LQ:178:ARG:HD2 | 2.04                     | 0.40              |
| 85:L5:4538:G:C4    | 85:L5:4539:U:C5   | 3.09                     | 0.40              |
| 85:L5:4708:A:N3    | 85:L5:4709:U:H5'  | 2.36                     | 0.40              |
| 85:L5:4737:G:C6    | 85:L5:4963:G:N1   | 2.89                     | 0.40              |
| 85:L5:4881:U:H4'   | 85:L5:4882:U:H5'  | 2.02                     | 0.40              |
| 85:L5:4883:C:H2'   | 85:L5:4884:G:C8   | 2.57                     | 0.40              |
| 85:L5:4977:A:H2'   | 85:L5:4978:G:H8   | 1.87                     | 0.40              |
| 20:L7:49:A:OP1     | 25:LD:225:GLN:HB2 | 2.21                     | 0.40              |
| 21:L8:83:C:H42     | 44:LY:50:ARG:NH2  | 2.08                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:LA:207:VAL:HG23 | 22:LA:208:GLU:HG3  | 2.04                     | 0.40              |
| 22:LA:242:ARG:CZ   | 22:LA:246:LEU:HD13 | 2.51                     | 0.40              |
| 23:LB:103:LYS:HB2  | 23:LB:153:MET:HE2  | 2.04                     | 0.40              |
| 23:LB:214:ASP:HA   | 23:LB:284:ILE:O    | 2.21                     | 0.40              |
| 23:LB:389:MET:HA   | 23:LB:389:MET:HE2  | 2.03                     | 0.40              |
| 24:LC:163:LYS:HB2  | 24:LC:166:GLU:HG2  | 2.02                     | 0.40              |
| 25:LD:166:ALA:O    | 25:LD:171:LEU:HB2  | 2.22                     | 0.40              |
| 25:LD:224:SER:OG   | 25:LD:225:GLN:N    | 2.55                     | 0.40              |
| 26:LE:150:LEU:N    | 26:LE:162:VAL:O    | 2.35                     | 0.40              |
| 28:LG:106:THR:O    | 28:LG:110:LYS:HB2  | 2.21                     | 0.40              |
| 31:LJ:115:LEU:HD22 | 31:LJ:116:GLY:HA2  | 2.04                     | 0.40              |
| 32:LL:59:VAL:HG23  | 32:LL:71:ARG:HG3   | 2.03                     | 0.40              |
| 33:LM:70:GLN:NE2   | 33:LM:74:ARG:HH21  | 2.19                     | 0.40              |
| 37:LQ:42:THR:HA    | 37:LQ:45:GLN:CD    | 2.47                     | 0.40              |
| 37:LQ:99:LYS:HE3   | 37:LQ:99:LYS:HB3   | 1.90                     | 0.40              |
| 38:LR:82:LYS:HE3   | 38:LR:82:LYS:HB3   | 1.91                     | 0.40              |
| 38:LR:104:ARG:HA   | 38:LR:107:ARG:HH12 | 1.86                     | 0.40              |
| 40:LT:111:GLU:HA   | 40:LT:114:GLN:CD   | 2.47                     | 0.40              |
| 43:LX:78:LYS:HG2   | 43:LX:100:VAL:HA   | 2.03                     | 0.40              |
| 46:La:145:VAL:HG23 | 54:Li:5:TYR:CE2    | 2.56                     | 0.40              |
| 52:Lg:85:LYS:HE2   | 52:Lg:88:ARG:NH1   | 2.36                     | 0.40              |
| 63:Lz:96:ASN:HD22  | 63:Lz:125:GLY:N    | 2.19                     | 0.40              |
| 66:SF:176:GLU:HA   | 66:SF:179:ASN:HB2  | 2.02                     | 0.40              |
| 67:SK:49:MET:HB2   | 67:SK:49:MET:HE3   | 1.72                     | 0.40              |
| 68:SP:72:LYS:HD3   | 68:SP:72:LYS:HA    | 1.93                     | 0.40              |
| 69:SQ:11:GLN:NE2   | 79:S2:1442:U:O2'   | 2.47                     | 0.40              |
| 69:SQ:131:LYS:HA   | 69:SQ:131:LYS:HD3  | 1.90                     | 0.40              |
| 70:SS:40:TYR:CD1   | 70:SS:71:MET:HE2   | 2.55                     | 0.40              |
| 71:ST:3:GLY:HA3    | 71:ST:4:VAL:HA     | 1.62                     | 0.40              |
| 71:ST:92:PHE:HD1   | 79:S2:1589:A:H5'   | 1.87                     | 0.40              |
| 72:SU:49:LYS:O     | 72:SU:91:LEU:HD22  | 2.21                     | 0.40              |
| 72:SU:66:ARG:NH2   | 72:SU:75:LYS:HA    | 2.31                     | 0.40              |
| 74:Sd:14:PHE:CD2   | 79:S2:1661:A:C8    | 3.08                     | 0.40              |
| 75:Sg:25:PRO:HD3   | 75:Sg:293:ALA:HB2  | 2.02                     | 0.40              |
| 75:Sg:88:ARG:NH2   | 79:S2:1398:G:O2'   | 2.55                     | 0.40              |
| 75:Sg:163:PRO:CB   | 75:Sg:179:LEU:HG   | 2.43                     | 0.40              |
| 76:SM:103:VAL:HG23 | 76:SM:104:VAL:O    | 2.21                     | 0.40              |
| 77:SZ:65:TYR:C     | 77:SZ:111:ARG:HE   | 2.28                     | 0.40              |
| 79:S2:92:A:N7      | 79:S2:447:A:C4     | 2.90                     | 0.40              |
| 79:S2:659:G:H5'    | 79:S2:660:C:OP1    | 2.21                     | 0.40              |
| 79:S2:969:U:O2     | 79:S2:971:G:N1     | 2.54                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 79:S2:1089:G:H2'   | 79:S2:1090:C:C6    | 2.56                     | 0.40              |
| 79:S2:1109:C:C2    | 79:S2:1110:G:H1'   | 2.56                     | 0.40              |
| 79:S2:1175:G:C4    | 79:S2:1176:G:C8    | 3.09                     | 0.40              |
| 79:S2:1177:U:C2    | 79:S2:1178:U:C5    | 3.09                     | 0.40              |
| 79:S2:1334:G:H2'   | 79:S2:1335:G:O4'   | 2.21                     | 0.40              |
| 79:S2:1512:C:H2'   | 79:S2:1513:C:C6    | 2.56                     | 0.40              |
| 79:S2:1646:C:N3    | 79:S2:1678:A:C4    | 2.90                     | 0.40              |
| 79:S2:1680:G:H2'   | 79:S2:1681:U:C6    | 2.57                     | 0.40              |
| 79:S2:1858:G:C2    | 79:S2:1859:A:C5    | 3.10                     | 0.40              |
| 81:AP:51:C:C2      | 81:AP:52:G:C8      | 3.09                     | 0.40              |
| 87:IW:96:GLN:HB2   | 87:IW:100:VAL:HB   | 2.03                     | 0.40              |
| 1:CH:58:THR:HB     | 65:SD:113:LEU:HG   | 2.04                     | 0.40              |
| 2:sE:7:LYS:NZ      | 79:s2:498:C:OP1    | 2.54                     | 0.40              |
| 2:sE:242:LYS:O     | 2:sE:244:ILE:N     | 2.54                     | 0.40              |
| 3:sI:11:ARG:HD3    | 3:sI:15:GLY:O      | 2.22                     | 0.40              |
| 6:sG:148:SER:OG    | 6:sG:149:LYS:HG2   | 2.21                     | 0.40              |
| 7:sJ:31:LEU:HA     | 7:sJ:31:LEU:HD23   | 1.85                     | 0.40              |
| 8:sY:40:ILE:H      | 8:sY:40:ILE:HG13   | 1.74                     | 0.40              |
| 10:sA:174:MET:HE2  | 10:sA:174:MET:C    | 2.46                     | 0.40              |
| 11:sB:134:LEU:HD21 | 11:sB:218:LEU:HB2  | 2.03                     | 0.40              |
| 11:sB:180:ASP:OD1  | 11:sB:181:LEU:N    | 2.48                     | 0.40              |
| 16:sN:54:LEU:HD12  | 16:sN:55:ARG:N     | 2.36                     | 0.40              |
| 20:l7:7:G:OP2      | 25:ID:28:THR:OG1   | 2.22                     | 0.40              |
| 20:l7:88:A:N1      | 85:l5:1942:A:H4'   | 2.37                     | 0.40              |
| 20:l7:119:U:H5     | 25:ID:258:LYS:NZ   | 2.18                     | 0.40              |
| 21:l8:123:U:N3     | 21:l8:125:C:H5''   | 2.36                     | 0.40              |
| 23:lB:108:GLU:HG3  | 23:lB:109:HIS:CE1  | 2.56                     | 0.40              |
| 24:lC:209:ILE:HB   | 24:lC:229:LEU:CD1  | 2.51                     | 0.40              |
| 25:ID:41:LYS:HG3   | 40:IT:93:ILE:HG13  | 2.04                     | 0.40              |
| 25:ID:167:VAL:HG11 | 25:ID:175:HIS:CE1  | 2.56                     | 0.40              |
| 27:lF:32:ARG:HH21  | 85:l5:1701:A:H61   | 1.68                     | 0.40              |
| 28:lG:109:GLU:C    | 28:lG:109:GLU:CD   | 2.89                     | 0.40              |
| 29:IH:68:ALA:HB1   | 85:l5:4691:A:N3    | 2.37                     | 0.40              |
| 29:IH:123:ILE:HD13 | 29:IH:123:ILE:HG21 | 1.74                     | 0.40              |
| 30:II:45:GLU:H     | 30:II:45:GLU:CD    | 2.28                     | 0.40              |
| 32:IL:65:ARG:HD3   | 46:la:66:ASN:OD1   | 2.21                     | 0.40              |
| 32:IL:198:ARG:NH2  | 85:l5:1485:C:N3    | 2.69                     | 0.40              |
| 34:IN:36:LEU:HD22  | 34:IN:36:LEU:HA    | 1.91                     | 0.40              |
| 40:IT:108:ARG:HH21 | 85:l5:1837:A:P     | 2.45                     | 0.40              |
| 40:IT:118:GLU:OE2  | 40:IT:122:LYS:HD2  | 2.21                     | 0.40              |
| 43:IX:72:ASP:OD1   | 43:IX:75:ALA:N     | 2.44                     | 0.40              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 45:lZ:42:LEU:HD23  | 45:lZ:43:VAL:N    | 2.36                     | 0.40              |
| 45:lZ:132:GLN:HA   | 45:lZ:132:GLN:OE1 | 2.22                     | 0.40              |
| 49:ld:83:ARG:NH1   | 85:l5:5046:U:OP2  | 2.42                     | 0.40              |
| 49:ld:118:GLN:HE22 | 85:l5:5055:G:H21  | 1.69                     | 0.40              |
| 50:le:58:ILE:HG22  | 85:l5:1664:U:OP1  | 2.20                     | 0.40              |
| 53:lh:14:LYS:HG3   | 53:lh:15:GLU:N    | 2.35                     | 0.40              |
| 56:lk:24:LYS:N     | 56:lk:35:LYS:O    | 2.46                     | 0.40              |
| 60:lo:62:THR:HG23  | 60:lo:63:THR:HG22 | 2.04                     | 0.40              |
| 62:lr:23:GLN:N     | 62:lr:23:GLN:OE1  | 2.54                     | 0.40              |
| 64:sR:5:ARG:HH12   | 64:sR:49:LYS:HD2  | 1.86                     | 0.40              |
| 64:sR:16:ILE:HD12  | 64:sR:20:TYR:HE2  | 1.86                     | 0.40              |
| 64:sR:53:TYR:CD2   | 79:s2:1466:G:C8   | 3.09                     | 0.40              |
| 64:sR:76:GLU:O     | 64:sR:80:ARG:HG2  | 2.20                     | 0.40              |
| 64:sR:79:GLU:CD    | 64:sR:80:ARG:HH12 | 2.30                     | 0.40              |
| 70:sS:74:PRO:HB2   | 70:sS:79:ILE:HB   | 2.04                     | 0.40              |
| 71:sT:7:LYS:HZ3    | 79:s2:1426:U:C5'  | 2.34                     | 0.40              |
| 72:sU:64:THR:HG23  | 72:sU:78:ASP:O    | 2.20                     | 0.40              |
| 75:sg:153:CYS:O    | 75:sg:168:CYS:HB3 | 2.21                     | 0.40              |
| 75:sg:257:LYS:HA   | 75:sg:269:GLU:HA  | 2.03                     | 0.40              |
| 75:sg:302:TYR:CE2  | 75:sg:308:ARG:HD2 | 2.56                     | 0.40              |
| 79:s2:320:G:H2'    | 79:s2:321:C:H6    | 1.86                     | 0.40              |
| 79:s2:614:C:H5     | 79:s2:625:G:H3'   | 1.86                     | 0.40              |
| 79:s2:748:C:O2'    | 79:s2:749:U:O5'   | 2.36                     | 0.40              |
| 79:s2:848:U:H2'    | 79:s2:849:A:C8    | 2.53                     | 0.40              |
| 79:s2:918:U:H2'    | 79:s2:919:A:N3    | 2.37                     | 0.40              |
| 79:s2:1373:C:C2    | 79:s2:1374:C:C5   | 3.10                     | 0.40              |
| 79:s2:1567:G:C5    | 79:s2:1568:C:C4   | 3.10                     | 0.40              |
| 79:s2:1610:G:C6    | 79:s2:1630:A:C5   | 3.09                     | 0.40              |
| 79:s2:1796:G:C6    | 79:s2:1797:U:C4   | 3.10                     | 0.40              |
| 80:cB:219:HIS:HB2  | 80:cB:221:TRP:NE1 | 2.36                     | 0.40              |
| 80:cB:769:HIS:HB3  | 85:l5:1981:G:N2   | 2.36                     | 0.40              |
| 82:pE:3:C:H2'      | 82:pE:4:C:O4'     | 2.20                     | 0.40              |
| 83:ls:77:LYS:O     | 83:ls:81:HIS:CE1  | 2.75                     | 0.40              |
| 84:lt:16:ARG:HD3   | 84:lt:61:LYS:HZ3  | 1.86                     | 0.40              |
| 85:l5:19:G:O2'     | 85:l5:20:U:H5'    | 2.21                     | 0.40              |
| 85:l5:247:G:C4     | 85:l5:248:C:C5    | 3.10                     | 0.40              |
| 85:l5:406:C:HO2'   | 85:l5:407:A:P     | 2.42                     | 0.40              |
| 85:l5:496:G:O6     | 85:l5:497:G:N2    | 2.55                     | 0.40              |
| 85:l5:497:G:N2     | 85:l5:658:C:H42   | 2.19                     | 0.40              |
| 85:l5:679:C:C2     | 85:l5:680:G:C8    | 3.09                     | 0.40              |
| 85:l5:965:G:N3     | 85:l5:965:G:H2'   | 2.36                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 85:L5:1171:G:OP2  | 85:L5:1171:G:H8   | 2.04                     | 0.40              |
| 85:L5:1204:C:N4   | 85:L5:1205:G:O6   | 2.53                     | 0.40              |
| 85:L5:1441:C:N3   | 85:L5:1442:C:H5   | 2.19                     | 0.40              |
| 85:L5:1466:G:H2'  | 85:L5:1467:C:H6   | 1.86                     | 0.40              |
| 85:L5:1470:G:H2'  | 85:L5:1471:U:C6   | 2.55                     | 0.40              |
| 85:L5:1696:C:H2'  | 85:L5:1697:G:O4'  | 2.21                     | 0.40              |
| 85:L5:1962:A:H2   | 85:L5:2024:G:H21  | 1.69                     | 0.40              |
| 85:L5:2004:U:H2'  | 85:L5:2005:G:O4'  | 2.21                     | 0.40              |
| 85:L5:2394:G:O2'  | 85:L5:2819:U:O4   | 2.35                     | 0.40              |
| 85:L5:2500:U:C2   | 85:L5:2501:C:C5   | 3.10                     | 0.40              |
| 85:L5:2720:C:H2'  | 85:L5:2721:G:O4'  | 2.21                     | 0.40              |
| 85:L5:2756:G:C6   | 85:L5:2757:A:C6   | 3.10                     | 0.40              |
| 85:L5:3970:G:H4'  | 85:L5:4052:C:C4   | 2.57                     | 0.40              |
| 85:L5:4489:G:C6   | 85:L5:4708:A:C5   | 3.10                     | 0.40              |
| 85:L5:4499:G:N3   | 85:L5:4529:G:H1'  | 2.35                     | 0.40              |
| 85:L5:4689:U:O4   | 85:L5:4698:C:H4'  | 2.21                     | 0.40              |
| 85:L5:4889:G:C6   | 85:L5:4931:G:C5   | 3.10                     | 0.40              |
| 80:CB:108:HIS:O   | 80:CB:138:GLN:NE2 | 2.55                     | 0.40              |
| 80:CB:535:GLN:OE1 | 80:CB:535:GLN:N   | 2.54                     | 0.40              |
| 80:CB:828:SER:O   | 80:CB:830:ARG:NH2 | 2.51                     | 0.40              |
| 80:CB:836:ALA:O   | 80:CB:840:LYS:HG3 | 2.22                     | 0.40              |
| 2:SE:63:LYS:HD2   | 79:S2:502:C:O2    | 2.21                     | 0.40              |
| 3:SI:145:ILE:HD12 | 79:S2:190:G:H5'   | 2.03                     | 0.40              |
| 4:SL:124:ASP:OD2  | 4:SL:147:LYS:HA   | 2.21                     | 0.40              |
| 5:SX:36:LEU:HD21  | 79:S2:407:G:C6    | 2.56                     | 0.40              |
| 6:SG:30:LYS:HA    | 6:SG:30:LYS:HD3   | 1.83                     | 0.40              |
| 6:SG:44:GLU:N     | 6:SG:44:GLU:OE1   | 2.55                     | 0.40              |
| 6:SG:70:HIS:HB2   | 6:SG:98:ARG:HH22  | 1.86                     | 0.40              |
| 10:SA:5:LEU:O     | 10:SA:9:GLN:NE2   | 2.53                     | 0.40              |
| 10:SA:158:ASP:O   | 13:SV:66:ASP:HA   | 2.22                     | 0.40              |
| 11:SB:133:TYR:CE1 | 11:SB:221:PRO:HD2 | 2.56                     | 0.40              |
| 14:Sa:42:ARG:HD3  | 14:Sa:42:ARG:HA   | 1.89                     | 0.40              |
| 85:L5:4:G:H2'     | 85:L5:5:A:H8      | 1.86                     | 0.40              |
| 85:L5:314:G:C6    | 85:L5:324:A:C6    | 3.08                     | 0.40              |
| 85:L5:358:C:H2'   | 85:L5:359:A:C8    | 2.56                     | 0.40              |
| 85:L5:1197:C:H2'  | 85:L5:1198:G:C8   | 2.57                     | 0.40              |
| 85:L5:1490:G:H2'  | 85:L5:1491:A:H8   | 1.87                     | 0.40              |
| 85:L5:1537:A:H2'  | 85:L5:1538:U:C6   | 2.56                     | 0.40              |
| 85:L5:1575:A:H2'  | 85:L5:1576:G:C8   | 2.56                     | 0.40              |
| 85:L5:1839:U:P    | 27:LF:202:LYS:HZ2 | 2.44                     | 0.40              |
| 85:L5:2034:G:C4   | 85:L5:2035:C:C5   | 3.10                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 85:L5:2656:U:H5''  | 45:LZ:38:TYR:HB3   | 2.03                     | 0.40              |
| 85:L5:2748:C:O2'   | 52:Lg:65:MET:HE1   | 2.22                     | 0.40              |
| 85:L5:2901:G:H2'   | 85:L5:2902:G:H5''  | 2.04                     | 0.40              |
| 85:L5:3799:A:N3    | 85:L5:4506:C:O2'   | 2.50                     | 0.40              |
| 85:L5:3799:A:C4    | 42:LV:40:ILE:HD13  | 2.57                     | 0.40              |
| 85:L5:3856:A:H5''  | 36:LP:83:TRP:O     | 2.21                     | 0.40              |
| 85:L5:3949:A:O2'   | 85:L5:3950:U:H6    | 2.05                     | 0.40              |
| 85:L5:4085:A:C5    | 28:LG:56:LYS:HD2   | 2.56                     | 0.40              |
| 85:L5:4410:G:C6    | 85:L5:4433:G:C6    | 3.09                     | 0.40              |
| 85:L5:4530:U:H2'   | 85:L5:4531:U:C6    | 2.56                     | 0.40              |
| 85:L5:4603:C:H2'   | 85:L5:4604:G:H8    | 1.86                     | 0.40              |
| 85:L5:5005:G:H1'   | 85:L5:5042:A:N6    | 2.37                     | 0.40              |
| 85:L5:5055:G:C2    | 85:L5:5056:A:C5    | 3.09                     | 0.40              |
| 20:L7:38:U:H5'     | 20:L7:39:C:OP2     | 2.21                     | 0.40              |
| 20:L7:41:G:N2      | 20:L7:45:U:C2      | 2.89                     | 0.40              |
| 21:L8:12:G:C6      | 21:L8:13:G:N7      | 2.89                     | 0.40              |
| 21:L8:86:U:OP1     | 21:L8:86:U:H4'     | 2.20                     | 0.40              |
| 22:LA:29:LEU:HD12  | 22:LA:124:GLY:H    | 1.85                     | 0.40              |
| 23:LB:50:LYS:HB2   | 23:LB:345:LEU:HD11 | 2.03                     | 0.40              |
| 23:LB:148:LYS:HB2  | 23:LB:148:LYS:HE2  | 1.79                     | 0.40              |
| 23:LB:386:LYS:HA   | 23:LB:386:LYS:HD2  | 1.90                     | 0.40              |
| 24:LC:141:GLY:O    | 24:LC:182:LYS:NZ   | 2.54                     | 0.40              |
| 24:LC:147:VAL:O    | 62:Lr:73:PRO:HG2   | 2.20                     | 0.40              |
| 24:LC:163:LYS:HD2  | 24:LC:163:LYS:HA   | 1.83                     | 0.40              |
| 25:LD:41:LYS:HD3   | 25:LD:41:LYS:HA    | 1.77                     | 0.40              |
| 25:LD:47:PRO:HB3   | 25:LD:68:ARG:HH21  | 1.86                     | 0.40              |
| 26:LE:93:THR:HA    | 26:LE:106:VAL:HA   | 2.03                     | 0.40              |
| 27:LF:92:VAL:O     | 27:LF:93:ILE:HG13  | 2.21                     | 0.40              |
| 28:LG:156:VAL:O    | 28:LG:201:THR:OG1  | 2.26                     | 0.40              |
| 29:LH:76:HIS:O     | 29:LH:80:MET:HG3   | 2.21                     | 0.40              |
| 29:LH:134:CYS:SG   | 29:LH:135:SER:N    | 2.94                     | 0.40              |
| 30:LI:31:ILE:HG22  | 30:LI:66:GLU:HB2   | 2.02                     | 0.40              |
| 30:LI:41:ALA:HB1   | 30:LI:45:GLU:CG    | 2.51                     | 0.40              |
| 31:LJ:92:TYR:N     | 31:LJ:92:TYR:CD2   | 2.89                     | 0.40              |
| 32:LL:96:ILE:HD11  | 32:LL:117:LEU:HD23 | 2.02                     | 0.40              |
| 33:LM:9:VAL:HG11   | 33:LM:66:HIS:HB2   | 2.03                     | 0.40              |
| 34:LN:37:HIS:HD2   | 34:LN:63:ARG:HH11  | 1.69                     | 0.40              |
| 34:LN:53:TYR:CD2   | 34:LN:53:TYR:C     | 3.00                     | 0.40              |
| 34:LN:184:ILE:HG23 | 34:LN:194:ARG:NH2  | 2.36                     | 0.40              |
| 35:LO:174:LEU:O    | 35:LO:177:LEU:HB2  | 2.21                     | 0.40              |
| 38:LR:151:ARG:O    | 38:LR:154:LEU:HG   | 2.21                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 40:LT:124:THR:OG1  | 40:LT:125:TRP:N    | 2.54                     | 0.40              |
| 41:LU:19:LEU:HA    | 41:LU:74:SER:H     | 1.86                     | 0.40              |
| 45:LZ:4:PHE:CZ     | 48:Lc:39:ARG:HA    | 2.56                     | 0.40              |
| 45:LZ:123:LYS:NZ   | 45:LZ:124:THR:H    | 2.19                     | 0.40              |
| 51:Lf:23:GLU:OE1   | 51:Lf:23:GLU:N     | 2.54                     | 0.40              |
| 51:Lf:88:PHE:CE2   | 51:Lf:92:LEU:HD11  | 2.57                     | 0.40              |
| 57:Ll:14:ALA:O     | 57:Ll:18:LYS:HG3   | 2.21                     | 0.40              |
| 64:SR:93:GLN:C     | 64:SR:95:ILE:H     | 2.29                     | 0.40              |
| 65:SD:65:ARG:O     | 65:SD:68:GLU:HG2   | 2.21                     | 0.40              |
| 65:SD:69:LEU:HD12  | 65:SD:69:LEU:HA    | 1.93                     | 0.40              |
| 65:SD:139:SER:O    | 65:SD:183:GLY:N    | 2.49                     | 0.40              |
| 65:SD:162:ASP:N    | 65:SD:163:PRO:HD2  | 2.36                     | 0.40              |
| 66:SF:28:VAL:HG13  | 66:SF:110:GLN:HA   | 2.02                     | 0.40              |
| 66:SF:49:LEU:HD23  | 66:SF:50:PRO:HD2   | 2.04                     | 0.40              |
| 66:SF:103:LEU:HD21 | 66:SF:178:ILE:HD13 | 2.04                     | 0.40              |
| 67:SK:21:MET:HE3   | 67:SK:21:MET:HB2   | 1.97                     | 0.40              |
| 68:SP:29:SER:OG    | 68:SP:30:TYR:N     | 2.54                     | 0.40              |
| 69:SQ:13:PHE:HE1   | 69:SQ:15:ARG:HD2   | 1.86                     | 0.40              |
| 69:SQ:25:CYS:SG    | 69:SQ:68:ILE:HD13  | 2.61                     | 0.40              |
| 71:ST:74:SER:O     | 71:ST:78:ILE:HG22  | 2.21                     | 0.40              |
| 72:SU:81:GLN:O     | 72:SU:82:MET:HE2   | 2.22                     | 0.40              |
| 73:Sc:18:LEU:CD1   | 73:Sc:29:GLN:HB2   | 2.51                     | 0.40              |
| 75:Sg:147:HIS:CE1  | 75:Sg:175:LYS:HG2  | 2.57                     | 0.40              |
| 78:Sf:141:CYS:N    | 78:Sf:146:LEU:O    | 2.36                     | 0.40              |
| 79:S2:26:U:C2      | 79:S2:27:A:C8      | 3.09                     | 0.40              |
| 79:S2:91:A:H5''    | 79:S2:92:A:H5''    | 2.04                     | 0.40              |
| 79:S2:108:G:C5     | 79:S2:109:U:C4     | 3.09                     | 0.40              |
| 79:S2:183:G:C2     | 79:S2:184:G:C8     | 3.08                     | 0.40              |
| 79:S2:476:A:H3'    | 79:S2:477:G:H8     | 1.86                     | 0.40              |
| 79:S2:793:G:H2'    | 79:S2:794:A:C8     | 2.51                     | 0.40              |
| 79:S2:851:C:O3'    | 79:S2:852:G:H8     | 2.03                     | 0.40              |
| 79:S2:1411:G:H2'   | 79:S2:1412:C:O4'   | 2.20                     | 0.40              |
| 79:S2:1604:G:C5    | 79:S2:1605:G:C5    | 3.09                     | 0.40              |
| 82:PE:2:C:H2'      | 82:PE:3:C:H6       | 1.87                     | 0.40              |
| 87:LW:31:PHE:CD2   | 87:LW:37:GLU:HG3   | 2.57                     | 0.40              |
| 1:CH:74:THR:OG1    | 1:CH:77:VAL:HG23   | 2.21                     | 0.40              |
| 1:CH:133:ARG:NH1   | 79:S2:533:A:O2'    | 2.51                     | 0.40              |
| 1:cH:100:ASN:OD1   | 79:s2:609:U:H1'    | 2.22                     | 0.40              |
| 2:sE:182:MET:N     | 2:sE:226:PHE:O     | 2.54                     | 0.40              |
| 3:sI:5:ARG:HH12    | 79:s2:380:G:H21    | 1.70                     | 0.40              |
| 3:sI:55:TYR:HD2    | 79:s2:305:U:C2     | 2.40                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:sI:65:PHE:HB2    | 3:sI:109:TYR:OH    | 2.22                     | 0.40              |
| 4:sL:91:ASP:OD2    | 4:sL:91:ASP:N      | 2.43                     | 0.40              |
| 5:sX:5:ARG:HH22    | 79:s2:1157:G:C4'   | 2.34                     | 0.40              |
| 11:sB:116:LYS:HA   | 79:s2:988:C:H5'    | 2.04                     | 0.40              |
| 14:sa:41:ILE:HG22  | 14:sa:41:ILE:O     | 2.21                     | 0.40              |
| 14:sa:82:LYS:NZ    | 79:s2:1210:G:OP1   | 2.48                     | 0.40              |
| 15:sC:60:TRP:CH2   | 15:sC:93:ILE:HG22  | 2.57                     | 0.40              |
| 15:sC:84:PHE:HB3   | 15:sC:86:LEU:HD22  | 2.03                     | 0.40              |
| 15:sC:139:LEU:HD23 | 15:sC:139:LEU:HA   | 1.88                     | 0.40              |
| 16:sN:18:TYR:HD1   | 18:sW:56:HIS:NE2   | 2.19                     | 0.40              |
| 21:l8:1:C:C4       | 21:l8:2:G:C5       | 3.09                     | 0.40              |
| 23:lB:257:TRP:C    | 23:lB:257:TRP:CD1  | 2.99                     | 0.40              |
| 26:lE:95:PRO:HG2   | 85:l5:687:U:N3     | 2.37                     | 0.40              |
| 26:lE:188:ARG:NH2  | 85:l5:4941:G:OP2   | 2.54                     | 0.40              |
| 27:lF:46:ARG:HE    | 85:l5:1705:G:N2    | 2.19                     | 0.40              |
| 28:lG:96:LEU:HD12  | 28:lG:96:LEU:HA    | 1.93                     | 0.40              |
| 29:lH:40:HIS:ND1   | 85:l5:4702:G:H5'   | 2.36                     | 0.40              |
| 29:lH:43:VAL:HG21  | 29:lH:73:ILE:HD13  | 2.04                     | 0.40              |
| 29:lH:140:GLN:NE2  | 29:lH:142:ASP:H    | 2.19                     | 0.40              |
| 30:lI:73:ASN:O     | 30:lI:77:VAL:HG13  | 2.22                     | 0.40              |
| 32:lL:57:PRO:HD3   | 32:lL:75:GLY:HA2   | 2.04                     | 0.40              |
| 32:lL:126:LEU:HD11 | 53:lh:117:ARG:NH2  | 2.36                     | 0.40              |
| 34:lN:114:ARG:O    | 34:lN:135:ILE:HG22 | 2.20                     | 0.40              |
| 47:lb:107:ARG:NH2  | 85:l5:1268:G:H3'   | 2.32                     | 0.40              |
| 49:ld:23:ARG:HD2   | 49:ld:25:TYR:OH    | 2.22                     | 0.40              |
| 53:lh:32:ARG:O     | 53:lh:35:LYS:HB3   | 2.22                     | 0.40              |
| 58:lm:78:ILE:O     | 58:lm:78:ILE:HG13  | 2.20                     | 0.40              |
| 61:lp:9:GLY:HA3    | 61:lp:27:LYS:NZ    | 2.37                     | 0.40              |
| 62:lr:3:ALA:HA     | 62:lr:6:GLN:NE2    | 2.37                     | 0.40              |
| 63:lz:196:LYS:HA   | 63:lz:196:LYS:HD2  | 1.84                     | 0.40              |
| 64:sR:17:ILE:CD1   | 64:sR:54:VAL:HG13  | 2.51                     | 0.40              |
| 64:sR:104:GLU:O    | 64:sR:107:LYS:HB2  | 2.22                     | 0.40              |
| 65:sD:7:LYS:HZ2    | 79:s2:1579:A:P     | 2.44                     | 0.40              |
| 65:sD:40:ARG:HG2   | 65:sD:49:ILE:HD11  | 2.02                     | 0.40              |
| 65:sD:106:ARG:CZ   | 65:sD:173:ARG:HD3  | 2.51                     | 0.40              |
| 66:sF:140:ASP:OD2  | 73:sc:46:VAL:HG22  | 2.20                     | 0.40              |
| 67:sK:16:PHE:CZ    | 67:sK:80:ARG:NH2   | 2.89                     | 0.40              |
| 68:sP:84:ILE:O     | 68:sP:86:LEU:HD23  | 2.22                     | 0.40              |
| 69:sQ:43:GLU:OE1   | 69:sQ:77:HIS:HB3   | 2.22                     | 0.40              |
| 71:sT:39:LEU:HD11  | 71:sT:52:TRP:CE3   | 2.57                     | 0.40              |
| 71:sT:128:GLN:HA   | 71:sT:131:LEU:HB2  | 2.01                     | 0.40              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 77:sZ:90:GLU:O    | 77:sZ:93:SER:OG    | 2.32                     | 0.40              |
| 79:s2:339:A:H2'   | 79:s2:340:C:H5     | 1.86                     | 0.40              |
| 79:s2:374:G:O6    | 79:s2:385:G:O6     | 2.39                     | 0.40              |
| 79:s2:610:G:C6    | 79:s2:634:A:C6     | 3.10                     | 0.40              |
| 79:s2:662:G:H5'   | 79:s2:1156:U:O2    | 2.21                     | 0.40              |
| 79:s2:1056:U:H2'  | 79:s2:1057:C:O4'   | 2.22                     | 0.40              |
| 79:s2:1077:A:C6   | 79:s2:1078:C:C5    | 3.09                     | 0.40              |
| 79:s2:1289:U:H2'  | 79:s2:1290:G:C8    | 2.56                     | 0.40              |
| 79:s2:1311:C:H2'  | 79:s2:1312:G:O4'   | 2.22                     | 0.40              |
| 79:s2:1563:G:C6   | 79:s2:1573:G:C6    | 3.09                     | 0.40              |
| 79:s2:1753:C:H5'  | 79:s2:1780:G:H1    | 1.86                     | 0.40              |
| 79:s2:1788:A:H2'  | 79:s2:1789:G:O4'   | 2.21                     | 0.40              |
| 79:s2:1812:U:N3   | 79:s2:1814:G:O6    | 2.54                     | 0.40              |
| 80:cB:117:ALA:O   | 80:cB:121:VAL:HG22 | 2.21                     | 0.40              |
| 80:cB:830:ARG:CA  | 80:cB:831:PRO:HG3  | 2.52                     | 0.40              |
| 83:ls:40:MET:HE2  | 85:l5:1999:A:N6    | 2.37                     | 0.40              |
| 83:ls:106:LYS:HD2 | 83:ls:106:LYS:HA   | 1.49                     | 0.40              |
| 85:l5:189:G:C2    | 85:l5:253:G:N1     | 2.90                     | 0.40              |
| 85:l5:229:G:C2    | 85:l5:240:G:C2     | 3.09                     | 0.40              |
| 85:l5:230:G:N1    | 85:l5:239:C:N3     | 2.70                     | 0.40              |
| 85:l5:437:G:C5    | 85:l5:1311:G:C2    | 3.09                     | 0.40              |
| 85:l5:468:U:C5    | 85:l5:469:C:H5     | 2.39                     | 0.40              |
| 85:l5:1296:G:HO2' | 85:l5:1297:U:C4'   | 2.35                     | 0.40              |
| 85:l5:1339:U:O4   | 85:l5:1518:A:H1'   | 2.22                     | 0.40              |
| 85:l5:1550:G:H2'  | 85:l5:1551:C:H6    | 1.86                     | 0.40              |
| 85:l5:1596:U:O2   | 85:l5:3861:A:O2'   | 2.29                     | 0.40              |
| 85:l5:1705:G:H3'  | 85:l5:1705:G:N3    | 2.36                     | 0.40              |
| 85:l5:2012:A:H2'  | 85:l5:2013:A:O4'   | 2.22                     | 0.40              |
| 85:l5:2092:G:C2   | 85:l5:2262:G:C6    | 3.10                     | 0.40              |
| 85:l5:2369:U:OP1  | 85:l5:2827:G:N2    | 2.53                     | 0.40              |
| 85:l5:2391:G:H2'  | 85:l5:2392:C:C6    | 2.56                     | 0.40              |
| 85:l5:2501:C:H2'  | 85:l5:2502:G:H8    | 1.84                     | 0.40              |
| 85:l5:2667:C:H2'  | 85:l5:2668:G:H8    | 1.87                     | 0.40              |
| 85:l5:2845:A:C8   | 85:l5:4671:C:N4    | 2.90                     | 0.40              |
| 85:l5:3619:G:H22  | 85:l5:3624:A:H1'   | 1.85                     | 0.40              |
| 85:l5:3706:C:H2'  | 85:l5:3707:U:O4'   | 2.22                     | 0.40              |
| 85:l5:3708:C:N4   | 85:l5:3742:G:O6    | 2.37                     | 0.40              |
| 85:l5:3784:A:HO2' | 85:l5:3785:A:H3'   | 1.85                     | 0.40              |
| 85:l5:3856:A:C4   | 85:l5:3857:G:C8    | 3.09                     | 0.40              |
| 85:l5:4414:A:H2'  | 85:l5:4422:A:C6    | 2.57                     | 0.40              |
| 80:CB:219:HIS:HB2 | 80:CB:221:TRP:CD1  | 2.57                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 80:CB:430:MET:HE3  | 80:CB:430:MET:HB2  | 1.93                     | 0.40              |
| 80:CB:801:ARG:HB3  | 85:L5:4605:A:C5    | 2.57                     | 0.40              |
| 2:SE:6:LYS:O       | 2:SE:30:ARG:NH2    | 2.55                     | 0.40              |
| 2:SE:60:GLU:O      | 2:SE:64:ILE:HG12   | 2.21                     | 0.40              |
| 4:SL:22:ARG:HH22   | 4:SL:26:GLY:C      | 2.30                     | 0.40              |
| 4:SL:31:GLU:CD     | 4:SL:31:GLU:C      | 2.89                     | 0.40              |
| 5:SX:20:GLN:O      | 79:S2:658:U:N3     | 2.55                     | 0.40              |
| 6:SG:92:ARG:O      | 79:S2:453:C:O2'    | 2.29                     | 0.40              |
| 8:SY:18:LEU:O      | 8:SY:20:ARG:HB3    | 2.21                     | 0.40              |
| 8:SY:33:ALA:HA     | 79:S2:581:U:O2'    | 2.22                     | 0.40              |
| 8:SY:44:LEU:HD12   | 8:SY:55:ILE:HD11   | 2.03                     | 0.40              |
| 10:SA:24:HIS:HB3   | 10:SA:51:LEU:HD21  | 2.04                     | 0.40              |
| 10:SA:68:ILE:HD12  | 10:SA:68:ILE:O     | 2.22                     | 0.40              |
| 10:SA:180:ARG:HH22 | 10:SA:184:ARG:NE   | 2.19                     | 0.40              |
| 11:SB:71:LEU:HD22  | 11:SB:84:PHE:HE1   | 1.85                     | 0.40              |
| 11:SB:206:PRO:O    | 11:SB:207:LEU:HD23 | 2.21                     | 0.40              |
| 15:SC:147:VAL:O    | 15:SC:151:ILE:HG12 | 2.21                     | 0.40              |
| 16:SN:72:LEU:HD12  | 16:SN:72:LEU:HA    | 1.83                     | 0.40              |
| 85:L5:37:U:H5''    | 46:La:32:ARG:HD2   | 2.03                     | 0.40              |
| 85:L5:176:G:C6     | 85:L5:261:G:C6     | 3.09                     | 0.40              |
| 85:L5:186:G:OP2    | 85:L5:186:G:H8     | 2.05                     | 0.40              |
| 85:L5:229:G:C2     | 85:L5:240:G:C2     | 3.09                     | 0.40              |
| 85:L5:282:C:C2     | 85:L5:283:G:C8     | 3.10                     | 0.40              |
| 85:L5:406:C:HO2'   | 85:L5:407:A:P      | 2.42                     | 0.40              |
| 85:L5:426:A:H2'    | 85:L5:427:A:C8     | 2.57                     | 0.40              |
| 85:L5:690:C:H2'    | 85:L5:691:C:H6     | 1.85                     | 0.40              |
| 85:L5:708:G:H2'    | 85:L5:709:C:C6     | 2.57                     | 0.40              |
| 85:L5:920:C:C2     | 85:L5:921:C:C5     | 3.09                     | 0.40              |
| 85:L5:1220:G:H2'   | 85:L5:1221:G:C8    | 2.57                     | 0.40              |
| 85:L5:1255:A:N6    | 85:L5:1257:A:O2'   | 2.54                     | 0.40              |
| 85:L5:1274:A:H8    | 85:L5:1274:A:OP2   | 2.04                     | 0.40              |
| 85:L5:1518:A:H61   | 32:LL:19:GLN:HE22  | 1.69                     | 0.40              |
| 85:L5:1923:A:P     | 39:LS:160:ARG:HH22 | 2.44                     | 0.40              |
| 85:L5:2308:A:H2'   | 85:L5:2309:G:O4'   | 2.20                     | 0.40              |
| 85:L5:2315:G:C2    | 85:L5:2325:C:C2    | 3.09                     | 0.40              |
| 85:L5:2635:U:C2    | 85:L5:2636:U:C5    | 3.10                     | 0.40              |
| 85:L5:2675:G:H1'   | 85:L5:2676:A:OP2   | 2.22                     | 0.40              |
| 85:L5:3670:C:O2'   | 34:LN:72:LYS:HD3   | 2.21                     | 0.40              |
| 85:L5:3969:G:N1    | 85:L5:4053:A:N3    | 2.69                     | 0.40              |
| 85:L5:3971:G:N1    | 85:L5:4050:A:N7    | 2.67                     | 0.40              |
| 85:L5:4089:G:C6    | 85:L5:4090:G:C6    | 3.10                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 85:L5:4342:C:H2'   | 85:L5:4343:U:H6    | 1.86                     | 0.40              |
| 85:L5:4354:U:N3    | 46:La:61:TYR:O     | 2.54                     | 0.40              |
| 85:L5:4640:C:H2'   | 85:L5:4641:U:H6    | 1.87                     | 0.40              |
| 85:L5:4664:A:C4    | 85:L5:4665:A:C8    | 3.09                     | 0.40              |
| 85:L5:4723:A:H2'   | 85:L5:4724:A:H8    | 1.84                     | 0.40              |
| 85:L5:4929:C:O4'   | 33:LM:118:MET:HE2  | 2.22                     | 0.40              |
| 85:L5:4976:U:N3    | 23:LB:342:LYS:O    | 2.55                     | 0.40              |
| 85:L5:4991:U:H2'   | 85:L5:4992:G:H8    | 1.86                     | 0.40              |
| 23:LB:108:GLU:OE1  | 23:LB:109:HIS:CD2  | 2.75                     | 0.40              |
| 26:LE:243:THR:OG1  | 26:LE:246:ARG:HG3  | 2.21                     | 0.40              |
| 28:LG:208:ASN:O    | 28:LG:212:LYS:HG3  | 2.22                     | 0.40              |
| 29:LH:127:ARG:HE   | 29:LH:127:ARG:HB2  | 1.76                     | 0.40              |
| 31:LJ:88:LYS:HG2   | 31:LJ:92:TYR:CE2   | 2.56                     | 0.40              |
| 34:LN:200:LEU:HD23 | 34:LN:200:LEU:HA   | 1.81                     | 0.40              |
| 35:LO:77:SER:N     | 35:LO:106:ASP:OD1  | 2.49                     | 0.40              |
| 36:LP:110:ASP:OD1  | 36:LP:110:ASP:N    | 2.54                     | 0.40              |
| 37:LQ:21:GLN:HE22  | 37:LQ:26:ARG:HH21  | 1.69                     | 0.40              |
| 37:LQ:170:LYS:HB2  | 37:LQ:170:LYS:HE2  | 1.76                     | 0.40              |
| 41:LU:41:GLN:HA    | 41:LU:44:GLN:HE22  | 1.86                     | 0.40              |
| 41:LU:107:LYS:C    | 41:LU:108:GLU:HG3  | 2.47                     | 0.40              |
| 43:LX:37:LYS:HA    | 43:LX:38:LYS:HA    | 1.68                     | 0.40              |
| 43:LX:72:ASP:O     | 43:LX:76:ILE:HD12  | 2.22                     | 0.40              |
| 45:LZ:13:VAL:HG23  | 45:LZ:21:ARG:O     | 2.21                     | 0.40              |
| 45:LZ:46:ILE:HD11  | 45:LZ:68:ILE:HB    | 2.04                     | 0.40              |
| 51:Lf:28:LEU:HD13  | 51:Lf:28:LEU:HA    | 1.87                     | 0.40              |
| 54:Li:12:ASN:ND2   | 54:Li:16:LYS:HE3   | 2.35                     | 0.40              |
| 62:Lr:47:LYS:HB3   | 62:Lr:102:TYR:CZ   | 2.56                     | 0.40              |
| 64:SR:125:GLY:N    | 79:S2:1109:C:O2    | 2.49                     | 0.40              |
| 66:SF:108:PRO:HA   | 66:SF:111:VAL:HG12 | 2.04                     | 0.40              |
| 66:SF:112:LEU:HD22 | 66:SF:177:LEU:HD12 | 2.03                     | 0.40              |
| 66:SF:201:LYS:HD3  | 66:SF:204:ARG:HB2  | 2.02                     | 0.40              |
| 72:SU:88:LEU:O     | 72:SU:89:ILE:HD13  | 2.22                     | 0.40              |
| 74:Sd:54:LYS:HZ1   | 79:S2:1482:C:P     | 2.45                     | 0.40              |
| 75:Sg:44:LYS:HG3   | 75:Sg:46:THR:HG23  | 2.03                     | 0.40              |
| 79:S2:97:U:H2'     | 79:S2:98:C:C6      | 2.56                     | 0.40              |
| 79:S2:377:G:N3     | 79:S2:377:G:H2'    | 2.36                     | 0.40              |
| 79:S2:613:G:O2'    | 79:S2:626:G:H4'    | 2.22                     | 0.40              |
| 79:S2:1142:G:H2'   | 79:S2:1144:A:OP2   | 2.22                     | 0.40              |
| 79:S2:1577:G:O2'   | 79:S2:1579:A:N3    | 2.52                     | 0.40              |
| 83:Ls:14:PHE:CE1   | 83:Ls:18:ILE:HG13  | 2.55                     | 0.40              |
| 83:Ls:54:LEU:HD23  | 83:Ls:54:LEU:HA    | 1.76                     | 0.40              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 83:Ls:78:LEU:HB3 | 83:Ls:82:ILE:HD11 | 2.03                     | 0.40              |
| 84:Lt:29:ALA:N   | 84:Lt:30:PRO:HD2  | 2.37                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 1   | CH    | 123/125 (98%) | 109 (89%) | 12 (10%) | 2 (2%)   | 7           | 36  |
| 1   | cH    | 123/125 (98%) | 106 (86%) | 16 (13%) | 1 (1%)   | 16          | 50  |
| 2   | SE    | 260/262 (99%) | 246 (95%) | 14 (5%)  | 0        | 100         | 100 |
| 2   | sE    | 260/262 (99%) | 243 (94%) | 16 (6%)  | 1 (0%)   | 30          | 62  |
| 3   | SI    | 204/206 (99%) | 191 (94%) | 13 (6%)  | 0        | 100         | 100 |
| 3   | sI    | 204/206 (99%) | 191 (94%) | 13 (6%)  | 0        | 100         | 100 |
| 4   | SL    | 151/153 (99%) | 137 (91%) | 14 (9%)  | 0        | 100         | 100 |
| 4   | sL    | 151/153 (99%) | 136 (90%) | 15 (10%) | 0        | 100         | 100 |
| 5   | SX    | 139/141 (99%) | 124 (89%) | 14 (10%) | 1 (1%)   | 18          | 52  |
| 5   | sX    | 139/141 (99%) | 121 (87%) | 17 (12%) | 1 (1%)   | 18          | 52  |
| 6   | SG    | 235/237 (99%) | 219 (93%) | 16 (7%)  | 0        | 100         | 100 |
| 6   | sG    | 235/237 (99%) | 220 (94%) | 14 (6%)  | 1 (0%)   | 30          | 62  |
| 7   | SJ    | 183/185 (99%) | 168 (92%) | 15 (8%)  | 0        | 100         | 100 |
| 7   | sJ    | 183/185 (99%) | 171 (93%) | 12 (7%)  | 0        | 100         | 100 |
| 8   | SY    | 129/131 (98%) | 116 (90%) | 13 (10%) | 0        | 100         | 100 |
| 8   | sY    | 129/131 (98%) | 117 (91%) | 12 (9%)  | 0        | 100         | 100 |
| 9   | se    | 56/58 (97%)   | 47 (84%)  | 9 (16%)  | 0        | 100         | 100 |
| 10  | SA    | 219/221 (99%) | 201 (92%) | 18 (8%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed       | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|----------------|-----------|----------|----------|-------------|-----|
| 10  | sA    | 219/221 (99%)  | 196 (90%) | 23 (10%) | 0        | 100         | 100 |
| 11  | SB    | 212/214 (99%)  | 204 (96%) | 8 (4%)   | 0        | 100         | 100 |
| 11  | sB    | 212/214 (99%)  | 199 (94%) | 13 (6%)  | 0        | 100         | 100 |
| 12  | SH    | 182/189 (96%)  | 159 (87%) | 23 (13%) | 0        | 100         | 100 |
| 12  | sH    | 182/189 (96%)  | 156 (86%) | 26 (14%) | 0        | 100         | 100 |
| 13  | SV    | 81/83 (98%)    | 74 (91%)  | 7 (9%)   | 0        | 100         | 100 |
| 13  | sV    | 81/83 (98%)    | 70 (86%)  | 11 (14%) | 0        | 100         | 100 |
| 14  | Sa    | 100/102 (98%)  | 81 (81%)  | 18 (18%) | 1 (1%)   | 12          | 45  |
| 14  | sa    | 100/102 (98%)  | 90 (90%)  | 10 (10%) | 0        | 100         | 100 |
| 15  | SC    | 220/222 (99%)  | 202 (92%) | 18 (8%)  | 0        | 100         | 100 |
| 15  | sC    | 220/222 (99%)  | 203 (92%) | 17 (8%)  | 0        | 100         | 100 |
| 16  | SN    | 148/150 (99%)  | 142 (96%) | 6 (4%)   | 0        | 100         | 100 |
| 16  | sN    | 148/150 (99%)  | 143 (97%) | 5 (3%)   | 0        | 100         | 100 |
| 17  | SO    | 138/140 (99%)  | 125 (91%) | 13 (9%)  | 0        | 100         | 100 |
| 17  | sO    | 138/140 (99%)  | 124 (90%) | 14 (10%) | 0        | 100         | 100 |
| 18  | SW    | 127/129 (98%)  | 117 (92%) | 10 (8%)  | 0        | 100         | 100 |
| 18  | sW    | 127/129 (98%)  | 117 (92%) | 10 (8%)  | 0        | 100         | 100 |
| 19  | Sb    | 81/83 (98%)    | 70 (86%)  | 11 (14%) | 0        | 100         | 100 |
| 19  | sb    | 81/83 (98%)    | 69 (85%)  | 12 (15%) | 0        | 100         | 100 |
| 22  | LA    | 246/248 (99%)  | 219 (89%) | 27 (11%) | 0        | 100         | 100 |
| 22  | lA    | 246/248 (99%)  | 225 (92%) | 21 (8%)  | 0        | 100         | 100 |
| 23  | LB    | 400/402 (100%) | 364 (91%) | 36 (9%)  | 0        | 100         | 100 |
| 23  | lB    | 400/402 (100%) | 371 (93%) | 29 (7%)  | 0        | 100         | 100 |
| 24  | LC    | 366/368 (100%) | 347 (95%) | 19 (5%)  | 0        | 100         | 100 |
| 24  | lC    | 366/368 (100%) | 340 (93%) | 26 (7%)  | 0        | 100         | 100 |
| 25  | LD    | 291/293 (99%)  | 279 (96%) | 12 (4%)  | 0        | 100         | 100 |
| 25  | lD    | 291/293 (99%)  | 271 (93%) | 20 (7%)  | 0        | 100         | 100 |
| 26  | LE    | 232/247 (94%)  | 212 (91%) | 20 (9%)  | 0        | 100         | 100 |
| 26  | lE    | 232/247 (94%)  | 210 (90%) | 22 (10%) | 0        | 100         | 100 |
| 27  | LF    | 223/225 (99%)  | 211 (95%) | 12 (5%)  | 0        | 100         | 100 |
| 27  | lF    | 223/225 (99%)  | 211 (95%) | 12 (5%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 28  | LG    | 239/241 (99%) | 224 (94%) | 15 (6%)  | 0        | 100         | 100 |
| 28  | IG    | 239/241 (99%) | 224 (94%) | 15 (6%)  | 0        | 100         | 100 |
| 29  | LH    | 188/190 (99%) | 174 (93%) | 14 (7%)  | 0        | 100         | 100 |
| 29  | IH    | 188/190 (99%) | 173 (92%) | 15 (8%)  | 0        | 100         | 100 |
| 30  | LI    | 198/213 (93%) | 183 (92%) | 15 (8%)  | 0        | 100         | 100 |
| 30  | II    | 198/213 (93%) | 188 (95%) | 10 (5%)  | 0        | 100         | 100 |
| 31  | LJ    | 174/176 (99%) | 158 (91%) | 16 (9%)  | 0        | 100         | 100 |
| 31  | IJ    | 174/176 (99%) | 155 (89%) | 19 (11%) | 0        | 100         | 100 |
| 32  | LL    | 208/210 (99%) | 190 (91%) | 18 (9%)  | 0        | 100         | 100 |
| 32  | IL    | 208/210 (99%) | 191 (92%) | 17 (8%)  | 0        | 100         | 100 |
| 33  | LM    | 137/139 (99%) | 127 (93%) | 9 (7%)   | 1 (1%)   | 18          | 52  |
| 33  | IM    | 137/139 (99%) | 126 (92%) | 10 (7%)  | 1 (1%)   | 18          | 52  |
| 34  | LN    | 201/203 (99%) | 184 (92%) | 16 (8%)  | 1 (0%)   | 24          | 59  |
| 34  | IN    | 201/203 (99%) | 190 (94%) | 10 (5%)  | 1 (0%)   | 24          | 59  |
| 35  | LO    | 199/201 (99%) | 191 (96%) | 8 (4%)   | 0        | 100         | 100 |
| 35  | IO    | 199/201 (99%) | 190 (96%) | 9 (4%)   | 0        | 100         | 100 |
| 36  | LP    | 151/153 (99%) | 140 (93%) | 11 (7%)  | 0        | 100         | 100 |
| 36  | IP    | 151/153 (99%) | 138 (91%) | 13 (9%)  | 0        | 100         | 100 |
| 37  | LQ    | 185/187 (99%) | 175 (95%) | 10 (5%)  | 0        | 100         | 100 |
| 37  | IQ    | 185/187 (99%) | 175 (95%) | 10 (5%)  | 0        | 100         | 100 |
| 38  | LR    | 185/187 (99%) | 179 (97%) | 6 (3%)   | 0        | 100         | 100 |
| 38  | IR    | 185/187 (99%) | 175 (95%) | 10 (5%)  | 0        | 100         | 100 |
| 39  | LS    | 173/175 (99%) | 160 (92%) | 13 (8%)  | 0        | 100         | 100 |
| 39  | IS    | 173/175 (99%) | 159 (92%) | 14 (8%)  | 0        | 100         | 100 |
| 40  | LT    | 157/159 (99%) | 149 (95%) | 8 (5%)   | 0        | 100         | 100 |
| 40  | IT    | 157/159 (99%) | 143 (91%) | 14 (9%)  | 0        | 100         | 100 |
| 41  | LU    | 99/101 (98%)  | 84 (85%)  | 15 (15%) | 0        | 100         | 100 |
| 41  | IU    | 99/101 (98%)  | 81 (82%)  | 18 (18%) | 0        | 100         | 100 |
| 42  | LV    | 129/131 (98%) | 121 (94%) | 8 (6%)   | 0        | 100         | 100 |
| 42  | IV    | 129/131 (98%) | 119 (92%) | 10 (8%)  | 0        | 100         | 100 |
| 43  | LX    | 118/120 (98%) | 114 (97%) | 4 (3%)   | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 43  | IX    | 118/120 (98%) | 113 (96%) | 5 (4%)   | 0        | 100         | 100 |
| 44  | LY    | 132/134 (98%) | 130 (98%) | 2 (2%)   | 0        | 100         | 100 |
| 44  | IY    | 132/134 (98%) | 128 (97%) | 4 (3%)   | 0        | 100         | 100 |
| 45  | LZ    | 133/135 (98%) | 123 (92%) | 10 (8%)  | 0        | 100         | 100 |
| 45  | IZ    | 133/135 (98%) | 120 (90%) | 13 (10%) | 0        | 100         | 100 |
| 46  | La    | 145/147 (99%) | 137 (94%) | 8 (6%)   | 0        | 100         | 100 |
| 46  | la    | 145/147 (99%) | 137 (94%) | 8 (6%)   | 0        | 100         | 100 |
| 47  | Lb    | 105/121 (87%) | 95 (90%)  | 10 (10%) | 0        | 100         | 100 |
| 47  | lb    | 105/121 (87%) | 94 (90%)  | 11 (10%) | 0        | 100         | 100 |
| 48  | Lc    | 96/98 (98%)   | 89 (93%)  | 7 (7%)   | 0        | 100         | 100 |
| 48  | lc    | 96/98 (98%)   | 90 (94%)  | 6 (6%)   | 0        | 100         | 100 |
| 49  | Ld    | 105/107 (98%) | 98 (93%)  | 7 (7%)   | 0        | 100         | 100 |
| 49  | ld    | 105/107 (98%) | 101 (96%) | 4 (4%)   | 0        | 100         | 100 |
| 50  | Le    | 126/128 (98%) | 119 (94%) | 7 (6%)   | 0        | 100         | 100 |
| 50  | le    | 126/128 (98%) | 116 (92%) | 10 (8%)  | 0        | 100         | 100 |
| 51  | Lf    | 107/109 (98%) | 97 (91%)  | 10 (9%)  | 0        | 100         | 100 |
| 51  | lf    | 107/109 (98%) | 97 (91%)  | 10 (9%)  | 0        | 100         | 100 |
| 52  | Lg    | 112/114 (98%) | 107 (96%) | 5 (4%)   | 0        | 100         | 100 |
| 52  | lg    | 112/114 (98%) | 100 (89%) | 12 (11%) | 0        | 100         | 100 |
| 53  | Lh    | 120/122 (98%) | 116 (97%) | 4 (3%)   | 0        | 100         | 100 |
| 53  | lh    | 120/122 (98%) | 119 (99%) | 1 (1%)   | 0        | 100         | 100 |
| 54  | Li    | 100/102 (98%) | 96 (96%)  | 4 (4%)   | 0        | 100         | 100 |
| 54  | li    | 100/102 (98%) | 97 (97%)  | 3 (3%)   | 0        | 100         | 100 |
| 55  | Lj    | 84/86 (98%)   | 76 (90%)  | 8 (10%)  | 0        | 100         | 100 |
| 55  | lj    | 84/86 (98%)   | 73 (87%)  | 11 (13%) | 0        | 100         | 100 |
| 56  | Lk    | 67/69 (97%)   | 65 (97%)  | 2 (3%)   | 0        | 100         | 100 |
| 56  | lk    | 67/69 (97%)   | 64 (96%)  | 3 (4%)   | 0        | 100         | 100 |
| 57  | Ll    | 48/50 (96%)   | 43 (90%)  | 5 (10%)  | 0        | 100         | 100 |
| 57  | ll    | 48/50 (96%)   | 46 (96%)  | 2 (4%)   | 0        | 100         | 100 |
| 58  | Lm    | 50/52 (96%)   | 49 (98%)  | 1 (2%)   | 0        | 100         | 100 |
| 58  | lm    | 50/52 (96%)   | 48 (96%)  | 2 (4%)   | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 59  | Ln    | 22/24 (92%)   | 22 (100%) | 0        | 0        | 100         | 100 |
| 59  | ln    | 22/24 (92%)   | 22 (100%) | 0        | 0        | 100         | 100 |
| 60  | Lo    | 103/105 (98%) | 94 (91%)  | 9 (9%)   | 0        | 100         | 100 |
| 60  | lo    | 103/105 (98%) | 99 (96%)  | 4 (4%)   | 0        | 100         | 100 |
| 61  | Lp    | 89/91 (98%)   | 84 (94%)  | 5 (6%)   | 0        | 100         | 100 |
| 61  | lp    | 89/91 (98%)   | 82 (92%)  | 7 (8%)   | 0        | 100         | 100 |
| 62  | Lr    | 123/125 (98%) | 116 (94%) | 7 (6%)   | 0        | 100         | 100 |
| 62  | lr    | 123/125 (98%) | 110 (89%) | 13 (11%) | 0        | 100         | 100 |
| 63  | Lz    | 215/217 (99%) | 166 (77%) | 49 (23%) | 0        | 100         | 100 |
| 63  | lz    | 215/217 (99%) | 172 (80%) | 43 (20%) | 0        | 100         | 100 |
| 64  | SR    | 133/135 (98%) | 114 (86%) | 18 (14%) | 1 (1%)   | 16          | 50  |
| 64  | sR    | 133/135 (98%) | 106 (80%) | 25 (19%) | 2 (2%)   | 8           | 37  |
| 65  | SD    | 225/227 (99%) | 208 (92%) | 17 (8%)  | 0        | 100         | 100 |
| 65  | sD    | 225/227 (99%) | 205 (91%) | 19 (8%)  | 1 (0%)   | 30          | 62  |
| 66  | SF    | 187/189 (99%) | 159 (85%) | 28 (15%) | 0        | 100         | 100 |
| 66  | sF    | 187/189 (99%) | 165 (88%) | 22 (12%) | 0        | 100         | 100 |
| 67  | SK    | 96/98 (98%)   | 85 (88%)  | 9 (9%)   | 2 (2%)   | 5           | 31  |
| 67  | sK    | 96/98 (98%)   | 85 (88%)  | 10 (10%) | 1 (1%)   | 12          | 45  |
| 68  | SP    | 119/121 (98%) | 112 (94%) | 7 (6%)   | 0        | 100         | 100 |
| 68  | sP    | 119/121 (98%) | 109 (92%) | 10 (8%)  | 0        | 100         | 100 |
| 69  | SQ    | 142/144 (99%) | 121 (85%) | 20 (14%) | 1 (1%)   | 18          | 52  |
| 69  | sQ    | 142/144 (99%) | 122 (86%) | 19 (13%) | 1 (1%)   | 18          | 52  |
| 70  | SS    | 143/145 (99%) | 132 (92%) | 11 (8%)  | 0        | 100         | 100 |
| 70  | sS    | 143/145 (99%) | 131 (92%) | 12 (8%)  | 0        | 100         | 100 |
| 71  | ST    | 141/143 (99%) | 127 (90%) | 13 (9%)  | 1 (1%)   | 18          | 52  |
| 71  | sT    | 141/143 (99%) | 128 (91%) | 12 (8%)  | 1 (1%)   | 18          | 52  |
| 72  | SU    | 102/104 (98%) | 91 (89%)  | 11 (11%) | 0        | 100         | 100 |
| 72  | sU    | 102/104 (98%) | 93 (91%)  | 9 (9%)   | 0        | 100         | 100 |
| 73  | Sc    | 62/64 (97%)   | 51 (82%)  | 11 (18%) | 0        | 100         | 100 |
| 73  | sc    | 62/64 (97%)   | 50 (81%)  | 12 (19%) | 0        | 100         | 100 |
| 74  | Sd    | 53/55 (96%)   | 49 (92%)  | 4 (8%)   | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Favoured    | Allowed   | Outliers | Percentiles |     |
|-----|-------|-------------------|-------------|-----------|----------|-------------|-----|
| 74  | sd    | 53/55 (96%)       | 48 (91%)    | 5 (9%)    | 0        | 100         | 100 |
| 75  | Sg    | 311/313 (99%)     | 275 (88%)   | 36 (12%)  | 0        | 100         | 100 |
| 75  | sg    | 311/313 (99%)     | 274 (88%)   | 37 (12%)  | 0        | 100         | 100 |
| 76  | SM    | 120/122 (98%)     | 101 (84%)   | 18 (15%)  | 1 (1%)   | 16          | 50  |
| 76  | sM    | 120/122 (98%)     | 109 (91%)   | 10 (8%)   | 1 (1%)   | 16          | 50  |
| 77  | SZ    | 73/75 (97%)       | 58 (80%)    | 15 (20%)  | 0        | 100         | 100 |
| 77  | sZ    | 73/75 (97%)       | 62 (85%)    | 11 (15%)  | 0        | 100         | 100 |
| 78  | Sf    | 65/67 (97%)       | 55 (85%)    | 10 (15%)  | 0        | 100         | 100 |
| 78  | sf    | 65/67 (97%)       | 55 (85%)    | 10 (15%)  | 0        | 100         | 100 |
| 80  | CB    | 842/856 (98%)     | 782 (93%)   | 57 (7%)   | 3 (0%)   | 30          | 62  |
| 80  | cB    | 842/856 (98%)     | 782 (93%)   | 57 (7%)   | 3 (0%)   | 30          | 62  |
| 83  | Ls    | 194/196 (99%)     | 184 (95%)   | 10 (5%)   | 0        | 100         | 100 |
| 83  | ls    | 194/196 (99%)     | 176 (91%)   | 18 (9%)   | 0        | 100         | 100 |
| 84  | Lt    | 137/141 (97%)     | 103 (75%)   | 32 (23%)  | 2 (2%)   | 8           | 37  |
| 84  | lt    | 137/141 (97%)     | 104 (76%)   | 31 (23%)  | 2 (2%)   | 8           | 37  |
| 86  | Se    | 45/47 (96%)       | 43 (96%)    | 2 (4%)    | 0        | 100         | 100 |
| 87  | LW    | 114/124 (92%)     | 109 (96%)   | 5 (4%)    | 0        | 100         | 100 |
| 87  | IW    | 114/124 (92%)     | 112 (98%)   | 2 (2%)    | 0        | 100         | 100 |
| All | All   | 25645/26099 (98%) | 23469 (92%) | 2141 (8%) | 35 (0%)  | 49          | 79  |

All (35) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | sG    | 217 | MET  |
| 67  | sK    | 96  | ARG  |
| 80  | cB    | 779 | THR  |
| 80  | CB    | 407 | LYS  |
| 80  | CB    | 779 | THR  |
| 67  | SK    | 96  | ARG  |
| 84  | Lt    | 144 | ASP  |
| 1   | CH    | 38  | VAL  |
| 1   | cH    | 38  | VAL  |
| 2   | sE    | 87  | MET  |
| 5   | sX    | 127 | ASN  |
| 71  | sT    | 41  | LYS  |
| 80  | cB    | 62  | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 80  | cB    | 407 | LYS  |
| 5   | SX    | 127 | ASN  |
| 64  | SR    | 124 | VAL  |
| 67  | SK    | 36  | ALA  |
| 69  | SQ    | 44  | PRO  |
| 71  | ST    | 39  | LEU  |
| 76  | sM    | 96  | ARG  |
| 84  | lt    | 24  | ALA  |
| 80  | CB    | 611 | ASP  |
| 76  | SM    | 96  | ARG  |
| 84  | Lt    | 24  | ALA  |
| 1   | CH    | 114 | ALA  |
| 69  | sQ    | 44  | PRO  |
| 34  | LN    | 124 | ASP  |
| 33  | IM    | 88  | ALA  |
| 34  | lN    | 124 | ASP  |
| 64  | sR    | 124 | VAL  |
| 64  | sR    | 128 | PHE  |
| 84  | lt    | 144 | ASP  |
| 33  | LM    | 88  | ALA  |
| 14  | Sa    | 46  | GLU  |
| 65  | sD    | 213 | PRO  |

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 1   | CH    | 100/100 (100%) | 100 (100%) | 0        | 100         | 100 |
| 1   | cH    | 100/100 (100%) | 100 (100%) | 0        | 100         | 100 |
| 2   | SE    | 224/224 (100%) | 223 (100%) | 1 (0%)   | 84          | 86  |
| 2   | sE    | 224/224 (100%) | 224 (100%) | 0        | 100         | 100 |
| 3   | SI    | 178/178 (100%) | 178 (100%) | 0        | 100         | 100 |
| 3   | sI    | 178/178 (100%) | 178 (100%) | 0        | 100         | 100 |
| 4   | SL    | 137/137 (100%) | 135 (98%)  | 2 (2%)   | 57          | 76  |

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| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 4   | sL    | 137/137 (100%) | 136 (99%)  | 1 (1%)   | 76          | 83  |
| 5   | SX    | 113/113 (100%) | 113 (100%) | 0        | 100         | 100 |
| 5   | sX    | 113/113 (100%) | 112 (99%)  | 1 (1%)   | 70          | 81  |
| 6   | SG    | 207/207 (100%) | 206 (100%) | 1 (0%)   | 81          | 85  |
| 6   | sG    | 207/207 (100%) | 207 (100%) | 0        | 100         | 100 |
| 7   | SJ    | 161/161 (100%) | 161 (100%) | 0        | 100         | 100 |
| 7   | sJ    | 161/161 (100%) | 161 (100%) | 0        | 100         | 100 |
| 8   | SY    | 113/113 (100%) | 113 (100%) | 0        | 100         | 100 |
| 8   | sY    | 113/113 (100%) | 112 (99%)  | 1 (1%)   | 70          | 81  |
| 9   | se    | 47/47 (100%)   | 47 (100%)  | 0        | 100         | 100 |
| 10  | SA    | 183/183 (100%) | 183 (100%) | 0        | 100         | 100 |
| 10  | sA    | 183/183 (100%) | 182 (100%) | 1 (0%)   | 81          | 85  |
| 11  | SB    | 195/195 (100%) | 194 (100%) | 1 (0%)   | 81          | 85  |
| 11  | sB    | 195/195 (100%) | 193 (99%)  | 2 (1%)   | 68          | 80  |
| 12  | SH    | 166/169 (98%)  | 166 (100%) | 0        | 100         | 100 |
| 12  | sH    | 166/169 (98%)  | 164 (99%)  | 2 (1%)   | 63          | 79  |
| 13  | SV    | 67/67 (100%)   | 67 (100%)  | 0        | 100         | 100 |
| 13  | sV    | 67/67 (100%)   | 67 (100%)  | 0        | 100         | 100 |
| 14  | Sa    | 89/89 (100%)   | 88 (99%)   | 1 (1%)   | 65          | 79  |
| 14  | sa    | 89/89 (100%)   | 87 (98%)   | 2 (2%)   | 45          | 71  |
| 15  | SC    | 188/188 (100%) | 187 (100%) | 1 (0%)   | 81          | 85  |
| 15  | sC    | 188/188 (100%) | 186 (99%)  | 2 (1%)   | 65          | 79  |
| 16  | SN    | 130/130 (100%) | 130 (100%) | 0        | 100         | 100 |
| 16  | sN    | 130/130 (100%) | 129 (99%)  | 1 (1%)   | 73          | 82  |
| 17  | SO    | 110/110 (100%) | 110 (100%) | 0        | 100         | 100 |
| 17  | sO    | 110/110 (100%) | 110 (100%) | 0        | 100         | 100 |
| 18  | SW    | 112/112 (100%) | 110 (98%)  | 2 (2%)   | 51          | 74  |
| 18  | sW    | 112/112 (100%) | 112 (100%) | 0        | 100         | 100 |
| 19  | Sb    | 75/75 (100%)   | 75 (100%)  | 0        | 100         | 100 |
| 19  | sb    | 75/75 (100%)   | 75 (100%)  | 0        | 100         | 100 |
| 22  | LA    | 190/190 (100%) | 190 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 22  | 1A    | 190/190 (100%) | 190 (100%) | 0        | 100         | 100 |
| 23  | LB    | 348/348 (100%) | 348 (100%) | 0        | 100         | 100 |
| 23  | 1B    | 348/348 (100%) | 347 (100%) | 1 (0%)   | 86          | 88  |
| 24  | LC    | 306/306 (100%) | 306 (100%) | 0        | 100         | 100 |
| 24  | 1C    | 306/306 (100%) | 305 (100%) | 1 (0%)   | 86          | 88  |
| 25  | LD    | 246/247 (100%) | 245 (100%) | 1 (0%)   | 84          | 86  |
| 25  | 1D    | 246/247 (100%) | 245 (100%) | 1 (0%)   | 84          | 86  |
| 26  | LE    | 209/220 (95%)  | 208 (100%) | 1 (0%)   | 81          | 85  |
| 26  | 1E    | 209/220 (95%)  | 208 (100%) | 1 (0%)   | 81          | 85  |
| 27  | LF    | 194/194 (100%) | 194 (100%) | 0        | 100         | 100 |
| 27  | 1F    | 194/194 (100%) | 191 (98%)  | 3 (2%)   | 57          | 76  |
| 28  | LG    | 203/205 (99%)  | 202 (100%) | 1 (0%)   | 81          | 85  |
| 28  | 1G    | 203/205 (99%)  | 203 (100%) | 0        | 100         | 100 |
| 29  | LH    | 169/169 (100%) | 169 (100%) | 0        | 100         | 100 |
| 29  | 1H    | 169/169 (100%) | 168 (99%)  | 1 (1%)   | 78          | 84  |
| 30  | LI    | 172/180 (96%)  | 171 (99%)  | 1 (1%)   | 78          | 84  |
| 30  | II    | 172/180 (96%)  | 171 (99%)  | 1 (1%)   | 78          | 84  |
| 31  | LJ    | 148/148 (100%) | 147 (99%)  | 1 (1%)   | 76          | 83  |
| 31  | 1J    | 148/148 (100%) | 147 (99%)  | 1 (1%)   | 76          | 83  |
| 32  | LL    | 176/176 (100%) | 176 (100%) | 0        | 100         | 100 |
| 32  | 1L    | 176/176 (100%) | 175 (99%)  | 1 (1%)   | 78          | 84  |
| 33  | LM    | 118/118 (100%) | 118 (100%) | 0        | 100         | 100 |
| 33  | 1M    | 118/118 (100%) | 116 (98%)  | 2 (2%)   | 53          | 75  |
| 34  | LN    | 171/171 (100%) | 170 (99%)  | 1 (1%)   | 78          | 84  |
| 34  | 1N    | 171/171 (100%) | 171 (100%) | 0        | 100         | 100 |
| 35  | LO    | 173/173 (100%) | 172 (99%)  | 1 (1%)   | 78          | 84  |
| 35  | 1O    | 173/173 (100%) | 172 (99%)  | 1 (1%)   | 78          | 84  |
| 36  | LP    | 134/134 (100%) | 134 (100%) | 0        | 100         | 100 |
| 36  | 1P    | 134/134 (100%) | 132 (98%)  | 2 (2%)   | 57          | 76  |
| 37  | LQ    | 164/164 (100%) | 164 (100%) | 0        | 100         | 100 |
| 37  | 1Q    | 164/164 (100%) | 164 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 38  | LR    | 166/166 (100%) | 166 (100%) | 0        | 100         | 100 |
| 38  | lR    | 166/166 (100%) | 166 (100%) | 0        | 100         | 100 |
| 39  | LS    | 156/156 (100%) | 156 (100%) | 0        | 100         | 100 |
| 39  | lS    | 156/156 (100%) | 155 (99%)  | 1 (1%)   | 78          | 84  |
| 40  | LT    | 139/139 (100%) | 138 (99%)  | 1 (1%)   | 76          | 83  |
| 40  | lT    | 139/139 (100%) | 138 (99%)  | 1 (1%)   | 76          | 83  |
| 41  | LU    | 91/91 (100%)   | 90 (99%)   | 1 (1%)   | 65          | 79  |
| 41  | lU    | 91/91 (100%)   | 91 (100%)  | 0        | 100         | 100 |
| 42  | LV    | 101/101 (100%) | 101 (100%) | 0        | 100         | 100 |
| 42  | lV    | 101/101 (100%) | 100 (99%)  | 1 (1%)   | 68          | 80  |
| 43  | LX    | 108/108 (100%) | 107 (99%)  | 1 (1%)   | 70          | 81  |
| 43  | lX    | 108/108 (100%) | 107 (99%)  | 1 (1%)   | 70          | 81  |
| 44  | LY    | 124/124 (100%) | 124 (100%) | 0        | 100         | 100 |
| 44  | lY    | 124/124 (100%) | 124 (100%) | 0        | 100         | 100 |
| 45  | LZ    | 117/117 (100%) | 117 (100%) | 0        | 100         | 100 |
| 45  | lZ    | 117/117 (100%) | 114 (97%)  | 3 (3%)   | 40          | 69  |
| 46  | La    | 120/120 (100%) | 120 (100%) | 0        | 100         | 100 |
| 46  | la    | 120/120 (100%) | 118 (98%)  | 2 (2%)   | 53          | 75  |
| 47  | Lb    | 88/101 (87%)   | 88 (100%)  | 0        | 100         | 100 |
| 47  | lb    | 88/101 (87%)   | 88 (100%)  | 0        | 100         | 100 |
| 48  | Lc    | 83/83 (100%)   | 82 (99%)   | 1 (1%)   | 63          | 79  |
| 48  | lc    | 83/83 (100%)   | 83 (100%)  | 0        | 100         | 100 |
| 49  | Ld    | 98/98 (100%)   | 97 (99%)   | 1 (1%)   | 68          | 80  |
| 49  | ld    | 98/98 (100%)   | 97 (99%)   | 1 (1%)   | 68          | 80  |
| 50  | Le    | 114/114 (100%) | 113 (99%)  | 1 (1%)   | 70          | 81  |
| 50  | le    | 114/114 (100%) | 113 (99%)  | 1 (1%)   | 70          | 81  |
| 51  | Lf    | 88/88 (100%)   | 88 (100%)  | 0        | 100         | 100 |
| 51  | lf    | 88/88 (100%)   | 87 (99%)   | 1 (1%)   | 65          | 79  |
| 52  | Lg    | 98/98 (100%)   | 98 (100%)  | 0        | 100         | 100 |
| 52  | lg    | 98/98 (100%)   | 97 (99%)   | 1 (1%)   | 68          | 80  |
| 53  | Lh    | 109/109 (100%) | 109 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 53  | lh    | 109/109 (100%) | 109 (100%) | 0        | 100         | 100 |
| 54  | Li    | 86/86 (100%)   | 85 (99%)   | 1 (1%)   | 63          | 79  |
| 54  | li    | 86/86 (100%)   | 86 (100%)  | 0        | 100         | 100 |
| 55  | Lj    | 73/73 (100%)   | 73 (100%)  | 0        | 100         | 100 |
| 55  | lj    | 73/73 (100%)   | 73 (100%)  | 0        | 100         | 100 |
| 56  | Lk    | 64/64 (100%)   | 64 (100%)  | 0        | 100         | 100 |
| 56  | lk    | 64/64 (100%)   | 64 (100%)  | 0        | 100         | 100 |
| 57  | Ll    | 47/47 (100%)   | 47 (100%)  | 0        | 100         | 100 |
| 57  | ll    | 47/47 (100%)   | 47 (100%)  | 0        | 100         | 100 |
| 58  | Lm    | 48/48 (100%)   | 47 (98%)   | 1 (2%)   | 47          | 71  |
| 58  | lm    | 48/48 (100%)   | 48 (100%)  | 0        | 100         | 100 |
| 59  | Ln    | 23/23 (100%)   | 23 (100%)  | 0        | 100         | 100 |
| 59  | ln    | 23/23 (100%)   | 23 (100%)  | 0        | 100         | 100 |
| 60  | Lo    | 93/93 (100%)   | 93 (100%)  | 0        | 100         | 100 |
| 60  | lo    | 93/93 (100%)   | 93 (100%)  | 0        | 100         | 100 |
| 61  | Lp    | 74/74 (100%)   | 74 (100%)  | 0        | 100         | 100 |
| 61  | lp    | 74/74 (100%)   | 74 (100%)  | 0        | 100         | 100 |
| 62  | Lr    | 109/109 (100%) | 107 (98%)  | 2 (2%)   | 51          | 74  |
| 62  | lr    | 109/109 (100%) | 109 (100%) | 0        | 100         | 100 |
| 63  | Lz    | 195/196 (100%) | 195 (100%) | 0        | 100         | 100 |
| 63  | lz    | 195/196 (100%) | 194 (100%) | 1 (0%)   | 81          | 85  |
| 64  | SR    | 122/122 (100%) | 122 (100%) | 0        | 100         | 100 |
| 64  | sR    | 122/122 (100%) | 122 (100%) | 0        | 100         | 100 |
| 65  | SD    | 190/190 (100%) | 190 (100%) | 0        | 100         | 100 |
| 65  | sD    | 190/190 (100%) | 187 (98%)  | 3 (2%)   | 55          | 75  |
| 66  | SF    | 159/159 (100%) | 157 (99%)  | 2 (1%)   | 61          | 78  |
| 66  | sF    | 159/159 (100%) | 159 (100%) | 0        | 100         | 100 |
| 67  | SK    | 89/89 (100%)   | 88 (99%)   | 1 (1%)   | 65          | 79  |
| 67  | sK    | 89/89 (100%)   | 89 (100%)  | 0        | 100         | 100 |
| 68  | SP    | 107/107 (100%) | 105 (98%)  | 2 (2%)   | 50          | 73  |
| 68  | sP    | 107/107 (100%) | 107 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed           | Rotameric    | Outliers | Percentiles |     |
|-----|-------|--------------------|--------------|----------|-------------|-----|
| 69  | SQ    | 119/119 (100%)     | 119 (100%)   | 0        | 100         | 100 |
| 69  | sQ    | 119/119 (100%)     | 117 (98%)    | 2 (2%)   | 53          | 75  |
| 70  | SS    | 126/126 (100%)     | 124 (98%)    | 2 (2%)   | 55          | 75  |
| 70  | sS    | 126/126 (100%)     | 125 (99%)    | 1 (1%)   | 73          | 82  |
| 71  | ST    | 113/113 (100%)     | 113 (100%)   | 0        | 100         | 100 |
| 71  | sT    | 113/113 (100%)     | 111 (98%)    | 2 (2%)   | 51          | 74  |
| 72  | SU    | 94/94 (100%)       | 93 (99%)     | 1 (1%)   | 65          | 79  |
| 72  | sU    | 94/94 (100%)       | 94 (100%)    | 0        | 100         | 100 |
| 73  | Sc    | 57/57 (100%)       | 57 (100%)    | 0        | 100         | 100 |
| 73  | sc    | 57/57 (100%)       | 57 (100%)    | 0        | 100         | 100 |
| 74  | Sd    | 48/48 (100%)       | 48 (100%)    | 0        | 100         | 100 |
| 74  | sd    | 48/48 (100%)       | 48 (100%)    | 0        | 100         | 100 |
| 75  | Sg    | 272/272 (100%)     | 271 (100%)   | 1 (0%)   | 84          | 86  |
| 75  | sg    | 272/272 (100%)     | 268 (98%)    | 4 (2%)   | 57          | 76  |
| 76  | SM    | 102/104 (98%)      | 102 (100%)   | 0        | 100         | 100 |
| 76  | sM    | 102/104 (98%)      | 101 (99%)    | 1 (1%)   | 68          | 80  |
| 77  | SZ    | 66/66 (100%)       | 66 (100%)    | 0        | 100         | 100 |
| 77  | sZ    | 66/66 (100%)       | 66 (100%)    | 0        | 100         | 100 |
| 78  | Sf    | 60/60 (100%)       | 59 (98%)     | 1 (2%)   | 53          | 75  |
| 78  | sf    | 60/60 (100%)       | 60 (100%)    | 0        | 100         | 100 |
| 80  | CB    | 722/728 (99%)      | 719 (100%)   | 3 (0%)   | 84          | 86  |
| 80  | cB    | 722/728 (99%)      | 720 (100%)   | 2 (0%)   | 86          | 88  |
| 83  | Ls    | 162/164 (99%)      | 162 (100%)   | 0        | 100         | 100 |
| 83  | ls    | 162/164 (99%)      | 162 (100%)   | 0        | 100         | 100 |
| 84  | Lt    | 112/115 (97%)      | 111 (99%)    | 1 (1%)   | 70          | 81  |
| 84  | lt    | 112/115 (97%)      | 112 (100%)   | 0        | 100         | 100 |
| 86  | Se    | 39/39 (100%)       | 39 (100%)    | 0        | 100         | 100 |
| 87  | LW    | 97/103 (94%)       | 97 (100%)    | 0        | 100         | 100 |
| 87  | IW    | 97/103 (94%)       | 95 (98%)     | 2 (2%)   | 47          | 71  |
| All | All   | 22282/22398 (100%) | 22182 (100%) | 100 (0%) | 81          | 86  |

All (100) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | sL    | 140 | PHE  |
| 5   | sX    | 98  | ASP  |
| 8   | sY    | 16  | ARG  |
| 10  | sA    | 65  | ILE  |
| 11  | sB    | 76  | ASN  |
| 11  | sB    | 78  | GLU  |
| 12  | sH    | 79  | LEU  |
| 12  | sH    | 180 | LEU  |
| 14  | sa    | 44  | ILE  |
| 14  | sa    | 79  | ILE  |
| 15  | sC    | 174 | ILE  |
| 15  | sC    | 256 | TRP  |
| 16  | sN    | 34  | LYS  |
| 23  | lB    | 305 | THR  |
| 24  | lC    | 223 | ASN  |
| 25  | lD    | 74  | ILE  |
| 26  | lE    | 279 | ASN  |
| 27  | lF    | 185 | ILE  |
| 27  | lF    | 187 | MET  |
| 27  | lF    | 189 | ASP  |
| 29  | lH    | 18  | ILE  |
| 30  | lI    | 142 | LEU  |
| 31  | lJ    | 171 | ASP  |
| 32  | lL    | 110 | LEU  |
| 33  | lM    | 6   | PHE  |
| 33  | lM    | 27  | ILE  |
| 35  | lO    | 189 | ILE  |
| 36  | lP    | 53  | LEU  |
| 36  | lP    | 148 | MET  |
| 39  | lS    | 85  | ASP  |
| 40  | lT    | 67  | VAL  |
| 42  | lV    | 36  | ASN  |
| 43  | lX    | 153 | ILE  |
| 45  | lZ    | 12  | LEU  |
| 45  | lZ    | 97  | ASN  |
| 45  | lZ    | 128 | LYS  |
| 46  | la    | 43  | ILE  |
| 46  | la    | 63  | LEU  |
| 49  | ld    | 49  | ILE  |
| 50  | le    | 78  | LEU  |
| 51  | lf    | 43  | LEU  |
| 52  | lg    | 64  | LEU  |
| 63  | lz    | 145 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 65  | sD    | 126 | ILE  |
| 65  | sD    | 193 | ASP  |
| 65  | sD    | 213 | PRO  |
| 69  | sQ    | 41  | MET  |
| 69  | sQ    | 130 | LYS  |
| 70  | sS    | 73  | ASN  |
| 71  | sT    | 18  | LEU  |
| 71  | sT    | 128 | GLN  |
| 75  | sg    | 32  | LEU  |
| 75  | sg    | 51  | ASN  |
| 75  | sg    | 105 | THR  |
| 75  | sg    | 235 | ILE  |
| 76  | sM    | 44  | LYS  |
| 80  | cB    | 611 | ASP  |
| 80  | cB    | 853 | ASN  |
| 80  | CB    | 362 | VAL  |
| 80  | CB    | 520 | LEU  |
| 80  | CB    | 746 | LEU  |
| 2   | SE    | 162 | ILE  |
| 4   | SL    | 82  | MET  |
| 4   | SL    | 86  | ILE  |
| 6   | SG    | 176 | ILE  |
| 11  | SB    | 43  | ASN  |
| 14  | Sa    | 75  | VAL  |
| 15  | SC    | 73  | MET  |
| 18  | SW    | 23  | ARG  |
| 18  | SW    | 85  | ASP  |
| 25  | LD    | 219 | TYR  |
| 26  | LE    | 119 | GLU  |
| 28  | LG    | 265 | LEU  |
| 30  | LI    | 181 | PHE  |
| 31  | LJ    | 24  | ILE  |
| 34  | LN    | 123 | GLU  |
| 35  | LO    | 58  | LEU  |
| 40  | LT    | 151 | LEU  |
| 41  | LU    | 50  | ASN  |
| 43  | LX    | 93  | ASN  |
| 48  | Lc    | 23  | LYS  |
| 49  | Ld    | 49  | ILE  |
| 50  | Le    | 7   | LEU  |
| 54  | Li    | 94  | LEU  |
| 58  | Lm    | 92  | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 62  | Lr    | 17  | LEU  |
| 62  | Lr    | 82  | ILE  |
| 66  | SF    | 39  | ILE  |
| 66  | SF    | 45  | TYR  |
| 67  | SK    | 78  | TYR  |
| 68  | SP    | 28  | MET  |
| 68  | SP    | 60  | LEU  |
| 70  | SS    | 101 | ASN  |
| 70  | SS    | 139 | THR  |
| 72  | SU    | 92  | HIS  |
| 75  | Sg    | 188 | HIS  |
| 78  | Sf    | 104 | LYS  |
| 84  | Lt    | 81  | ILE  |
| 87  | IW    | 12  | LYS  |
| 87  | IW    | 32  | LEU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (248) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | cH    | 51  | GLN  |
| 1   | cH    | 70  | HIS  |
| 1   | cH    | 82  | GLN  |
| 2   | sE    | 17  | HIS  |
| 2   | sE    | 197 | ASN  |
| 4   | sL    | 94  | HIS  |
| 6   | sG    | 146 | ASN  |
| 7   | sJ    | 132 | GLN  |
| 8   | sY    | 19  | GLN  |
| 8   | sY    | 85  | ASN  |
| 8   | sY    | 112 | ASN  |
| 9   | se    | 15  | GLN  |
| 9   | se    | 56  | ASN  |
| 9   | se    | 58  | ASN  |
| 10  | sA    | 132 | GLN  |
| 10  | sA    | 141 | ASN  |
| 11  | sB    | 99  | ASN  |
| 11  | sB    | 101 | HIS  |
| 11  | sB    | 157 | GLN  |
| 12  | sH    | 25  | GLN  |
| 12  | sH    | 76  | GLN  |
| 13  | sV    | 2   | GLN  |
| 13  | sV    | 21  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 13  | sV    | 29  | HIS  |
| 14  | sa    | 25  | ASN  |
| 17  | sO    | 38  | ASN  |
| 17  | sO    | 103 | ASN  |
| 18  | sW    | 24  | GLN  |
| 18  | sW    | 44  | HIS  |
| 18  | sW    | 90  | GLN  |
| 18  | sW    | 92  | ASN  |
| 19  | sb    | 19  | HIS  |
| 19  | sb    | 51  | GLN  |
| 19  | sb    | 83  | GLN  |
| 23  | lB    | 3   | HIS  |
| 23  | lB    | 145 | GLN  |
| 23  | lB    | 165 | HIS  |
| 23  | lB    | 302 | ASN  |
| 24  | lC    | 38  | ASN  |
| 24  | lC    | 43  | ASN  |
| 24  | lC    | 89  | GLN  |
| 24  | lC    | 299 | GLN  |
| 25  | lD    | 195 | HIS  |
| 25  | lD    | 222 | GLN  |
| 25  | lD    | 291 | GLN  |
| 26  | lE    | 266 | GLN  |
| 27  | lF    | 131 | ASN  |
| 27  | lF    | 151 | ASN  |
| 27  | lF    | 206 | ASN  |
| 28  | lG    | 64  | GLN  |
| 28  | lG    | 90  | GLN  |
| 28  | lG    | 94  | GLN  |
| 28  | lG    | 240 | ASN  |
| 30  | lI    | 133 | GLN  |
| 31  | lJ    | 10  | ASN  |
| 31  | lJ    | 42  | GLN  |
| 31  | lJ    | 46  | GLN  |
| 31  | lJ    | 71  | HIS  |
| 32  | lL    | 188 | ASN  |
| 33  | lM    | 56  | GLN  |
| 34  | lN    | 37  | HIS  |
| 34  | lN    | 57  | GLN  |
| 34  | lN    | 99  | GLN  |
| 34  | lN    | 117 | ASN  |
| 35  | lO    | 150 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 36  | lP    | 34  | GLN  |
| 36  | lP    | 101 | ASN  |
| 36  | lP    | 133 | HIS  |
| 37  | lQ    | 188 | ASN  |
| 38  | lR    | 134 | ASN  |
| 38  | lR    | 158 | GLN  |
| 39  | lS    | 23  | HIS  |
| 39  | lS    | 92  | ASN  |
| 39  | lS    | 144 | GLN  |
| 40  | lT    | 49  | GLN  |
| 40  | lT    | 90  | ASN  |
| 40  | lT    | 98  | HIS  |
| 41  | lU    | 44  | GLN  |
| 42  | lV    | 135 | ASN  |
| 43  | lX    | 93  | ASN  |
| 43  | lX    | 108 | GLN  |
| 43  | lX    | 125 | ASN  |
| 44  | lY    | 65  | GLN  |
| 45  | lZ    | 97  | ASN  |
| 48  | lc    | 15  | ASN  |
| 48  | lc    | 40  | GLN  |
| 49  | ld    | 69  | ASN  |
| 50  | le    | 102 | ASN  |
| 53  | lh    | 98  | HIS  |
| 53  | lh    | 101 | ASN  |
| 54  | li    | 26  | HIS  |
| 54  | li    | 80  | HIS  |
| 57  | ll    | 25  | GLN  |
| 58  | lm    | 90  | ASN  |
| 60  | lo    | 45  | GLN  |
| 61  | lp    | 33  | GLN  |
| 62  | lr    | 6   | GLN  |
| 62  | lr    | 100 | ASN  |
| 62  | lr    | 121 | GLN  |
| 63  | lz    | 143 | ASN  |
| 63  | lz    | 182 | ASN  |
| 63  | lz    | 197 | ASN  |
| 65  | sD    | 207 | HIS  |
| 66  | sF    | 29  | GLN  |
| 66  | sF    | 149 | GLN  |
| 67  | sK    | 73  | ASN  |
| 68  | sP    | 54  | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 69  | sQ    | 35  | ASN  |
| 69  | sQ    | 114 | GLN  |
| 70  | sS    | 10  | GLN  |
| 70  | sS    | 120 | HIS  |
| 71  | sT    | 42  | HIS  |
| 74  | sd    | 5   | GLN  |
| 75  | sg    | 15  | ASN  |
| 75  | sg    | 64  | HIS  |
| 75  | sg    | 143 | GLN  |
| 75  | sg    | 162 | ASN  |
| 75  | sg    | 222 | ASN  |
| 75  | sg    | 285 | GLN  |
| 75  | sg    | 296 | GLN  |
| 77  | sZ    | 64  | ASN  |
| 77  | sZ    | 103 | HIS  |
| 80  | cB    | 21  | ASN  |
| 80  | cB    | 138 | GLN  |
| 80  | cB    | 306 | ASN  |
| 80  | cB    | 433 | ASN  |
| 80  | cB    | 448 | GLN  |
| 80  | cB    | 468 | ASN  |
| 80  | cB    | 750 | GLN  |
| 80  | cB    | 803 | ASN  |
| 80  | cB    | 807 | GLN  |
| 83  | ls    | 127 | ASN  |
| 83  | ls    | 176 | ASN  |
| 84  | lt    | 68  | GLN  |
| 84  | lt    | 111 | ASN  |
| 80  | CB    | 18  | ASN  |
| 80  | CB    | 21  | ASN  |
| 80  | CB    | 176 | GLN  |
| 80  | CB    | 565 | HIS  |
| 80  | CB    | 737 | GLN  |
| 4   | SL    | 11  | GLN  |
| 4   | SL    | 39  | ASN  |
| 4   | SL    | 112 | HIS  |
| 5   | SX    | 97  | ASN  |
| 6   | SG    | 177 | GLN  |
| 6   | SG    | 197 | GLN  |
| 6   | SG    | 225 | GLN  |
| 7   | SJ    | 140 | GLN  |
| 8   | SY    | 19  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8   | SY    | 63  | HIS  |
| 8   | SY    | 89  | HIS  |
| 10  | SA    | 33  | GLN  |
| 10  | SA    | 165 | ASN  |
| 12  | SH    | 44  | ASN  |
| 12  | SH    | 76  | GLN  |
| 12  | SH    | 163 | GLN  |
| 12  | SH    | 193 | GLN  |
| 14  | Sa    | 7   | ASN  |
| 15  | SC    | 113 | GLN  |
| 15  | SC    | 178 | HIS  |
| 16  | SN    | 123 | HIS  |
| 17  | SO    | 32  | HIS  |
| 17  | SO    | 83  | GLN  |
| 18  | SW    | 64  | ASN  |
| 18  | SW    | 90  | GLN  |
| 18  | SW    | 92  | ASN  |
| 18  | SW    | 113 | HIS  |
| 19  | Sb    | 51  | GLN  |
| 19  | Sb    | 83  | GLN  |
| 22  | LA    | 19  | HIS  |
| 22  | LA    | 140 | ASN  |
| 23  | LB    | 3   | HIS  |
| 23  | LB    | 123 | HIS  |
| 23  | LB    | 184 | GLN  |
| 23  | LB    | 203 | GLN  |
| 23  | LB    | 354 | GLN  |
| 24  | LC    | 38  | ASN  |
| 24  | LC    | 48  | ASN  |
| 24  | LC    | 142 | HIS  |
| 24  | LC    | 212 | ASN  |
| 25  | LD    | 63  | GLN  |
| 25  | LD    | 111 | ASN  |
| 25  | LD    | 195 | HIS  |
| 26  | LE    | 191 | GLN  |
| 26  | LE    | 266 | GLN  |
| 27  | LF    | 119 | ASN  |
| 27  | LF    | 226 | HIS  |
| 27  | LF    | 239 | GLN  |
| 28  | LG    | 64  | GLN  |
| 28  | LG    | 81  | ASN  |
| 28  | LG    | 82  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 28  | LG    | 108 | GLN  |
| 28  | LG    | 159 | HIS  |
| 28  | LG    | 195 | HIS  |
| 28  | LG    | 236 | HIS  |
| 29  | LH    | 149 | ASN  |
| 30  | LI    | 100 | ASN  |
| 30  | LI    | 147 | HIS  |
| 31  | LJ    | 42  | GLN  |
| 32  | LL    | 19  | GLN  |
| 32  | LL    | 67  | HIS  |
| 33  | LM    | 33  | GLN  |
| 33  | LM    | 34  | ASN  |
| 34  | LN    | 37  | HIS  |
| 34  | LN    | 86  | HIS  |
| 35  | LO    | 63  | ASN  |
| 35  | LO    | 173 | GLN  |
| 36  | LP    | 118 | GLN  |
| 37  | LQ    | 188 | ASN  |
| 38  | LR    | 75  | HIS  |
| 39  | LS    | 108 | GLN  |
| 39  | LS    | 117 | HIS  |
| 40  | LT    | 3   | ASN  |
| 40  | LT    | 69  | GLN  |
| 40  | LT    | 127 | GLN  |
| 41  | LU    | 41  | GLN  |
| 42  | LV    | 101 | ASN  |
| 43  | LX    | 111 | GLN  |
| 44  | LY    | 14  | ASN  |
| 44  | LY    | 96  | HIS  |
| 44  | LY    | 100 | HIS  |
| 46  | La    | 34  | ASN  |
| 46  | La    | 40  | HIS  |
| 46  | La    | 62  | HIS  |
| 47  | Lb    | 6   | ASN  |
| 48  | Lc    | 73  | HIS  |
| 49  | Ld    | 116 | ASN  |
| 50  | Le    | 34  | ASN  |
| 50  | Le    | 52  | GLN  |
| 50  | Le    | 124 | ASN  |
| 53  | Lh    | 65  | GLN  |
| 53  | Lh    | 107 | GLN  |
| 53  | Lh    | 108 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 55  | Lj    | 48  | ASN  |
| 61  | Lp    | 56  | HIS  |
| 63  | Lz    | 96  | ASN  |
| 65  | SD    | 101 | GLN  |
| 66  | SF    | 149 | GLN  |
| 67  | SK    | 32  | HIS  |
| 69  | SQ    | 97  | GLN  |
| 73  | Sc    | 29  | GLN  |
| 75  | Sg    | 26  | GLN  |
| 75  | Sg    | 162 | ASN  |
| 76  | SM    | 28  | HIS  |
| 77  | SZ    | 45  | ASN  |
| 77  | SZ    | 64  | ASN  |
| 84  | Lt    | 68  | GLN  |
| 87  | IW    | 79  | GLN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed          | Backbone Outliers | Pucker Outliers |
|-----|-------|-------------------|-------------------|-----------------|
| 20  | L7    | 119/120 (99%)     | 15 (12%)          | 0               |
| 20  | l7    | 119/120 (99%)     | 16 (13%)          | 0               |
| 21  | L8    | 155/156 (99%)     | 28 (18%)          | 0               |
| 21  | l8    | 155/156 (99%)     | 35 (22%)          | 0               |
| 79  | S2    | 1714/1740 (98%)   | 495 (28%)         | 12 (0%)         |
| 79  | s2    | 1712/1740 (98%)   | 546 (31%)         | 0               |
| 81  | AP    | 69/73 (94%)       | 25 (36%)          | 1 (1%)          |
| 81  | aP    | 69/73 (94%)       | 25 (36%)          | 0               |
| 82  | PE    | 74/76 (97%)       | 40 (54%)          | 3 (4%)          |
| 82  | pE    | 73/76 (96%)       | 35 (47%)          | 0               |
| 85  | L5    | 3696/3740 (98%)   | 969 (26%)         | 34 (0%)         |
| 85  | l5    | 3696/3740 (98%)   | 929 (25%)         | 0               |
| All | All   | 11651/11810 (98%) | 3158 (27%)        | 50 (0%)         |

All (3158) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 20  | l7    | 2   | U    |
| 20  | l7    | 7   | G    |
| 20  | l7    | 22  | A    |
| 20  | l7    | 24  | C    |
| 20  | l7    | 33  | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 20  | 17    | 37  | G    |
| 20  | 17    | 38  | U    |
| 20  | 17    | 39  | C    |
| 20  | 17    | 54  | A    |
| 20  | 17    | 63  | C    |
| 20  | 17    | 64  | G    |
| 20  | 17    | 66  | G    |
| 20  | 17    | 89  | G    |
| 20  | 17    | 97  | G    |
| 20  | 17    | 100 | A    |
| 20  | 17    | 111 | C    |
| 21  | 18    | 3   | A    |
| 21  | 18    | 34  | U    |
| 21  | 18    | 35  | C    |
| 21  | 18    | 38  | U    |
| 21  | 18    | 39  | G    |
| 21  | 18    | 46  | G    |
| 21  | 18    | 48  | A    |
| 21  | 18    | 49  | G    |
| 21  | 18    | 51  | U    |
| 21  | 18    | 59  | A    |
| 21  | 18    | 60  | G    |
| 21  | 18    | 61  | A    |
| 21  | 18    | 62  | A    |
| 21  | 18    | 63  | U    |
| 21  | 18    | 68  | G    |
| 21  | 18    | 80  | A    |
| 21  | 18    | 82  | A    |
| 21  | 18    | 83  | C    |
| 21  | 18    | 84  | A    |
| 21  | 18    | 85  | U    |
| 21  | 18    | 86  | U    |
| 21  | 18    | 87  | G    |
| 21  | 18    | 94  | G    |
| 21  | 18    | 103 | A    |
| 21  | 18    | 105 | C    |
| 21  | 18    | 110 | U    |
| 21  | 18    | 111 | U    |
| 21  | 18    | 114 | G    |
| 21  | 18    | 123 | U    |
| 21  | 18    | 124 | U    |
| 21  | 18    | 125 | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 21  | l8    | 126 | C    |
| 21  | l8    | 127 | U    |
| 21  | l8    | 147 | G    |
| 21  | l8    | 151 | G    |
| 79  | s2    | 2   | A    |
| 79  | s2    | 3   | C    |
| 79  | s2    | 4   | C    |
| 79  | s2    | 25  | A    |
| 79  | s2    | 26  | U    |
| 79  | s2    | 33  | G    |
| 79  | s2    | 34  | U    |
| 79  | s2    | 37  | C    |
| 79  | s2    | 41  | G    |
| 79  | s2    | 42  | A    |
| 79  | s2    | 43  | U    |
| 79  | s2    | 44  | U    |
| 79  | s2    | 45  | A    |
| 79  | s2    | 46  | A    |
| 79  | s2    | 56  | G    |
| 79  | s2    | 62  | G    |
| 79  | s2    | 64  | A    |
| 79  | s2    | 65  | C    |
| 79  | s2    | 66  | G    |
| 79  | s2    | 67  | C    |
| 79  | s2    | 68  | A    |
| 79  | s2    | 72  | C    |
| 79  | s2    | 73  | C    |
| 79  | s2    | 74  | G    |
| 79  | s2    | 76  | U    |
| 79  | s2    | 92  | A    |
| 79  | s2    | 99  | A    |
| 79  | s2    | 103 | A    |
| 79  | s2    | 113 | G    |
| 79  | s2    | 114 | G    |
| 79  | s2    | 115 | U    |
| 79  | s2    | 116 | U    |
| 79  | s2    | 126 | G    |
| 79  | s2    | 130 | G    |
| 79  | s2    | 140 | C    |
| 79  | s2    | 142 | C    |
| 79  | s2    | 143 | U    |
| 79  | s2    | 147 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 79  | s2    | 149 | A    |
| 79  | s2    | 155 | G    |
| 79  | s2    | 158 | A    |
| 79  | s2    | 161 | U    |
| 79  | s2    | 162 | C    |
| 79  | s2    | 163 | U    |
| 79  | s2    | 168 | C    |
| 79  | s2    | 175 | A    |
| 79  | s2    | 179 | C    |
| 79  | s2    | 187 | G    |
| 79  | s2    | 190 | G    |
| 79  | s2    | 191 | A    |
| 79  | s2    | 192 | C    |
| 79  | s2    | 196 | C    |
| 79  | s2    | 197 | U    |
| 79  | s2    | 198 | U    |
| 79  | s2    | 199 | C    |
| 79  | s2    | 200 | G    |
| 79  | s2    | 202 | G    |
| 79  | s2    | 203 | G    |
| 79  | s2    | 204 | G    |
| 79  | s2    | 206 | G    |
| 79  | s2    | 207 | G    |
| 79  | s2    | 208 | G    |
| 79  | s2    | 212 | C    |
| 79  | s2    | 214 | U    |
| 79  | s2    | 220 | U    |
| 79  | s2    | 291 | G    |
| 79  | s2    | 292 | A    |
| 79  | s2    | 293 | C    |
| 79  | s2    | 294 | U    |
| 79  | s2    | 295 | C    |
| 79  | s2    | 301 | A    |
| 79  | s2    | 303 | C    |
| 79  | s2    | 305 | U    |
| 79  | s2    | 306 | C    |
| 79  | s2    | 307 | G    |
| 79  | s2    | 308 | G    |
| 79  | s2    | 309 | G    |
| 79  | s2    | 310 | C    |
| 79  | s2    | 311 | C    |
| 79  | s2    | 312 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 79  | s2    | 314 | U    |
| 79  | s2    | 317 | C    |
| 79  | s2    | 318 | A    |
| 79  | s2    | 319 | C    |
| 79  | s2    | 322 | C    |
| 79  | s2    | 323 | C    |
| 79  | s2    | 324 | C    |
| 79  | s2    | 325 | C    |
| 79  | s2    | 326 | C    |
| 79  | s2    | 327 | G    |
| 79  | s2    | 328 | U    |
| 79  | s2    | 329 | G    |
| 79  | s2    | 332 | G    |
| 79  | s2    | 338 | G    |
| 79  | s2    | 339 | A    |
| 79  | s2    | 340 | C    |
| 79  | s2    | 347 | G    |
| 79  | s2    | 351 | G    |
| 79  | s2    | 360 | A    |
| 79  | s2    | 361 | U    |
| 79  | s2    | 362 | C    |
| 79  | s2    | 364 | A    |
| 79  | s2    | 368 | U    |
| 79  | s2    | 370 | G    |
| 79  | s2    | 372 | U    |
| 79  | s2    | 374 | G    |
| 79  | s2    | 375 | U    |
| 79  | s2    | 385 | G    |
| 79  | s2    | 386 | C    |
| 79  | s2    | 391 | C    |
| 79  | s2    | 407 | G    |
| 79  | s2    | 408 | A    |
| 79  | s2    | 409 | C    |
| 79  | s2    | 421 | G    |
| 79  | s2    | 426 | A    |
| 79  | s2    | 428 | U    |
| 79  | s2    | 429 | C    |
| 79  | s2    | 437 | G    |
| 79  | s2    | 442 | C    |
| 79  | s2    | 448 | A    |
| 79  | s2    | 449 | A    |
| 79  | s2    | 450 | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 79  | s2    | 452 | G    |
| 79  | s2    | 464 | A    |
| 79  | s2    | 465 | A    |
| 79  | s2    | 471 | G    |
| 79  | s2    | 472 | C    |
| 79  | s2    | 473 | A    |
| 79  | s2    | 474 | G    |
| 79  | s2    | 476 | A    |
| 79  | s2    | 478 | G    |
| 79  | s2    | 487 | U    |
| 79  | s2    | 488 | U    |
| 79  | s2    | 492 | C    |
| 79  | s2    | 493 | A    |
| 79  | s2    | 496 | C    |
| 79  | s2    | 502 | C    |
| 79  | s2    | 503 | C    |
| 79  | s2    | 516 | A    |
| 79  | s2    | 517 | C    |
| 79  | s2    | 523 | A    |
| 79  | s2    | 532 | C    |
| 79  | s2    | 533 | A    |
| 79  | s2    | 534 | G    |
| 79  | s2    | 535 | G    |
| 79  | s2    | 536 | A    |
| 79  | s2    | 537 | C    |
| 79  | s2    | 538 | U    |
| 79  | s2    | 540 | U    |
| 79  | s2    | 541 | U    |
| 79  | s2    | 542 | U    |
| 79  | s2    | 544 | G    |
| 79  | s2    | 546 | G    |
| 79  | s2    | 547 | G    |
| 79  | s2    | 551 | U    |
| 79  | s2    | 552 | G    |
| 79  | s2    | 553 | U    |
| 79  | s2    | 555 | A    |
| 79  | s2    | 557 | U    |
| 79  | s2    | 558 | G    |
| 79  | s2    | 559 | G    |
| 79  | s2    | 560 | A    |
| 79  | s2    | 563 | G    |
| 79  | s2    | 564 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 79  | s2    | 566 | U    |
| 79  | s2    | 583 | A    |
| 79  | s2    | 585 | C    |
| 79  | s2    | 587 | A    |
| 79  | s2    | 589 | G    |
| 79  | s2    | 590 | A    |
| 79  | s2    | 591 | U    |
| 79  | s2    | 593 | C    |
| 79  | s2    | 594 | A    |
| 79  | s2    | 603 | C    |
| 79  | s2    | 604 | A    |
| 79  | s2    | 608 | C    |
| 79  | s2    | 610 | G    |
| 79  | s2    | 612 | U    |
| 79  | s2    | 614 | C    |
| 79  | s2    | 617 | G    |
| 79  | s2    | 623 | G    |
| 79  | s2    | 627 | U    |
| 79  | s2    | 628 | A    |
| 79  | s2    | 629 | A    |
| 79  | s2    | 631 | U    |
| 79  | s2    | 638 | C    |
| 79  | s2    | 641 | A    |
| 79  | s2    | 643 | A    |
| 79  | s2    | 644 | G    |
| 79  | s2    | 660 | C    |
| 79  | s2    | 668 | A    |
| 79  | s2    | 669 | A    |
| 79  | s2    | 671 | A    |
| 79  | s2    | 672 | A    |
| 79  | s2    | 673 | G    |
| 79  | s2    | 684 | G    |
| 79  | s2    | 688 | U    |
| 79  | s2    | 689 | U    |
| 79  | s2    | 692 | G    |
| 79  | s2    | 693 | A    |
| 79  | s2    | 695 | C    |
| 79  | s2    | 696 | G    |
| 79  | s2    | 697 | G    |
| 79  | s2    | 698 | G    |
| 79  | s2    | 731 | G    |
| 79  | s2    | 732 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 79  | s2    | 734 | C    |
| 79  | s2    | 736 | C    |
| 79  | s2    | 738 | C    |
| 79  | s2    | 749 | U    |
| 79  | s2    | 750 | C    |
| 79  | s2    | 751 | G    |
| 79  | s2    | 752 | G    |
| 79  | s2    | 753 | C    |
| 79  | s2    | 787 | G    |
| 79  | s2    | 788 | G    |
| 79  | s2    | 791 | C    |
| 79  | s2    | 792 | C    |
| 79  | s2    | 794 | A    |
| 79  | s2    | 798 | G    |
| 79  | s2    | 799 | U    |
| 79  | s2    | 801 | U    |
| 79  | s2    | 819 | G    |
| 79  | s2    | 821 | G    |
| 79  | s2    | 822 | U    |
| 79  | s2    | 823 | U    |
| 79  | s2    | 824 | C    |
| 79  | s2    | 827 | A    |
| 79  | s2    | 830 | A    |
| 79  | s2    | 833 | C    |
| 79  | s2    | 834 | C    |
| 79  | s2    | 835 | C    |
| 79  | s2    | 836 | G    |
| 79  | s2    | 837 | A    |
| 79  | s2    | 838 | G    |
| 79  | s2    | 839 | C    |
| 79  | s2    | 842 | C    |
| 79  | s2    | 844 | U    |
| 79  | s2    | 847 | A    |
| 79  | s2    | 859 | G    |
| 79  | s2    | 862 | A    |
| 79  | s2    | 869 | A    |
| 79  | s2    | 870 | A    |
| 79  | s2    | 871 | U    |
| 79  | s2    | 872 | A    |
| 79  | s2    | 873 | G    |
| 79  | s2    | 874 | G    |
| 79  | s2    | 877 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 79  | s2    | 878  | G    |
| 79  | s2    | 882  | U    |
| 79  | s2    | 888  | U    |
| 79  | s2    | 889  | U    |
| 79  | s2    | 890  | U    |
| 79  | s2    | 891  | G    |
| 79  | s2    | 892  | U    |
| 79  | s2    | 893  | U    |
| 79  | s2    | 894  | G    |
| 79  | s2    | 896  | U    |
| 79  | s2    | 898  | U    |
| 79  | s2    | 899  | U    |
| 79  | s2    | 900  | C    |
| 79  | s2    | 901  | G    |
| 79  | s2    | 903  | A    |
| 79  | s2    | 913  | A    |
| 79  | s2    | 914  | U    |
| 79  | s2    | 917  | U    |
| 79  | s2    | 918  | U    |
| 79  | s2    | 919  | A    |
| 79  | s2    | 920  | A    |
| 79  | s2    | 925  | G    |
| 79  | s2    | 926  | A    |
| 79  | s2    | 933  | G    |
| 79  | s2    | 934  | G    |
| 79  | s2    | 949  | G    |
| 79  | s2    | 954  | U    |
| 79  | s2    | 955  | A    |
| 79  | s2    | 956  | G    |
| 79  | s2    | 963  | A    |
| 79  | s2    | 969  | U    |
| 79  | s2    | 971  | G    |
| 79  | s2    | 978  | G    |
| 79  | s2    | 979  | C    |
| 79  | s2    | 988  | C    |
| 79  | s2    | 989  | C    |
| 79  | s2    | 990  | A    |
| 79  | s2    | 992  | A    |
| 79  | s2    | 999  | G    |
| 79  | s2    | 1001 | A    |
| 79  | s2    | 1002 | U    |
| 79  | s2    | 1008 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 79  | s2    | 1017 | U    |
| 79  | s2    | 1019 | C    |
| 79  | s2    | 1023 | A    |
| 79  | s2    | 1024 | A    |
| 79  | s2    | 1027 | A    |
| 79  | s2    | 1042 | A    |
| 79  | s2    | 1044 | G    |
| 79  | s2    | 1045 | U    |
| 79  | s2    | 1058 | A    |
| 79  | s2    | 1060 | A    |
| 79  | s2    | 1061 | U    |
| 79  | s2    | 1062 | A    |
| 79  | s2    | 1067 | C    |
| 79  | s2    | 1078 | C    |
| 79  | s2    | 1083 | A    |
| 79  | s2    | 1085 | C    |
| 79  | s2    | 1087 | A    |
| 79  | s2    | 1088 | U    |
| 79  | s2    | 1093 | A    |
| 79  | s2    | 1100 | A    |
| 79  | s2    | 1107 | G    |
| 79  | s2    | 1108 | G    |
| 79  | s2    | 1109 | C    |
| 79  | s2    | 1110 | G    |
| 79  | s2    | 1113 | A    |
| 79  | s2    | 1114 | U    |
| 79  | s2    | 1115 | U    |
| 79  | s2    | 1116 | C    |
| 79  | s2    | 1118 | C    |
| 79  | s2    | 1119 | A    |
| 79  | s2    | 1121 | G    |
| 79  | s2    | 1124 | C    |
| 79  | s2    | 1125 | C    |
| 79  | s2    | 1128 | C    |
| 79  | s2    | 1133 | A    |
| 79  | s2    | 1138 | C    |
| 79  | s2    | 1148 | A    |
| 79  | s2    | 1150 | A    |
| 79  | s2    | 1153 | C    |
| 79  | s2    | 1154 | U    |
| 79  | s2    | 1155 | U    |
| 79  | s2    | 1170 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 79  | s2    | 1172 | U    |
| 79  | s2    | 1195 | A    |
| 79  | s2    | 1200 | A    |
| 79  | s2    | 1207 | G    |
| 79  | s2    | 1208 | A    |
| 79  | s2    | 1213 | C    |
| 79  | s2    | 1215 | C    |
| 79  | s2    | 1216 | C    |
| 79  | s2    | 1217 | A    |
| 79  | s2    | 1220 | A    |
| 79  | s2    | 1224 | G    |
| 79  | s2    | 1227 | G    |
| 79  | s2    | 1237 | C    |
| 79  | s2    | 1240 | A    |
| 79  | s2    | 1242 | U    |
| 79  | s2    | 1243 | U    |
| 79  | s2    | 1251 | A    |
| 79  | s2    | 1253 | A    |
| 79  | s2    | 1256 | G    |
| 79  | s2    | 1257 | G    |
| 79  | s2    | 1259 | A    |
| 79  | s2    | 1264 | C    |
| 79  | s2    | 1274 | G    |
| 79  | s2    | 1275 | G    |
| 79  | s2    | 1281 | G    |
| 79  | s2    | 1283 | C    |
| 79  | s2    | 1284 | A    |
| 79  | s2    | 1286 | G    |
| 79  | s2    | 1287 | A    |
| 79  | s2    | 1290 | G    |
| 79  | s2    | 1294 | G    |
| 79  | s2    | 1295 | A    |
| 79  | s2    | 1301 | A    |
| 79  | s2    | 1302 | G    |
| 79  | s2    | 1303 | C    |
| 79  | s2    | 1306 | U    |
| 79  | s2    | 1308 | U    |
| 79  | s2    | 1313 | A    |
| 79  | s2    | 1320 | G    |
| 79  | s2    | 1333 | U    |
| 79  | s2    | 1342 | U    |
| 79  | s2    | 1345 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 79  | s2    | 1348 | G    |
| 79  | s2    | 1351 | G    |
| 79  | s2    | 1354 | G    |
| 79  | s2    | 1355 | C    |
| 79  | s2    | 1356 | G    |
| 79  | s2    | 1357 | A    |
| 79  | s2    | 1364 | U    |
| 79  | s2    | 1369 | A    |
| 79  | s2    | 1370 | A    |
| 79  | s2    | 1371 | U    |
| 79  | s2    | 1372 | U    |
| 79  | s2    | 1373 | C    |
| 79  | s2    | 1375 | G    |
| 79  | s2    | 1376 | A    |
| 79  | s2    | 1378 | A    |
| 79  | s2    | 1388 | A    |
| 79  | s2    | 1389 | C    |
| 79  | s2    | 1396 | A    |
| 79  | s2    | 1401 | A    |
| 79  | s2    | 1402 | A    |
| 79  | s2    | 1406 | G    |
| 79  | s2    | 1407 | U    |
| 79  | s2    | 1411 | G    |
| 79  | s2    | 1412 | C    |
| 79  | s2    | 1414 | A    |
| 79  | s2    | 1415 | C    |
| 79  | s2    | 1419 | C    |
| 79  | s2    | 1420 | G    |
| 79  | s2    | 1421 | A    |
| 79  | s2    | 1422 | G    |
| 79  | s2    | 1423 | C    |
| 79  | s2    | 1425 | G    |
| 79  | s2    | 1428 | G    |
| 79  | s2    | 1433 | C    |
| 79  | s2    | 1434 | C    |
| 79  | s2    | 1435 | C    |
| 79  | s2    | 1436 | C    |
| 79  | s2    | 1438 | A    |
| 79  | s2    | 1442 | U    |
| 79  | s2    | 1449 | G    |
| 79  | s2    | 1450 | G    |
| 79  | s2    | 1452 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 79  | s2    | 1453 | C    |
| 79  | s2    | 1454 | A    |
| 79  | s2    | 1459 | G    |
| 79  | s2    | 1462 | U    |
| 79  | s2    | 1463 | U    |
| 79  | s2    | 1464 | C    |
| 79  | s2    | 1465 | A    |
| 79  | s2    | 1472 | C    |
| 79  | s2    | 1473 | G    |
| 79  | s2    | 1476 | A    |
| 79  | s2    | 1478 | U    |
| 79  | s2    | 1479 | G    |
| 79  | s2    | 1484 | A    |
| 79  | s2    | 1486 | A    |
| 79  | s2    | 1489 | A    |
| 79  | s2    | 1490 | G    |
| 79  | s2    | 1494 | U    |
| 79  | s2    | 1495 | G    |
| 79  | s2    | 1497 | G    |
| 79  | s2    | 1498 | A    |
| 79  | s2    | 1507 | G    |
| 79  | s2    | 1508 | A    |
| 79  | s2    | 1520 | G    |
| 79  | s2    | 1521 | C    |
| 79  | s2    | 1522 | A    |
| 79  | s2    | 1533 | A    |
| 79  | s2    | 1535 | U    |
| 79  | s2    | 1536 | G    |
| 79  | s2    | 1537 | A    |
| 79  | s2    | 1544 | C    |
| 79  | s2    | 1546 | G    |
| 79  | s2    | 1551 | U    |
| 79  | s2    | 1552 | G    |
| 79  | s2    | 1556 | A    |
| 79  | s2    | 1560 | U    |
| 79  | s2    | 1570 | G    |
| 79  | s2    | 1572 | C    |
| 79  | s2    | 1578 | U    |
| 79  | s2    | 1579 | A    |
| 79  | s2    | 1580 | A    |
| 79  | s2    | 1581 | C    |
| 79  | s2    | 1585 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 79  | s2    | 1586 | U    |
| 79  | s2    | 1587 | G    |
| 79  | s2    | 1588 | A    |
| 79  | s2    | 1594 | A    |
| 79  | s2    | 1598 | G    |
| 79  | s2    | 1599 | U    |
| 79  | s2    | 1600 | G    |
| 79  | s2    | 1601 | A    |
| 79  | s2    | 1602 | U    |
| 79  | s2    | 1603 | G    |
| 79  | s2    | 1604 | G    |
| 79  | s2    | 1606 | G    |
| 79  | s2    | 1621 | U    |
| 79  | s2    | 1623 | A    |
| 79  | s2    | 1629 | C    |
| 79  | s2    | 1630 | A    |
| 79  | s2    | 1633 | A    |
| 79  | s2    | 1634 | A    |
| 79  | s2    | 1637 | A    |
| 79  | s2    | 1638 | G    |
| 79  | s2    | 1639 | G    |
| 79  | s2    | 1640 | A    |
| 79  | s2    | 1646 | C    |
| 79  | s2    | 1648 | G    |
| 79  | s2    | 1649 | U    |
| 79  | s2    | 1654 | G    |
| 79  | s2    | 1662 | U    |
| 79  | s2    | 1663 | A    |
| 79  | s2    | 1664 | A    |
| 79  | s2    | 1665 | G    |
| 79  | s2    | 1671 | G    |
| 79  | s2    | 1680 | G    |
| 79  | s2    | 1683 | C    |
| 79  | s2    | 1694 | U    |
| 79  | s2    | 1696 | C    |
| 79  | s2    | 1699 | A    |
| 79  | s2    | 1706 | G    |
| 79  | s2    | 1712 | A    |
| 79  | s2    | 1715 | A    |
| 79  | s2    | 1722 | G    |
| 79  | s2    | 1726 | G    |
| 79  | s2    | 1729 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 79  | s2    | 1742 | C    |
| 79  | s2    | 1743 | G    |
| 79  | s2    | 1744 | G    |
| 79  | s2    | 1745 | A    |
| 79  | s2    | 1747 | C    |
| 79  | s2    | 1752 | C    |
| 79  | s2    | 1753 | C    |
| 79  | s2    | 1754 | G    |
| 79  | s2    | 1755 | C    |
| 79  | s2    | 1757 | G    |
| 79  | s2    | 1758 | G    |
| 79  | s2    | 1759 | G    |
| 79  | s2    | 1760 | G    |
| 79  | s2    | 1761 | U    |
| 79  | s2    | 1772 | C    |
| 79  | s2    | 1773 | C    |
| 79  | s2    | 1774 | C    |
| 79  | s2    | 1777 | G    |
| 79  | s2    | 1782 | G    |
| 79  | s2    | 1783 | C    |
| 79  | s2    | 1784 | G    |
| 79  | s2    | 1785 | C    |
| 79  | s2    | 1787 | G    |
| 79  | s2    | 1788 | A    |
| 79  | s2    | 1798 | C    |
| 79  | s2    | 1809 | A    |
| 79  | s2    | 1810 | U    |
| 79  | s2    | 1812 | U    |
| 79  | s2    | 1813 | A    |
| 79  | s2    | 1819 | A    |
| 79  | s2    | 1820 | G    |
| 79  | s2    | 1822 | A    |
| 79  | s2    | 1823 | A    |
| 79  | s2    | 1824 | A    |
| 79  | s2    | 1825 | A    |
| 79  | s2    | 1826 | G    |
| 79  | s2    | 1835 | A    |
| 79  | s2    | 1838 | U    |
| 79  | s2    | 1839 | U    |
| 79  | s2    | 1849 | G    |
| 79  | s2    | 1852 | C    |
| 79  | s2    | 1861 | G    |

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| Mol | Chain | Res   | Type |
|-----|-------|-------|------|
| 79  | s2    | 1863  | A    |
| 79  | s2    | 1864  | U    |
| 79  | s2    | 1865  | C    |
| 79  | s2    | 1866  | A    |
| 81  | aP    | 9     | A    |
| 81  | aP    | 10    | G    |
| 81  | aP    | 11    | U    |
| 81  | aP    | 13    | U    |
| 81  | aP    | 14    | A    |
| 81  | aP    | 19    | G    |
| 81  | aP    | 20(A) | U    |
| 81  | aP    | 21    | A    |
| 81  | aP    | 26    | G    |
| 81  | aP    | 30    | G    |
| 81  | aP    | 31    | C    |
| 81  | aP    | 34    | A    |
| 81  | aP    | 47    | U    |
| 81  | aP    | 48    | C    |
| 81  | aP    | 49    | C    |
| 81  | aP    | 54    | U    |
| 81  | aP    | 55    | U    |
| 81  | aP    | 56    | C    |
| 81  | aP    | 58    | A    |
| 81  | aP    | 61    | C    |
| 81  | aP    | 64    | G    |
| 81  | aP    | 66    | C    |
| 81  | aP    | 67    | G    |
| 81  | aP    | 70    | A    |
| 81  | aP    | 71    | A    |
| 82  | pE    | 5     | G    |
| 82  | pE    | 7     | A    |
| 82  | pE    | 8     | U    |
| 82  | pE    | 9     | A    |
| 82  | pE    | 10    | G    |
| 82  | pE    | 11    | C    |
| 82  | pE    | 16    | C    |
| 82  | pE    | 19    | G    |
| 82  | pE    | 20    | U    |
| 82  | pE    | 21    | A    |
| 82  | pE    | 22    | G    |
| 82  | pE    | 25    | C    |
| 82  | pE    | 26    | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 82  | pE    | 27  | U    |
| 82  | pE    | 31  | A    |
| 82  | pE    | 34  | U    |
| 82  | pE    | 35  | U    |
| 82  | pE    | 38  | A    |
| 82  | pE    | 39  | U    |
| 82  | pE    | 40  | C    |
| 82  | pE    | 46  | G    |
| 82  | pE    | 47  | U    |
| 82  | pE    | 48  | C    |
| 82  | pE    | 50  | A    |
| 82  | pE    | 52  | G    |
| 82  | pE    | 54  | U    |
| 82  | pE    | 55  | U    |
| 82  | pE    | 56  | C    |
| 82  | pE    | 58  | A    |
| 82  | pE    | 61  | C    |
| 82  | pE    | 65  | G    |
| 82  | pE    | 67  | U    |
| 82  | pE    | 69  | G    |
| 82  | pE    | 70  | G    |
| 82  | pE    | 76  | A    |
| 85  | l5    | 2   | G    |
| 85  | l5    | 13  | U    |
| 85  | l5    | 17  | A    |
| 85  | l5    | 25  | A    |
| 85  | l5    | 26  | C    |
| 85  | l5    | 30  | C    |
| 85  | l5    | 39  | A    |
| 85  | l5    | 42  | A    |
| 85  | l5    | 48  | G    |
| 85  | l5    | 56  | A    |
| 85  | l5    | 59  | A    |
| 85  | l5    | 64  | A    |
| 85  | l5    | 65  | A    |
| 85  | l5    | 67  | C    |
| 85  | l5    | 73  | A    |
| 85  | l5    | 74  | G    |
| 85  | l5    | 91  | G    |
| 85  | l5    | 95  | G    |
| 85  | l5    | 104 | G    |
| 85  | l5    | 108 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 85  | l5    | 109 | G    |
| 85  | l5    | 110 | C    |
| 85  | l5    | 116 | G    |
| 85  | l5    | 119 | G    |
| 85  | l5    | 120 | A    |
| 85  | l5    | 127 | G    |
| 85  | l5    | 132 | G    |
| 85  | l5    | 133 | C    |
| 85  | l5    | 134 | G    |
| 85  | l5    | 135 | G    |
| 85  | l5    | 144 | G    |
| 85  | l5    | 145 | G    |
| 85  | l5    | 152 | U    |
| 85  | l5    | 159 | C    |
| 85  | l5    | 164 | G    |
| 85  | l5    | 165 | A    |
| 85  | l5    | 170 | C    |
| 85  | l5    | 172 | C    |
| 85  | l5    | 181 | C    |
| 85  | l5    | 183 | C    |
| 85  | l5    | 184 | U    |
| 85  | l5    | 185 | C    |
| 85  | l5    | 187 | U    |
| 85  | l5    | 188 | G    |
| 85  | l5    | 189 | G    |
| 85  | l5    | 197 | A    |
| 85  | l5    | 200 | U    |
| 85  | l5    | 209 | U    |
| 85  | l5    | 210 | C    |
| 85  | l5    | 211 | G    |
| 85  | l5    | 213 | G    |
| 85  | l5    | 216 | C    |
| 85  | l5    | 218 | A    |
| 85  | l5    | 220 | C    |
| 85  | l5    | 234 | G    |
| 85  | l5    | 235 | A    |
| 85  | l5    | 250 | C    |
| 85  | l5    | 255 | C    |
| 85  | l5    | 256 | G    |
| 85  | l5    | 261 | G    |
| 85  | l5    | 263 | G    |
| 85  | l5    | 264 | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 85  | l5    | 265 | C    |
| 85  | l5    | 266 | C    |
| 85  | l5    | 267 | G    |
| 85  | l5    | 269 | G    |
| 85  | l5    | 274 | C    |
| 85  | l5    | 275 | C    |
| 85  | l5    | 276 | C    |
| 85  | l5    | 280 | G    |
| 85  | l5    | 281 | U    |
| 85  | l5    | 297 | U    |
| 85  | l5    | 306 | A    |
| 85  | l5    | 310 | G    |
| 85  | l5    | 315 | G    |
| 85  | l5    | 316 | U    |
| 85  | l5    | 340 | C    |
| 85  | l5    | 350 | C    |
| 85  | l5    | 373 | G    |
| 85  | l5    | 385 | A    |
| 85  | l5    | 387 | G    |
| 85  | l5    | 388 | A    |
| 85  | l5    | 396 | A    |
| 85  | l5    | 401 | G    |
| 85  | l5    | 407 | A    |
| 85  | l5    | 409 | G    |
| 85  | l5    | 410 | A    |
| 85  | l5    | 411 | G    |
| 85  | l5    | 412 | G    |
| 85  | l5    | 413 | G    |
| 85  | l5    | 414 | C    |
| 85  | l5    | 431 | G    |
| 85  | l5    | 432 | U    |
| 85  | l5    | 436 | C    |
| 85  | l5    | 440 | U    |
| 85  | l5    | 449 | C    |
| 85  | l5    | 450 | G    |
| 85  | l5    | 452 | A    |
| 85  | l5    | 453 | G    |
| 85  | l5    | 454 | U    |
| 85  | l5    | 456 | C    |
| 85  | l5    | 457 | G    |
| 85  | l5    | 462 | G    |
| 85  | l5    | 464 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 85  | l5    | 467 | U    |
| 85  | l5    | 468 | U    |
| 85  | l5    | 469 | C    |
| 85  | l5    | 472 | C    |
| 85  | l5    | 485 | C    |
| 85  | l5    | 486 | C    |
| 85  | l5    | 489 | C    |
| 85  | l5    | 493 | G    |
| 85  | l5    | 494 | U    |
| 85  | l5    | 497 | G    |
| 85  | l5    | 498 | C    |
| 85  | l5    | 499 | G    |
| 85  | l5    | 500 | G    |
| 85  | l5    | 501 | C    |
| 85  | l5    | 502 | C    |
| 85  | l5    | 503 | C    |
| 85  | l5    | 504 | G    |
| 85  | l5    | 505 | G    |
| 85  | l5    | 506 | C    |
| 85  | l5    | 509 | A    |
| 85  | l5    | 510 | U    |
| 85  | l5    | 511 | C    |
| 85  | l5    | 512 | U    |
| 85  | l5    | 513 | U    |
| 85  | l5    | 514 | U    |
| 85  | l5    | 518 | G    |
| 85  | l5    | 519 | C    |
| 85  | l5    | 643 | C    |
| 85  | l5    | 644 | G    |
| 85  | l5    | 646 | G    |
| 85  | l5    | 654 | C    |
| 85  | l5    | 656 | C    |
| 85  | l5    | 657 | C    |
| 85  | l5    | 659 | G    |
| 85  | l5    | 666 | G    |
| 85  | l5    | 667 | A    |
| 85  | l5    | 668 | C    |
| 85  | l5    | 669 | C    |
| 85  | l5    | 672 | C    |
| 85  | l5    | 673 | C    |
| 85  | l5    | 685 | C    |
| 85  | l5    | 686 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 85  | 15    | 687 | U    |
| 85  | 15    | 696 | C    |
| 85  | 15    | 700 | G    |
| 85  | 15    | 703 | G    |
| 85  | 15    | 704 | C    |
| 85  | 15    | 706 | C    |
| 85  | 15    | 708 | G    |
| 85  | 15    | 731 | G    |
| 85  | 15    | 738 | C    |
| 85  | 15    | 739 | G    |
| 85  | 15    | 741 | C    |
| 85  | 15    | 742 | G    |
| 85  | 15    | 750 | U    |
| 85  | 15    | 753 | C    |
| 85  | 15    | 754 | U    |
| 85  | 15    | 758 | G    |
| 85  | 15    | 759 | G    |
| 85  | 15    | 760 | G    |
| 85  | 15    | 904 | C    |
| 85  | 15    | 906 | C    |
| 85  | 15    | 907 | C    |
| 85  | 15    | 910 | G    |
| 85  | 15    | 911 | U    |
| 85  | 15    | 912 | G    |
| 85  | 15    | 913 | U    |
| 85  | 15    | 914 | U    |
| 85  | 15    | 915 | A    |
| 85  | 15    | 917 | A    |
| 85  | 15    | 918 | G    |
| 85  | 15    | 923 | C    |
| 85  | 15    | 924 | C    |
| 85  | 15    | 926 | G    |
| 85  | 15    | 932 | A    |
| 85  | 15    | 933 | G    |
| 85  | 15    | 935 | A    |
| 85  | 15    | 936 | C    |
| 85  | 15    | 937 | U    |
| 85  | 15    | 941 | C    |
| 85  | 15    | 944 | A    |
| 85  | 15    | 945 | U    |
| 85  | 15    | 946 | C    |
| 85  | 15    | 957 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 85  | l5    | 959  | G    |
| 85  | l5    | 960  | A    |
| 85  | l5    | 961  | G    |
| 85  | l5    | 962  | C    |
| 85  | l5    | 965  | G    |
| 85  | l5    | 967  | C    |
| 85  | l5    | 969  | C    |
| 85  | l5    | 970  | G    |
| 85  | l5    | 977  | C    |
| 85  | l5    | 982  | U    |
| 85  | l5    | 985  | C    |
| 85  | l5    | 989  | U    |
| 85  | l5    | 990  | C    |
| 85  | l5    | 992  | C    |
| 85  | l5    | 993  | G    |
| 85  | l5    | 995  | C    |
| 85  | l5    | 1048 | G    |
| 85  | l5    | 1049 | C    |
| 85  | l5    | 1050 | C    |
| 85  | l5    | 1051 | G    |
| 85  | l5    | 1066 | G    |
| 85  | l5    | 1070 | G    |
| 85  | l5    | 1071 | C    |
| 85  | l5    | 1072 | C    |
| 85  | l5    | 1075 | G    |
| 85  | l5    | 1076 | C    |
| 85  | l5    | 1082 | C    |
| 85  | l5    | 1083 | U    |
| 85  | l5    | 1094 | G    |
| 85  | l5    | 1095 | A    |
| 85  | l5    | 1168 | G    |
| 85  | l5    | 1171 | G    |
| 85  | l5    | 1172 | C    |
| 85  | l5    | 1173 | G    |
| 85  | l5    | 1178 | G    |
| 85  | l5    | 1179 | U    |
| 85  | l5    | 1180 | C    |
| 85  | l5    | 1182 | C    |
| 85  | l5    | 1183 | C    |
| 85  | l5    | 1200 | G    |
| 85  | l5    | 1202 | C    |
| 85  | l5    | 1203 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 85  | l5    | 1204 | C    |
| 85  | l5    | 1205 | G    |
| 85  | l5    | 1210 | C    |
| 85  | l5    | 1211 | G    |
| 85  | l5    | 1214 | C    |
| 85  | l5    | 1215 | C    |
| 85  | l5    | 1216 | C    |
| 85  | l5    | 1217 | G    |
| 85  | l5    | 1218 | G    |
| 85  | l5    | 1219 | G    |
| 85  | l5    | 1221 | G    |
| 85  | l5    | 1222 | A    |
| 85  | l5    | 1235 | G    |
| 85  | l5    | 1241 | C    |
| 85  | l5    | 1242 | G    |
| 85  | l5    | 1245 | C    |
| 85  | l5    | 1246 | G    |
| 85  | l5    | 1247 | U    |
| 85  | l5    | 1253 | G    |
| 85  | l5    | 1254 | A    |
| 85  | l5    | 1257 | A    |
| 85  | l5    | 1258 | G    |
| 85  | l5    | 1261 | G    |
| 85  | l5    | 1262 | G    |
| 85  | l5    | 1266 | G    |
| 85  | l5    | 1267 | C    |
| 85  | l5    | 1269 | G    |
| 85  | l5    | 1270 | A    |
| 85  | l5    | 1271 | G    |
| 85  | l5    | 1272 | C    |
| 85  | l5    | 1273 | G    |
| 85  | l5    | 1274 | A    |
| 85  | l5    | 1275 | G    |
| 85  | l5    | 1277 | G    |
| 85  | l5    | 1280 | C    |
| 85  | l5    | 1284 | G    |
| 85  | l5    | 1285 | U    |
| 85  | l5    | 1287 | G    |
| 85  | l5    | 1293 | G    |
| 85  | l5    | 1294 | A    |
| 85  | l5    | 1295 | C    |
| 85  | l5    | 1296 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 85  | l5    | 1301 | C    |
| 85  | l5    | 1324 | A    |
| 85  | l5    | 1326 | A    |
| 85  | l5    | 1337 | A    |
| 85  | l5    | 1344 | C    |
| 85  | l5    | 1345 | A    |
| 85  | l5    | 1354 | A    |
| 85  | l5    | 1358 | G    |
| 85  | l5    | 1359 | G    |
| 85  | l5    | 1365 | C    |
| 85  | l5    | 1367 | C    |
| 85  | l5    | 1370 | G    |
| 85  | l5    | 1378 | C    |
| 85  | l5    | 1381 | U    |
| 85  | l5    | 1387 | A    |
| 85  | l5    | 1394 | G    |
| 85  | l5    | 1397 | A    |
| 85  | l5    | 1404 | G    |
| 85  | l5    | 1405 | C    |
| 85  | l5    | 1407 | C    |
| 85  | l5    | 1408 | G    |
| 85  | l5    | 1409 | C    |
| 85  | l5    | 1410 | U    |
| 85  | l5    | 1411 | C    |
| 85  | l5    | 1414 | C    |
| 85  | l5    | 1415 | G    |
| 85  | l5    | 1417 | C    |
| 85  | l5    | 1418 | C    |
| 85  | l5    | 1420 | A    |
| 85  | l5    | 1425 | G    |
| 85  | l5    | 1437 | C    |
| 85  | l5    | 1439 | C    |
| 85  | l5    | 1443 | A    |
| 85  | l5    | 1444 | G    |
| 85  | l5    | 1446 | C    |
| 85  | l5    | 1447 | C    |
| 85  | l5    | 1452 | A    |
| 85  | l5    | 1457 | G    |
| 85  | l5    | 1465 | G    |
| 85  | l5    | 1482 | G    |
| 85  | l5    | 1483 | C    |
| 85  | l5    | 1493 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 85  | l5    | 1497 | A    |
| 85  | l5    | 1498 | G    |
| 85  | l5    | 1501 | C    |
| 85  | l5    | 1502 | G    |
| 85  | l5    | 1517 | G    |
| 85  | l5    | 1518 | A    |
| 85  | l5    | 1523 | A    |
| 85  | l5    | 1534 | A    |
| 85  | l5    | 1547 | A    |
| 85  | l5    | 1549 | G    |
| 85  | l5    | 1564 | A    |
| 85  | l5    | 1566 | C    |
| 85  | l5    | 1574 | G    |
| 85  | l5    | 1578 | U    |
| 85  | l5    | 1582 | U    |
| 85  | l5    | 1591 | U    |
| 85  | l5    | 1596 | U    |
| 85  | l5    | 1624 | G    |
| 85  | l5    | 1625 | G    |
| 85  | l5    | 1626 | G    |
| 85  | l5    | 1631 | A    |
| 85  | l5    | 1633 | G    |
| 85  | l5    | 1634 | A    |
| 85  | l5    | 1641 | G    |
| 85  | l5    | 1654 | G    |
| 85  | l5    | 1661 | C    |
| 85  | l5    | 1676 | C    |
| 85  | l5    | 1677 | U    |
| 85  | l5    | 1678 | C    |
| 85  | l5    | 1681 | G    |
| 85  | l5    | 1691 | G    |
| 85  | l5    | 1698 | C    |
| 85  | l5    | 1699 | A    |
| 85  | l5    | 1700 | G    |
| 85  | l5    | 1703 | C    |
| 85  | l5    | 1704 | C    |
| 85  | l5    | 1705 | G    |
| 85  | l5    | 1707 | C    |
| 85  | l5    | 1715 | C    |
| 85  | l5    | 1718 | C    |
| 85  | l5    | 1730 | U    |
| 85  | l5    | 1740 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 85  | l5    | 1741 | G    |
| 85  | l5    | 1742 | A    |
| 85  | l5    | 1750 | G    |
| 85  | l5    | 1753 | G    |
| 85  | l5    | 1754 | U    |
| 85  | l5    | 1757 | U    |
| 85  | l5    | 1758 | G    |
| 85  | l5    | 1760 | G    |
| 85  | l5    | 1761 | G    |
| 85  | l5    | 1762 | C    |
| 85  | l5    | 1763 | C    |
| 85  | l5    | 1764 | G    |
| 85  | l5    | 1765 | A    |
| 85  | l5    | 1766 | A    |
| 85  | l5    | 1767 | A    |
| 85  | l5    | 1768 | C    |
| 85  | l5    | 1769 | G    |
| 85  | l5    | 1770 | A    |
| 85  | l5    | 1775 | A    |
| 85  | l5    | 1787 | A    |
| 85  | l5    | 1803 | G    |
| 85  | l5    | 1804 | A    |
| 85  | l5    | 1806 | G    |
| 85  | l5    | 1810 | G    |
| 85  | l5    | 1820 | C    |
| 85  | l5    | 1821 | G    |
| 85  | l5    | 1822 | U    |
| 85  | l5    | 1833 | G    |
| 85  | l5    | 1836 | G    |
| 85  | l5    | 1837 | A    |
| 85  | l5    | 1842 | G    |
| 85  | l5    | 1843 | A    |
| 85  | l5    | 1855 | G    |
| 85  | l5    | 1869 | G    |
| 85  | l5    | 1882 | U    |
| 85  | l5    | 1897 | A    |
| 85  | l5    | 1917 | A    |
| 85  | l5    | 1918 | U    |
| 85  | l5    | 1919 | G    |
| 85  | l5    | 1920 | C    |
| 85  | l5    | 1921 | C    |
| 85  | l5    | 1922 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 85  | l5    | 1925 | G    |
| 85  | l5    | 1931 | C    |
| 85  | l5    | 1932 | A    |
| 85  | l5    | 1936 | C    |
| 85  | l5    | 1940 | G    |
| 85  | l5    | 1948 | G    |
| 85  | l5    | 1959 | U    |
| 85  | l5    | 1960 | A    |
| 85  | l5    | 1961 | G    |
| 85  | l5    | 1962 | A    |
| 85  | l5    | 1974 | U    |
| 85  | l5    | 1975 | G    |
| 85  | l5    | 1976 | G    |
| 85  | l5    | 1978 | C    |
| 85  | l5    | 1980 | U    |
| 85  | l5    | 1981 | G    |
| 85  | l5    | 1982 | G    |
| 85  | l5    | 1983 | A    |
| 85  | l5    | 1984 | A    |
| 85  | l5    | 1985 | G    |
| 85  | l5    | 1989 | G    |
| 85  | l5    | 1991 | A    |
| 85  | l5    | 1992 | U    |
| 85  | l5    | 1993 | C    |
| 85  | l5    | 1997 | U    |
| 85  | l5    | 1998 | A    |
| 85  | l5    | 2001 | G    |
| 85  | l5    | 2002 | A    |
| 85  | l5    | 2004 | U    |
| 85  | l5    | 2011 | C    |
| 85  | l5    | 2014 | C    |
| 85  | l5    | 2017 | A    |
| 85  | l5    | 2018 | C    |
| 85  | l5    | 2022 | C    |
| 85  | l5    | 2024 | G    |
| 85  | l5    | 2026 | A    |
| 85  | l5    | 2033 | A    |
| 85  | l5    | 2034 | G    |
| 85  | l5    | 2046 | G    |
| 85  | l5    | 2048 | U    |
| 85  | l5    | 2052 | G    |
| 85  | l5    | 2055 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 85  | l5    | 2056 | G    |
| 85  | l5    | 2069 | A    |
| 85  | l5    | 2084 | C    |
| 85  | l5    | 2085 | G    |
| 85  | l5    | 2092 | G    |
| 85  | l5    | 2093 | A    |
| 85  | l5    | 2095 | A    |
| 85  | l5    | 2096 | G    |
| 85  | l5    | 2097 | U    |
| 85  | l5    | 2098 | G    |
| 85  | l5    | 2101 | C    |
| 85  | l5    | 2102 | G    |
| 85  | l5    | 2103 | G    |
| 85  | l5    | 2106 | G    |
| 85  | l5    | 2107 | C    |
| 85  | l5    | 2108 | G    |
| 85  | l5    | 2112 | G    |
| 85  | l5    | 2250 | C    |
| 85  | l5    | 2252 | G    |
| 85  | l5    | 2253 | A    |
| 85  | l5    | 2255 | C    |
| 85  | l5    | 2256 | C    |
| 85  | l5    | 2257 | C    |
| 85  | l5    | 2258 | C    |
| 85  | l5    | 2259 | G    |
| 85  | l5    | 2260 | C    |
| 85  | l5    | 2289 | C    |
| 85  | l5    | 2300 | A    |
| 85  | l5    | 2301 | G    |
| 85  | l5    | 2306 | G    |
| 85  | l5    | 2313 | A    |
| 85  | l5    | 2331 | G    |
| 85  | l5    | 2332 | A    |
| 85  | l5    | 2333 | G    |
| 85  | l5    | 2348 | G    |
| 85  | l5    | 2349 | A    |
| 85  | l5    | 2351 | C    |
| 85  | l5    | 2360 | A    |
| 85  | l5    | 2364 | G    |
| 85  | l5    | 2389 | A    |
| 85  | l5    | 2395 | A    |
| 85  | l5    | 2397 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 85  | 15    | 2398 | U    |
| 85  | 15    | 2402 | G    |
| 85  | 15    | 2404 | A    |
| 85  | 15    | 2410 | C    |
| 85  | 15    | 2417 | A    |
| 85  | 15    | 2421 | G    |
| 85  | 15    | 2425 | U    |
| 85  | 15    | 2441 | C    |
| 85  | 15    | 2450 | G    |
| 85  | 15    | 2453 | A    |
| 85  | 15    | 2463 | G    |
| 85  | 15    | 2464 | C    |
| 85  | 15    | 2465 | C    |
| 85  | 15    | 2471 | G    |
| 85  | 15    | 2474 | G    |
| 85  | 15    | 2475 | G    |
| 85  | 15    | 2478 | C    |
| 85  | 15    | 2479 | G    |
| 85  | 15    | 2483 | G    |
| 85  | 15    | 2484 | A    |
| 85  | 15    | 2485 | U    |
| 85  | 15    | 2487 | G    |
| 85  | 15    | 2488 | C    |
| 85  | 15    | 2489 | C    |
| 85  | 15    | 2490 | U    |
| 85  | 15    | 2491 | C    |
| 85  | 15    | 2494 | U    |
| 85  | 15    | 2503 | G    |
| 85  | 15    | 2504 | C    |
| 85  | 15    | 2505 | C    |
| 85  | 15    | 2506 | G    |
| 85  | 15    | 2511 | A    |
| 85  | 15    | 2513 | A    |
| 85  | 15    | 2518 | G    |
| 85  | 15    | 2519 | U    |
| 85  | 15    | 2520 | C    |
| 85  | 15    | 2529 | A    |
| 85  | 15    | 2537 | A    |
| 85  | 15    | 2544 | G    |
| 85  | 15    | 2546 | G    |
| 85  | 15    | 2547 | G    |
| 85  | 15    | 2554 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 85  | 15    | 2555 | G    |
| 85  | 15    | 2557 | G    |
| 85  | 15    | 2560 | C    |
| 85  | 15    | 2565 | A    |
| 85  | 15    | 2568 | C    |
| 85  | 15    | 2583 | C    |
| 85  | 15    | 2586 | G    |
| 85  | 15    | 2587 | A    |
| 85  | 15    | 2588 | C    |
| 85  | 15    | 2589 | C    |
| 85  | 15    | 2601 | A    |
| 85  | 15    | 2618 | G    |
| 85  | 15    | 2627 | C    |
| 85  | 15    | 2638 | G    |
| 85  | 15    | 2643 | G    |
| 85  | 15    | 2652 | G    |
| 85  | 15    | 2653 | C    |
| 85  | 15    | 2662 | G    |
| 85  | 15    | 2669 | C    |
| 85  | 15    | 2673 | G    |
| 85  | 15    | 2676 | A    |
| 85  | 15    | 2687 | U    |
| 85  | 15    | 2694 | G    |
| 85  | 15    | 2695 | A    |
| 85  | 15    | 2696 | A    |
| 85  | 15    | 2703 | G    |
| 85  | 15    | 2707 | U    |
| 85  | 15    | 2708 | U    |
| 85  | 15    | 2710 | C    |
| 85  | 15    | 2711 | G    |
| 85  | 15    | 2719 | C    |
| 85  | 15    | 2721 | G    |
| 85  | 15    | 2724 | G    |
| 85  | 15    | 2726 | G    |
| 85  | 15    | 2730 | U    |
| 85  | 15    | 2739 | C    |
| 85  | 15    | 2742 | G    |
| 85  | 15    | 2743 | A    |
| 85  | 15    | 2746 | A    |
| 85  | 15    | 2761 | U    |
| 85  | 15    | 2763 | U    |
| 85  | 15    | 2764 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 85  | 15    | 2769 | U    |
| 85  | 15    | 2770 | C    |
| 85  | 15    | 2787 | A    |
| 85  | 15    | 2788 | U    |
| 85  | 15    | 2790 | U    |
| 85  | 15    | 2794 | C    |
| 85  | 15    | 2802 | C    |
| 85  | 15    | 2826 | U    |
| 85  | 15    | 2827 | G    |
| 85  | 15    | 2829 | U    |
| 85  | 15    | 2833 | A    |
| 85  | 15    | 2835 | A    |
| 85  | 15    | 2847 | G    |
| 85  | 15    | 2855 | G    |
| 85  | 15    | 2867 | C    |
| 85  | 15    | 2877 | G    |
| 85  | 15    | 2894 | A    |
| 85  | 15    | 2895 | A    |
| 85  | 15    | 2897 | G    |
| 85  | 15    | 2900 | U    |
| 85  | 15    | 2901 | G    |
| 85  | 15    | 2902 | G    |
| 85  | 15    | 2903 | G    |
| 85  | 15    | 2904 | U    |
| 85  | 15    | 2905 | C    |
| 85  | 15    | 2906 | G    |
| 85  | 15    | 2908 | U    |
| 85  | 15    | 3590 | G    |
| 85  | 15    | 3591 | C    |
| 85  | 15    | 3594 | C    |
| 85  | 15    | 3595 | U    |
| 85  | 15    | 3596 | A    |
| 85  | 15    | 3597 | G    |
| 85  | 15    | 3599 | A    |
| 85  | 15    | 3605 | C    |
| 85  | 15    | 3615 | G    |
| 85  | 15    | 3618 | C    |
| 85  | 15    | 3626 | G    |
| 85  | 15    | 3630 | A    |
| 85  | 15    | 3635 | A    |
| 85  | 15    | 3644 | U    |
| 85  | 15    | 3646 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 85  | 15    | 3652 | A    |
| 85  | 15    | 3662 | A    |
| 85  | 15    | 3664 | G    |
| 85  | 15    | 3670 | C    |
| 85  | 15    | 3673 | C    |
| 85  | 15    | 3674 | G    |
| 85  | 15    | 3685 | C    |
| 85  | 15    | 3692 | A    |
| 85  | 15    | 3710 | G    |
| 85  | 15    | 3711 | A    |
| 85  | 15    | 3713 | U    |
| 85  | 15    | 3726 | A    |
| 85  | 15    | 3727 | A    |
| 85  | 15    | 3735 | G    |
| 85  | 15    | 3748 | A    |
| 85  | 15    | 3750 | G    |
| 85  | 15    | 3756 | A    |
| 85  | 15    | 3759 | A    |
| 85  | 15    | 3772 | U    |
| 85  | 15    | 3773 | U    |
| 85  | 15    | 3776 | G    |
| 85  | 15    | 3777 | G    |
| 85  | 15    | 3778 | U    |
| 85  | 15    | 3784 | A    |
| 85  | 15    | 3786 | U    |
| 85  | 15    | 3801 | U    |
| 85  | 15    | 3802 | U    |
| 85  | 15    | 3810 | C    |
| 85  | 15    | 3811 | G    |
| 85  | 15    | 3812 | C    |
| 85  | 15    | 3817 | A    |
| 85  | 15    | 3818 | U    |
| 85  | 15    | 3819 | G    |
| 85  | 15    | 3823 | G    |
| 85  | 15    | 3839 | G    |
| 85  | 15    | 3840 | U    |
| 85  | 15    | 3841 | C    |
| 85  | 15    | 3867 | A    |
| 85  | 15    | 3876 | A    |
| 85  | 15    | 3877 | A    |
| 85  | 15    | 3878 | C    |
| 85  | 15    | 3879 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 85  | 15    | 3887 | C    |
| 85  | 15    | 3890 | A    |
| 85  | 15    | 3892 | U    |
| 85  | 15    | 3897 | G    |
| 85  | 15    | 3898 | G    |
| 85  | 15    | 3901 | A    |
| 85  | 15    | 3902 | A    |
| 85  | 15    | 3906 | A    |
| 85  | 15    | 3907 | G    |
| 85  | 15    | 3908 | A    |
| 85  | 15    | 3915 | U    |
| 85  | 15    | 3922 | G    |
| 85  | 15    | 3923 | A    |
| 85  | 15    | 3938 | G    |
| 85  | 15    | 3939 | G    |
| 85  | 15    | 3940 | U    |
| 85  | 15    | 3943 | A    |
| 85  | 15    | 3944 | G    |
| 85  | 15    | 3947 | A    |
| 85  | 15    | 3948 | C    |
| 85  | 15    | 3949 | A    |
| 85  | 15    | 3950 | U    |
| 85  | 15    | 3951 | G    |
| 85  | 15    | 3953 | G    |
| 85  | 15    | 3955 | G    |
| 85  | 15    | 3956 | G    |
| 85  | 15    | 3957 | U    |
| 85  | 15    | 3959 | U    |
| 85  | 15    | 3960 | A    |
| 85  | 15    | 3961 | G    |
| 85  | 15    | 3962 | A    |
| 85  | 15    | 3963 | A    |
| 85  | 15    | 3964 | U    |
| 85  | 15    | 3965 | A    |
| 85  | 15    | 3966 | A    |
| 85  | 15    | 3967 | G    |
| 85  | 15    | 3968 | U    |
| 85  | 15    | 3969 | G    |
| 85  | 15    | 3970 | G    |
| 85  | 15    | 3972 | A    |
| 85  | 15    | 3973 | G    |
| 85  | 15    | 4039 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 85  | l5    | 4041 | C    |
| 85  | l5    | 4042 | G    |
| 85  | l5    | 4043 | G    |
| 85  | l5    | 4044 | U    |
| 85  | l5    | 4046 | A    |
| 85  | l5    | 4047 | A    |
| 85  | l5    | 4048 | A    |
| 85  | l5    | 4049 | U    |
| 85  | l5    | 4050 | A    |
| 85  | l5    | 4051 | C    |
| 85  | l5    | 4052 | C    |
| 85  | l5    | 4053 | A    |
| 85  | l5    | 4054 | C    |
| 85  | l5    | 4055 | U    |
| 85  | l5    | 4056 | A    |
| 85  | l5    | 4057 | C    |
| 85  | l5    | 4058 | U    |
| 85  | l5    | 4059 | C    |
| 85  | l5    | 4060 | U    |
| 85  | l5    | 4062 | A    |
| 85  | l5    | 4063 | U    |
| 85  | l5    | 4064 | C    |
| 85  | l5    | 4065 | G    |
| 85  | l5    | 4067 | U    |
| 85  | l5    | 4068 | U    |
| 85  | l5    | 4069 | U    |
| 85  | l5    | 4076 | G    |
| 85  | l5    | 4084 | G    |
| 85  | l5    | 4096 | C    |
| 85  | l5    | 4097 | G    |
| 85  | l5    | 4098 | A    |
| 85  | l5    | 4099 | G    |
| 85  | l5    | 4101 | C    |
| 85  | l5    | 4102 | C    |
| 85  | l5    | 4103 | C    |
| 85  | l5    | 4104 | G    |
| 85  | l5    | 4108 | G    |
| 85  | l5    | 4111 | U    |
| 85  | l5    | 4114 | C    |
| 85  | l5    | 4115 | G    |
| 85  | l5    | 4116 | C    |
| 85  | l5    | 4117 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 85  | l5    | 4119 | C    |
| 85  | l5    | 4120 | U    |
| 85  | l5    | 4121 | G    |
| 85  | l5    | 4127 | A    |
| 85  | l5    | 4133 | C    |
| 85  | l5    | 4134 | C    |
| 85  | l5    | 4140 | C    |
| 85  | l5    | 4141 | G    |
| 85  | l5    | 4142 | C    |
| 85  | l5    | 4143 | G    |
| 85  | l5    | 4144 | C    |
| 85  | l5    | 4146 | G    |
| 85  | l5    | 4149 | C    |
| 85  | l5    | 4157 | A    |
| 85  | l5    | 4160 | C    |
| 85  | l5    | 4162 | C    |
| 85  | l5    | 4163 | U    |
| 85  | l5    | 4168 | G    |
| 85  | l5    | 4170 | A    |
| 85  | l5    | 4183 | G    |
| 85  | l5    | 4184 | G    |
| 85  | l5    | 4191 | G    |
| 85  | l5    | 4196 | G    |
| 85  | l5    | 4201 | G    |
| 85  | l5    | 4203 | A    |
| 85  | l5    | 4212 | A    |
| 85  | l5    | 4213 | A    |
| 85  | l5    | 4222 | G    |
| 85  | l5    | 4225 | G    |
| 85  | l5    | 4229 | U    |
| 85  | l5    | 4233 | A    |
| 85  | l5    | 4241 | C    |
| 85  | l5    | 4242 | U    |
| 85  | l5    | 4249 | G    |
| 85  | l5    | 4251 | A    |
| 85  | l5    | 4254 | G    |
| 85  | l5    | 4255 | A    |
| 85  | l5    | 4265 | U    |
| 85  | l5    | 4268 | A    |
| 85  | l5    | 4273 | A    |
| 85  | l5    | 4279 | A    |
| 85  | l5    | 4281 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 85  | l5    | 4290 | U    |
| 85  | l5    | 4291 | G    |
| 85  | l5    | 4297 | G    |
| 85  | l5    | 4304 | A    |
| 85  | l5    | 4305 | G    |
| 85  | l5    | 4306 | U    |
| 85  | l5    | 4314 | C    |
| 85  | l5    | 4319 | C    |
| 85  | l5    | 4326 | G    |
| 85  | l5    | 4330 | G    |
| 85  | l5    | 4332 | C    |
| 85  | l5    | 4349 | C    |
| 85  | l5    | 4354 | U    |
| 85  | l5    | 4373 | G    |
| 85  | l5    | 4376 | A    |
| 85  | l5    | 4377 | G    |
| 85  | l5    | 4378 | A    |
| 85  | l5    | 4380 | A    |
| 85  | l5    | 4387 | C    |
| 85  | l5    | 4391 | G    |
| 85  | l5    | 4393 | G    |
| 85  | l5    | 4394 | A    |
| 85  | l5    | 4422 | A    |
| 85  | l5    | 4426 | C    |
| 85  | l5    | 4433 | G    |
| 85  | l5    | 4438 | U    |
| 85  | l5    | 4448 | G    |
| 85  | l5    | 4449 | A    |
| 85  | l5    | 4452 | U    |
| 85  | l5    | 4453 | C    |
| 85  | l5    | 4464 | A    |
| 85  | l5    | 4466 | C    |
| 85  | l5    | 4488 | A    |
| 85  | l5    | 4500 | U    |
| 85  | l5    | 4512 | U    |
| 85  | l5    | 4513 | A    |
| 85  | l5    | 4518 | A    |
| 85  | l5    | 4522 | G    |
| 85  | l5    | 4524 | G    |
| 85  | l5    | 4528 | G    |
| 85  | l5    | 4545 | G    |
| 85  | l5    | 4548 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 85  | 15    | 4549 | G    |
| 85  | 15    | 4556 | U    |
| 85  | 15    | 4557 | U    |
| 85  | 15    | 4560 | C    |
| 85  | 15    | 4567 | G    |
| 85  | 15    | 4572 | U    |
| 85  | 15    | 4573 | G    |
| 85  | 15    | 4575 | G    |
| 85  | 15    | 4581 | G    |
| 85  | 15    | 4584 | A    |
| 85  | 15    | 4589 | A    |
| 85  | 15    | 4590 | A    |
| 85  | 15    | 4600 | G    |
| 85  | 15    | 4601 | U    |
| 85  | 15    | 4617 | G    |
| 85  | 15    | 4636 | U    |
| 85  | 15    | 4637 | G    |
| 85  | 15    | 4652 | G    |
| 85  | 15    | 4656 | A    |
| 85  | 15    | 4659 | G    |
| 85  | 15    | 4670 | C    |
| 85  | 15    | 4672 | A    |
| 85  | 15    | 4682 | U    |
| 85  | 15    | 4687 | A    |
| 85  | 15    | 4695 | C    |
| 85  | 15    | 4700 | A    |
| 85  | 15    | 4707 | A    |
| 85  | 15    | 4708 | A    |
| 85  | 15    | 4709 | U    |
| 85  | 15    | 4719 | G    |
| 85  | 15    | 4733 | C    |
| 85  | 15    | 4734 | A    |
| 85  | 15    | 4740 | G    |
| 85  | 15    | 4741 | C    |
| 85  | 15    | 4742 | G    |
| 85  | 15    | 4745 | G    |
| 85  | 15    | 4747 | C    |
| 85  | 15    | 4750 | G    |
| 85  | 15    | 4754 | G    |
| 85  | 15    | 4757 | C    |
| 85  | 15    | 4759 | C    |
| 85  | 15    | 4761 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 85  | 15    | 4764 | A    |
| 85  | 15    | 4765 | G    |
| 85  | 15    | 4771 | C    |
| 85  | 15    | 4772 | C    |
| 85  | 15    | 4773 | C    |
| 85  | 15    | 4775 | C    |
| 85  | 15    | 4776 | G    |
| 85  | 15    | 4859 | C    |
| 85  | 15    | 4860 | G    |
| 85  | 15    | 4862 | G    |
| 85  | 15    | 4863 | G    |
| 85  | 15    | 4865 | C    |
| 85  | 15    | 4870 | G    |
| 85  | 15    | 4871 | C    |
| 85  | 15    | 4875 | G    |
| 85  | 15    | 4877 | G    |
| 85  | 15    | 4880 | C    |
| 85  | 15    | 4881 | U    |
| 85  | 15    | 4882 | U    |
| 85  | 15    | 4883 | C    |
| 85  | 15    | 4887 | C    |
| 85  | 15    | 4889 | G    |
| 85  | 15    | 4895 | C    |
| 85  | 15    | 4896 | G    |
| 85  | 15    | 4897 | G    |
| 85  | 15    | 4900 | C    |
| 85  | 15    | 4901 | G    |
| 85  | 15    | 4902 | C    |
| 85  | 15    | 4910 | G    |
| 85  | 15    | 4912 | G    |
| 85  | 15    | 4914 | C    |
| 85  | 15    | 4922 | C    |
| 85  | 15    | 4923 | C    |
| 85  | 15    | 4925 | U    |
| 85  | 15    | 4926 | C    |
| 85  | 15    | 4927 | G    |
| 85  | 15    | 4928 | C    |
| 85  | 15    | 4931 | G    |
| 85  | 15    | 4941 | G    |
| 85  | 15    | 4943 | A    |
| 85  | 15    | 4944 | C    |
| 85  | 15    | 4947 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 85  | l5    | 4951 | G    |
| 85  | l5    | 4960 | G    |
| 85  | l5    | 4973 | U    |
| 85  | l5    | 4976 | U    |
| 85  | l5    | 4985 | U    |
| 85  | l5    | 4988 | U    |
| 85  | l5    | 4989 | U    |
| 85  | l5    | 4990 | C    |
| 85  | l5    | 4991 | U    |
| 85  | l5    | 5006 | U    |
| 85  | l5    | 5014 | A    |
| 85  | l5    | 5017 | G    |
| 85  | l5    | 5020 | G    |
| 85  | l5    | 5024 | C    |
| 85  | l5    | 5026 | U    |
| 85  | l5    | 5027 | C    |
| 85  | l5    | 5028 | G    |
| 85  | l5    | 5029 | C    |
| 85  | l5    | 5030 | U    |
| 85  | l5    | 5034 | A    |
| 85  | l5    | 5041 | G    |
| 85  | l5    | 5050 | C    |
| 85  | l5    | 5054 | C    |
| 85  | l5    | 5055 | G    |
| 85  | l5    | 5060 | A    |
| 85  | l5    | 5061 | A    |
| 85  | l5    | 5069 | U    |
| 85  | L5    | 2    | G    |
| 85  | L5    | 4    | G    |
| 85  | L5    | 13   | U    |
| 85  | L5    | 25   | A    |
| 85  | L5    | 26   | C    |
| 85  | L5    | 30   | C    |
| 85  | L5    | 39   | A    |
| 85  | L5    | 42   | A    |
| 85  | L5    | 48   | G    |
| 85  | L5    | 49   | U    |
| 85  | L5    | 56   | A    |
| 85  | L5    | 59   | A    |
| 85  | L5    | 64   | A    |
| 85  | L5    | 65   | A    |
| 85  | L5    | 67   | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 85  | L5    | 73  | A    |
| 85  | L5    | 91  | G    |
| 85  | L5    | 95  | G    |
| 85  | L5    | 104 | G    |
| 85  | L5    | 108 | A    |
| 85  | L5    | 109 | G    |
| 85  | L5    | 110 | C    |
| 85  | L5    | 116 | G    |
| 85  | L5    | 119 | G    |
| 85  | L5    | 120 | A    |
| 85  | L5    | 127 | G    |
| 85  | L5    | 132 | G    |
| 85  | L5    | 133 | C    |
| 85  | L5    | 134 | G    |
| 85  | L5    | 144 | G    |
| 85  | L5    | 145 | G    |
| 85  | L5    | 152 | U    |
| 85  | L5    | 159 | C    |
| 85  | L5    | 165 | A    |
| 85  | L5    | 166 | C    |
| 85  | L5    | 170 | C    |
| 85  | L5    | 171 | U    |
| 85  | L5    | 172 | C    |
| 85  | L5    | 181 | C    |
| 85  | L5    | 183 | C    |
| 85  | L5    | 184 | U    |
| 85  | L5    | 185 | C    |
| 85  | L5    | 188 | G    |
| 85  | L5    | 189 | G    |
| 85  | L5    | 200 | U    |
| 85  | L5    | 209 | U    |
| 85  | L5    | 213 | G    |
| 85  | L5    | 216 | C    |
| 85  | L5    | 218 | A    |
| 85  | L5    | 220 | C    |
| 85  | L5    | 232 | G    |
| 85  | L5    | 234 | G    |
| 85  | L5    | 235 | A    |
| 85  | L5    | 237 | G    |
| 85  | L5    | 250 | C    |
| 85  | L5    | 255 | C    |
| 85  | L5    | 256 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 85  | L5    | 261 | G    |
| 85  | L5    | 262 | G    |
| 85  | L5    | 264 | C    |
| 85  | L5    | 265 | C    |
| 85  | L5    | 266 | C    |
| 85  | L5    | 267 | G    |
| 85  | L5    | 269 | G    |
| 85  | L5    | 270 | U    |
| 85  | L5    | 274 | C    |
| 85  | L5    | 275 | C    |
| 85  | L5    | 276 | C    |
| 85  | L5    | 280 | G    |
| 85  | L5    | 281 | U    |
| 85  | L5    | 297 | U    |
| 85  | L5    | 306 | A    |
| 85  | L5    | 310 | G    |
| 85  | L5    | 315 | G    |
| 85  | L5    | 316 | U    |
| 85  | L5    | 332 | C    |
| 85  | L5    | 340 | C    |
| 85  | L5    | 350 | C    |
| 85  | L5    | 365 | U    |
| 85  | L5    | 372 | A    |
| 85  | L5    | 373 | G    |
| 85  | L5    | 385 | A    |
| 85  | L5    | 387 | G    |
| 85  | L5    | 388 | A    |
| 85  | L5    | 396 | A    |
| 85  | L5    | 401 | G    |
| 85  | L5    | 407 | A    |
| 85  | L5    | 409 | G    |
| 85  | L5    | 410 | A    |
| 85  | L5    | 411 | G    |
| 85  | L5    | 412 | G    |
| 85  | L5    | 413 | G    |
| 85  | L5    | 431 | G    |
| 85  | L5    | 438 | G    |
| 85  | L5    | 440 | U    |
| 85  | L5    | 447 | C    |
| 85  | L5    | 449 | C    |
| 85  | L5    | 450 | G    |
| 85  | L5    | 452 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 85  | L5    | 453 | G    |
| 85  | L5    | 454 | U    |
| 85  | L5    | 456 | C    |
| 85  | L5    | 457 | G    |
| 85  | L5    | 465 | G    |
| 85  | L5    | 467 | U    |
| 85  | L5    | 468 | U    |
| 85  | L5    | 472 | C    |
| 85  | L5    | 478 | G    |
| 85  | L5    | 484 | U    |
| 85  | L5    | 485 | C    |
| 85  | L5    | 486 | C    |
| 85  | L5    | 493 | G    |
| 85  | L5    | 494 | U    |
| 85  | L5    | 497 | G    |
| 85  | L5    | 498 | C    |
| 85  | L5    | 499 | G    |
| 85  | L5    | 500 | G    |
| 85  | L5    | 501 | C    |
| 85  | L5    | 502 | C    |
| 85  | L5    | 503 | C    |
| 85  | L5    | 504 | G    |
| 85  | L5    | 505 | G    |
| 85  | L5    | 506 | C    |
| 85  | L5    | 509 | A    |
| 85  | L5    | 510 | U    |
| 85  | L5    | 512 | U    |
| 85  | L5    | 513 | U    |
| 85  | L5    | 514 | U    |
| 85  | L5    | 515 | C    |
| 85  | L5    | 518 | G    |
| 85  | L5    | 643 | C    |
| 85  | L5    | 644 | G    |
| 85  | L5    | 646 | G    |
| 85  | L5    | 654 | C    |
| 85  | L5    | 655 | C    |
| 85  | L5    | 656 | C    |
| 85  | L5    | 657 | C    |
| 85  | L5    | 658 | C    |
| 85  | L5    | 659 | G    |
| 85  | L5    | 666 | G    |
| 85  | L5    | 667 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 85  | L5    | 668 | C    |
| 85  | L5    | 669 | C    |
| 85  | L5    | 672 | C    |
| 85  | L5    | 673 | C    |
| 85  | L5    | 674 | G    |
| 85  | L5    | 678 | C    |
| 85  | L5    | 679 | C    |
| 85  | L5    | 682 | G    |
| 85  | L5    | 685 | C    |
| 85  | L5    | 686 | A    |
| 85  | L5    | 687 | U    |
| 85  | L5    | 696 | C    |
| 85  | L5    | 703 | G    |
| 85  | L5    | 704 | C    |
| 85  | L5    | 706 | C    |
| 85  | L5    | 708 | G    |
| 85  | L5    | 729 | G    |
| 85  | L5    | 730 | G    |
| 85  | L5    | 731 | G    |
| 85  | L5    | 733 | A    |
| 85  | L5    | 738 | C    |
| 85  | L5    | 739 | G    |
| 85  | L5    | 742 | G    |
| 85  | L5    | 750 | U    |
| 85  | L5    | 753 | C    |
| 85  | L5    | 754 | U    |
| 85  | L5    | 758 | G    |
| 85  | L5    | 759 | G    |
| 85  | L5    | 904 | C    |
| 85  | L5    | 905 | C    |
| 85  | L5    | 906 | C    |
| 85  | L5    | 907 | C    |
| 85  | L5    | 910 | G    |
| 85  | L5    | 911 | U    |
| 85  | L5    | 912 | G    |
| 85  | L5    | 913 | U    |
| 85  | L5    | 914 | U    |
| 85  | L5    | 915 | A    |
| 85  | L5    | 917 | A    |
| 85  | L5    | 918 | G    |
| 85  | L5    | 923 | C    |
| 85  | L5    | 924 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 85  | L5    | 926  | G    |
| 85  | L5    | 932  | A    |
| 85  | L5    | 933  | G    |
| 85  | L5    | 935  | A    |
| 85  | L5    | 936  | C    |
| 85  | L5    | 937  | U    |
| 85  | L5    | 941  | C    |
| 85  | L5    | 943  | A    |
| 85  | L5    | 944  | A    |
| 85  | L5    | 945  | U    |
| 85  | L5    | 957  | G    |
| 85  | L5    | 959  | G    |
| 85  | L5    | 960  | A    |
| 85  | L5    | 961  | G    |
| 85  | L5    | 962  | C    |
| 85  | L5    | 965  | G    |
| 85  | L5    | 966  | A    |
| 85  | L5    | 967  | C    |
| 85  | L5    | 968  | C    |
| 85  | L5    | 969  | C    |
| 85  | L5    | 970  | G    |
| 85  | L5    | 982  | U    |
| 85  | L5    | 985  | C    |
| 85  | L5    | 989  | U    |
| 85  | L5    | 990  | C    |
| 85  | L5    | 992  | C    |
| 85  | L5    | 993  | G    |
| 85  | L5    | 995  | C    |
| 85  | L5    | 1048 | G    |
| 85  | L5    | 1049 | C    |
| 85  | L5    | 1050 | C    |
| 85  | L5    | 1051 | G    |
| 85  | L5    | 1066 | G    |
| 85  | L5    | 1070 | G    |
| 85  | L5    | 1071 | C    |
| 85  | L5    | 1072 | C    |
| 85  | L5    | 1075 | G    |
| 85  | L5    | 1082 | C    |
| 85  | L5    | 1083 | U    |
| 85  | L5    | 1095 | A    |
| 85  | L5    | 1168 | G    |
| 85  | L5    | 1171 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 85  | L5    | 1172 | C    |
| 85  | L5    | 1173 | G    |
| 85  | L5    | 1179 | U    |
| 85  | L5    | 1180 | C    |
| 85  | L5    | 1181 | C    |
| 85  | L5    | 1182 | C    |
| 85  | L5    | 1183 | C    |
| 85  | L5    | 1184 | A    |
| 85  | L5    | 1202 | C    |
| 85  | L5    | 1203 | G    |
| 85  | L5    | 1205 | G    |
| 85  | L5    | 1210 | C    |
| 85  | L5    | 1211 | G    |
| 85  | L5    | 1215 | C    |
| 85  | L5    | 1216 | C    |
| 85  | L5    | 1217 | G    |
| 85  | L5    | 1218 | G    |
| 85  | L5    | 1219 | G    |
| 85  | L5    | 1222 | A    |
| 85  | L5    | 1241 | C    |
| 85  | L5    | 1242 | G    |
| 85  | L5    | 1245 | C    |
| 85  | L5    | 1246 | G    |
| 85  | L5    | 1253 | G    |
| 85  | L5    | 1254 | A    |
| 85  | L5    | 1257 | A    |
| 85  | L5    | 1258 | G    |
| 85  | L5    | 1261 | G    |
| 85  | L5    | 1262 | G    |
| 85  | L5    | 1266 | G    |
| 85  | L5    | 1267 | C    |
| 85  | L5    | 1269 | G    |
| 85  | L5    | 1270 | A    |
| 85  | L5    | 1271 | G    |
| 85  | L5    | 1272 | C    |
| 85  | L5    | 1273 | G    |
| 85  | L5    | 1274 | A    |
| 85  | L5    | 1275 | G    |
| 85  | L5    | 1280 | C    |
| 85  | L5    | 1284 | G    |
| 85  | L5    | 1287 | G    |
| 85  | L5    | 1293 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 85  | L5    | 1294 | A    |
| 85  | L5    | 1295 | C    |
| 85  | L5    | 1296 | G    |
| 85  | L5    | 1301 | C    |
| 85  | L5    | 1314 | C    |
| 85  | L5    | 1322 | A    |
| 85  | L5    | 1325 | C    |
| 85  | L5    | 1326 | A    |
| 85  | L5    | 1337 | A    |
| 85  | L5    | 1345 | A    |
| 85  | L5    | 1354 | A    |
| 85  | L5    | 1358 | G    |
| 85  | L5    | 1359 | G    |
| 85  | L5    | 1365 | C    |
| 85  | L5    | 1366 | G    |
| 85  | L5    | 1367 | C    |
| 85  | L5    | 1370 | G    |
| 85  | L5    | 1378 | C    |
| 85  | L5    | 1381 | U    |
| 85  | L5    | 1387 | A    |
| 85  | L5    | 1394 | G    |
| 85  | L5    | 1397 | A    |
| 85  | L5    | 1404 | G    |
| 85  | L5    | 1405 | C    |
| 85  | L5    | 1407 | C    |
| 85  | L5    | 1409 | C    |
| 85  | L5    | 1410 | U    |
| 85  | L5    | 1414 | C    |
| 85  | L5    | 1415 | G    |
| 85  | L5    | 1417 | C    |
| 85  | L5    | 1418 | C    |
| 85  | L5    | 1420 | A    |
| 85  | L5    | 1425 | G    |
| 85  | L5    | 1434 | G    |
| 85  | L5    | 1435 | G    |
| 85  | L5    | 1437 | C    |
| 85  | L5    | 1439 | C    |
| 85  | L5    | 1443 | A    |
| 85  | L5    | 1444 | G    |
| 85  | L5    | 1446 | C    |
| 85  | L5    | 1447 | C    |
| 85  | L5    | 1452 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 85  | L5    | 1457 | G    |
| 85  | L5    | 1465 | G    |
| 85  | L5    | 1472 | C    |
| 85  | L5    | 1475 | G    |
| 85  | L5    | 1482 | G    |
| 85  | L5    | 1483 | C    |
| 85  | L5    | 1497 | A    |
| 85  | L5    | 1498 | G    |
| 85  | L5    | 1502 | G    |
| 85  | L5    | 1516 | G    |
| 85  | L5    | 1517 | G    |
| 85  | L5    | 1518 | A    |
| 85  | L5    | 1523 | A    |
| 85  | L5    | 1525 | A    |
| 85  | L5    | 1534 | A    |
| 85  | L5    | 1535 | C    |
| 85  | L5    | 1547 | A    |
| 85  | L5    | 1562 | G    |
| 85  | L5    | 1563 | A    |
| 85  | L5    | 1564 | A    |
| 85  | L5    | 1566 | C    |
| 85  | L5    | 1574 | G    |
| 85  | L5    | 1578 | U    |
| 85  | L5    | 1582 | U    |
| 85  | L5    | 1591 | U    |
| 85  | L5    | 1592 | G    |
| 85  | L5    | 1596 | U    |
| 85  | L5    | 1597 | G    |
| 85  | L5    | 1598 | C    |
| 85  | L5    | 1612 | G    |
| 85  | L5    | 1624 | G    |
| 85  | L5    | 1625 | G    |
| 85  | L5    | 1631 | A    |
| 85  | L5    | 1633 | G    |
| 85  | L5    | 1634 | A    |
| 85  | L5    | 1638 | A    |
| 85  | L5    | 1640 | C    |
| 85  | L5    | 1641 | G    |
| 85  | L5    | 1654 | G    |
| 85  | L5    | 1661 | C    |
| 85  | L5    | 1663 | C    |
| 85  | L5    | 1676 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 85  | L5    | 1677 | U    |
| 85  | L5    | 1678 | C    |
| 85  | L5    | 1681 | G    |
| 85  | L5    | 1691 | G    |
| 85  | L5    | 1698 | C    |
| 85  | L5    | 1699 | A    |
| 85  | L5    | 1700 | G    |
| 85  | L5    | 1701 | A    |
| 85  | L5    | 1703 | C    |
| 85  | L5    | 1704 | C    |
| 85  | L5    | 1705 | G    |
| 85  | L5    | 1707 | C    |
| 85  | L5    | 1718 | C    |
| 85  | L5    | 1730 | U    |
| 85  | L5    | 1732 | C    |
| 85  | L5    | 1734 | G    |
| 85  | L5    | 1740 | C    |
| 85  | L5    | 1741 | G    |
| 85  | L5    | 1742 | A    |
| 85  | L5    | 1750 | G    |
| 85  | L5    | 1753 | G    |
| 85  | L5    | 1754 | U    |
| 85  | L5    | 1757 | U    |
| 85  | L5    | 1758 | G    |
| 85  | L5    | 1760 | G    |
| 85  | L5    | 1761 | G    |
| 85  | L5    | 1762 | C    |
| 85  | L5    | 1763 | C    |
| 85  | L5    | 1764 | G    |
| 85  | L5    | 1765 | A    |
| 85  | L5    | 1766 | A    |
| 85  | L5    | 1767 | A    |
| 85  | L5    | 1768 | C    |
| 85  | L5    | 1770 | A    |
| 85  | L5    | 1781 | U    |
| 85  | L5    | 1787 | A    |
| 85  | L5    | 1804 | A    |
| 85  | L5    | 1806 | G    |
| 85  | L5    | 1810 | G    |
| 85  | L5    | 1820 | C    |
| 85  | L5    | 1821 | G    |
| 85  | L5    | 1822 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 85  | L5    | 1826 | G    |
| 85  | L5    | 1833 | G    |
| 85  | L5    | 1834 | U    |
| 85  | L5    | 1836 | G    |
| 85  | L5    | 1837 | A    |
| 85  | L5    | 1842 | G    |
| 85  | L5    | 1843 | A    |
| 85  | L5    | 1855 | G    |
| 85  | L5    | 1869 | G    |
| 85  | L5    | 1897 | A    |
| 85  | L5    | 1917 | A    |
| 85  | L5    | 1918 | U    |
| 85  | L5    | 1919 | G    |
| 85  | L5    | 1920 | C    |
| 85  | L5    | 1921 | C    |
| 85  | L5    | 1922 | G    |
| 85  | L5    | 1925 | G    |
| 85  | L5    | 1931 | C    |
| 85  | L5    | 1932 | A    |
| 85  | L5    | 1936 | C    |
| 85  | L5    | 1940 | G    |
| 85  | L5    | 1948 | G    |
| 85  | L5    | 1959 | U    |
| 85  | L5    | 1960 | A    |
| 85  | L5    | 1961 | G    |
| 85  | L5    | 1962 | A    |
| 85  | L5    | 1974 | U    |
| 85  | L5    | 1975 | G    |
| 85  | L5    | 1978 | C    |
| 85  | L5    | 1980 | U    |
| 85  | L5    | 1981 | G    |
| 85  | L5    | 1982 | G    |
| 85  | L5    | 1984 | A    |
| 85  | L5    | 1985 | G    |
| 85  | L5    | 1989 | G    |
| 85  | L5    | 1991 | A    |
| 85  | L5    | 1992 | U    |
| 85  | L5    | 1993 | C    |
| 85  | L5    | 1997 | U    |
| 85  | L5    | 1998 | A    |
| 85  | L5    | 2001 | G    |
| 85  | L5    | 2002 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 85  | L5    | 2004 | U    |
| 85  | L5    | 2011 | C    |
| 85  | L5    | 2014 | C    |
| 85  | L5    | 2017 | A    |
| 85  | L5    | 2018 | C    |
| 85  | L5    | 2022 | C    |
| 85  | L5    | 2024 | G    |
| 85  | L5    | 2026 | A    |
| 85  | L5    | 2033 | A    |
| 85  | L5    | 2034 | G    |
| 85  | L5    | 2046 | G    |
| 85  | L5    | 2048 | U    |
| 85  | L5    | 2055 | G    |
| 85  | L5    | 2056 | G    |
| 85  | L5    | 2062 | C    |
| 85  | L5    | 2069 | A    |
| 85  | L5    | 2084 | C    |
| 85  | L5    | 2085 | G    |
| 85  | L5    | 2092 | G    |
| 85  | L5    | 2093 | A    |
| 85  | L5    | 2095 | A    |
| 85  | L5    | 2096 | G    |
| 85  | L5    | 2097 | U    |
| 85  | L5    | 2098 | G    |
| 85  | L5    | 2101 | C    |
| 85  | L5    | 2102 | G    |
| 85  | L5    | 2103 | G    |
| 85  | L5    | 2107 | C    |
| 85  | L5    | 2108 | G    |
| 85  | L5    | 2112 | G    |
| 85  | L5    | 2250 | C    |
| 85  | L5    | 2252 | G    |
| 85  | L5    | 2253 | A    |
| 85  | L5    | 2256 | C    |
| 85  | L5    | 2258 | C    |
| 85  | L5    | 2259 | G    |
| 85  | L5    | 2260 | C    |
| 85  | L5    | 2263 | A    |
| 85  | L5    | 2264 | C    |
| 85  | L5    | 2289 | C    |
| 85  | L5    | 2300 | A    |
| 85  | L5    | 2301 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 85  | L5    | 2306 | G    |
| 85  | L5    | 2313 | A    |
| 85  | L5    | 2316 | G    |
| 85  | L5    | 2331 | G    |
| 85  | L5    | 2332 | A    |
| 85  | L5    | 2333 | G    |
| 85  | L5    | 2348 | G    |
| 85  | L5    | 2349 | A    |
| 85  | L5    | 2351 | C    |
| 85  | L5    | 2360 | A    |
| 85  | L5    | 2382 | A    |
| 85  | L5    | 2392 | C    |
| 85  | L5    | 2395 | A    |
| 85  | L5    | 2397 | G    |
| 85  | L5    | 2398 | U    |
| 85  | L5    | 2402 | G    |
| 85  | L5    | 2404 | A    |
| 85  | L5    | 2410 | C    |
| 85  | L5    | 2412 | A    |
| 85  | L5    | 2417 | A    |
| 85  | L5    | 2421 | G    |
| 85  | L5    | 2425 | U    |
| 85  | L5    | 2441 | C    |
| 85  | L5    | 2450 | G    |
| 85  | L5    | 2453 | A    |
| 85  | L5    | 2463 | G    |
| 85  | L5    | 2464 | C    |
| 85  | L5    | 2465 | C    |
| 85  | L5    | 2469 | C    |
| 85  | L5    | 2471 | G    |
| 85  | L5    | 2474 | G    |
| 85  | L5    | 2475 | G    |
| 85  | L5    | 2478 | C    |
| 85  | L5    | 2479 | G    |
| 85  | L5    | 2483 | G    |
| 85  | L5    | 2484 | A    |
| 85  | L5    | 2485 | U    |
| 85  | L5    | 2486 | G    |
| 85  | L5    | 2487 | G    |
| 85  | L5    | 2488 | C    |
| 85  | L5    | 2489 | C    |
| 85  | L5    | 2490 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 85  | L5    | 2491 | C    |
| 85  | L5    | 2494 | U    |
| 85  | L5    | 2503 | G    |
| 85  | L5    | 2504 | C    |
| 85  | L5    | 2506 | G    |
| 85  | L5    | 2511 | A    |
| 85  | L5    | 2513 | A    |
| 85  | L5    | 2518 | G    |
| 85  | L5    | 2519 | U    |
| 85  | L5    | 2529 | A    |
| 85  | L5    | 2537 | A    |
| 85  | L5    | 2544 | G    |
| 85  | L5    | 2546 | G    |
| 85  | L5    | 2547 | G    |
| 85  | L5    | 2554 | U    |
| 85  | L5    | 2555 | G    |
| 85  | L5    | 2557 | G    |
| 85  | L5    | 2559 | G    |
| 85  | L5    | 2560 | C    |
| 85  | L5    | 2565 | A    |
| 85  | L5    | 2568 | C    |
| 85  | L5    | 2583 | C    |
| 85  | L5    | 2586 | G    |
| 85  | L5    | 2587 | A    |
| 85  | L5    | 2589 | C    |
| 85  | L5    | 2601 | A    |
| 85  | L5    | 2602 | G    |
| 85  | L5    | 2618 | G    |
| 85  | L5    | 2627 | C    |
| 85  | L5    | 2632 | U    |
| 85  | L5    | 2652 | G    |
| 85  | L5    | 2653 | C    |
| 85  | L5    | 2662 | G    |
| 85  | L5    | 2669 | C    |
| 85  | L5    | 2673 | G    |
| 85  | L5    | 2676 | A    |
| 85  | L5    | 2686 | G    |
| 85  | L5    | 2687 | U    |
| 85  | L5    | 2694 | G    |
| 85  | L5    | 2695 | A    |
| 85  | L5    | 2696 | A    |
| 85  | L5    | 2701 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 85  | L5    | 2703 | G    |
| 85  | L5    | 2707 | U    |
| 85  | L5    | 2708 | U    |
| 85  | L5    | 2710 | C    |
| 85  | L5    | 2711 | G    |
| 85  | L5    | 2712 | G    |
| 85  | L5    | 2719 | C    |
| 85  | L5    | 2721 | G    |
| 85  | L5    | 2724 | G    |
| 85  | L5    | 2726 | G    |
| 85  | L5    | 2730 | U    |
| 85  | L5    | 2739 | C    |
| 85  | L5    | 2742 | G    |
| 85  | L5    | 2743 | A    |
| 85  | L5    | 2746 | A    |
| 85  | L5    | 2754 | G    |
| 85  | L5    | 2759 | G    |
| 85  | L5    | 2761 | U    |
| 85  | L5    | 2763 | U    |
| 85  | L5    | 2764 | A    |
| 85  | L5    | 2769 | U    |
| 85  | L5    | 2770 | C    |
| 85  | L5    | 2786 | C    |
| 85  | L5    | 2787 | A    |
| 85  | L5    | 2788 | U    |
| 85  | L5    | 2790 | U    |
| 85  | L5    | 2799 | G    |
| 85  | L5    | 2825 | A    |
| 85  | L5    | 2826 | U    |
| 85  | L5    | 2827 | G    |
| 85  | L5    | 2828 | U    |
| 85  | L5    | 2829 | U    |
| 85  | L5    | 2833 | A    |
| 85  | L5    | 2835 | A    |
| 85  | L5    | 2846 | G    |
| 85  | L5    | 2855 | G    |
| 85  | L5    | 2867 | C    |
| 85  | L5    | 2877 | G    |
| 85  | L5    | 2894 | A    |
| 85  | L5    | 2895 | A    |
| 85  | L5    | 2897 | G    |
| 85  | L5    | 2899 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 85  | L5    | 2900 | U    |
| 85  | L5    | 2902 | G    |
| 85  | L5    | 2903 | G    |
| 85  | L5    | 2904 | U    |
| 85  | L5    | 2905 | C    |
| 85  | L5    | 2906 | G    |
| 85  | L5    | 2908 | U    |
| 85  | L5    | 3588 | C    |
| 85  | L5    | 3590 | G    |
| 85  | L5    | 3591 | C    |
| 85  | L5    | 3594 | C    |
| 85  | L5    | 3595 | U    |
| 85  | L5    | 3596 | A    |
| 85  | L5    | 3597 | G    |
| 85  | L5    | 3599 | A    |
| 85  | L5    | 3605 | C    |
| 85  | L5    | 3615 | G    |
| 85  | L5    | 3618 | C    |
| 85  | L5    | 3626 | G    |
| 85  | L5    | 3630 | A    |
| 85  | L5    | 3635 | A    |
| 85  | L5    | 3646 | A    |
| 85  | L5    | 3662 | A    |
| 85  | L5    | 3664 | G    |
| 85  | L5    | 3670 | C    |
| 85  | L5    | 3673 | C    |
| 85  | L5    | 3674 | G    |
| 85  | L5    | 3680 | U    |
| 85  | L5    | 3685 | C    |
| 85  | L5    | 3692 | A    |
| 85  | L5    | 3696 | C    |
| 85  | L5    | 3698 | G    |
| 85  | L5    | 3706 | C    |
| 85  | L5    | 3710 | G    |
| 85  | L5    | 3711 | A    |
| 85  | L5    | 3713 | U    |
| 85  | L5    | 3726 | A    |
| 85  | L5    | 3727 | A    |
| 85  | L5    | 3748 | A    |
| 85  | L5    | 3750 | G    |
| 85  | L5    | 3756 | A    |
| 85  | L5    | 3759 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 85  | L5    | 3772 | U    |
| 85  | L5    | 3773 | U    |
| 85  | L5    | 3774 | A    |
| 85  | L5    | 3776 | G    |
| 85  | L5    | 3777 | G    |
| 85  | L5    | 3778 | U    |
| 85  | L5    | 3784 | A    |
| 85  | L5    | 3786 | U    |
| 85  | L5    | 3788 | C    |
| 85  | L5    | 3801 | U    |
| 85  | L5    | 3802 | U    |
| 85  | L5    | 3810 | C    |
| 85  | L5    | 3811 | G    |
| 85  | L5    | 3812 | C    |
| 85  | L5    | 3814 | U    |
| 85  | L5    | 3817 | A    |
| 85  | L5    | 3818 | U    |
| 85  | L5    | 3819 | G    |
| 85  | L5    | 3823 | G    |
| 85  | L5    | 3838 | U    |
| 85  | L5    | 3839 | G    |
| 85  | L5    | 3840 | U    |
| 85  | L5    | 3843 | C    |
| 85  | L5    | 3867 | A    |
| 85  | L5    | 3876 | A    |
| 85  | L5    | 3877 | A    |
| 85  | L5    | 3878 | C    |
| 85  | L5    | 3879 | G    |
| 85  | L5    | 3887 | C    |
| 85  | L5    | 3890 | A    |
| 85  | L5    | 3892 | U    |
| 85  | L5    | 3897 | G    |
| 85  | L5    | 3898 | G    |
| 85  | L5    | 3901 | A    |
| 85  | L5    | 3906 | A    |
| 85  | L5    | 3907 | G    |
| 85  | L5    | 3908 | A    |
| 85  | L5    | 3915 | U    |
| 85  | L5    | 3920 | U    |
| 85  | L5    | 3922 | G    |
| 85  | L5    | 3923 | A    |
| 85  | L5    | 3928 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 85  | L5    | 3938 | G    |
| 85  | L5    | 3939 | G    |
| 85  | L5    | 3943 | A    |
| 85  | L5    | 3944 | G    |
| 85  | L5    | 3947 | A    |
| 85  | L5    | 3948 | C    |
| 85  | L5    | 3949 | A    |
| 85  | L5    | 3950 | U    |
| 85  | L5    | 3951 | G    |
| 85  | L5    | 3953 | G    |
| 85  | L5    | 3955 | G    |
| 85  | L5    | 3956 | G    |
| 85  | L5    | 3957 | U    |
| 85  | L5    | 3959 | U    |
| 85  | L5    | 3960 | A    |
| 85  | L5    | 3962 | A    |
| 85  | L5    | 3963 | A    |
| 85  | L5    | 3964 | U    |
| 85  | L5    | 3965 | A    |
| 85  | L5    | 3966 | A    |
| 85  | L5    | 3967 | G    |
| 85  | L5    | 3968 | U    |
| 85  | L5    | 3969 | G    |
| 85  | L5    | 3970 | G    |
| 85  | L5    | 3972 | A    |
| 85  | L5    | 3973 | G    |
| 85  | L5    | 4039 | G    |
| 85  | L5    | 4041 | C    |
| 85  | L5    | 4042 | G    |
| 85  | L5    | 4043 | G    |
| 85  | L5    | 4044 | U    |
| 85  | L5    | 4046 | A    |
| 85  | L5    | 4047 | A    |
| 85  | L5    | 4048 | A    |
| 85  | L5    | 4049 | U    |
| 85  | L5    | 4050 | A    |
| 85  | L5    | 4051 | C    |
| 85  | L5    | 4052 | C    |
| 85  | L5    | 4053 | A    |
| 85  | L5    | 4054 | C    |
| 85  | L5    | 4055 | U    |
| 85  | L5    | 4056 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 85  | L5    | 4057 | C    |
| 85  | L5    | 4058 | U    |
| 85  | L5    | 4059 | C    |
| 85  | L5    | 4060 | U    |
| 85  | L5    | 4061 | G    |
| 85  | L5    | 4062 | A    |
| 85  | L5    | 4063 | U    |
| 85  | L5    | 4064 | C    |
| 85  | L5    | 4065 | G    |
| 85  | L5    | 4067 | U    |
| 85  | L5    | 4068 | U    |
| 85  | L5    | 4069 | U    |
| 85  | L5    | 4076 | G    |
| 85  | L5    | 4088 | C    |
| 85  | L5    | 4092 | G    |
| 85  | L5    | 4093 | G    |
| 85  | L5    | 4094 | G    |
| 85  | L5    | 4095 | G    |
| 85  | L5    | 4096 | C    |
| 85  | L5    | 4097 | G    |
| 85  | L5    | 4099 | G    |
| 85  | L5    | 4101 | C    |
| 85  | L5    | 4102 | C    |
| 85  | L5    | 4103 | C    |
| 85  | L5    | 4104 | G    |
| 85  | L5    | 4105 | A    |
| 85  | L5    | 4106 | G    |
| 85  | L5    | 4107 | G    |
| 85  | L5    | 4108 | G    |
| 85  | L5    | 4109 | G    |
| 85  | L5    | 4110 | C    |
| 85  | L5    | 4111 | U    |
| 85  | L5    | 4112 | C    |
| 85  | L5    | 4113 | U    |
| 85  | L5    | 4114 | C    |
| 85  | L5    | 4115 | G    |
| 85  | L5    | 4116 | C    |
| 85  | L5    | 4117 | U    |
| 85  | L5    | 4119 | C    |
| 85  | L5    | 4122 | G    |
| 85  | L5    | 4127 | A    |
| 85  | L5    | 4128 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 85  | L5    | 4133 | C    |
| 85  | L5    | 4134 | C    |
| 85  | L5    | 4140 | C    |
| 85  | L5    | 4141 | G    |
| 85  | L5    | 4142 | C    |
| 85  | L5    | 4143 | G    |
| 85  | L5    | 4144 | C    |
| 85  | L5    | 4146 | G    |
| 85  | L5    | 4149 | C    |
| 85  | L5    | 4160 | C    |
| 85  | L5    | 4162 | C    |
| 85  | L5    | 4163 | U    |
| 85  | L5    | 4168 | G    |
| 85  | L5    | 4170 | A    |
| 85  | L5    | 4183 | G    |
| 85  | L5    | 4184 | G    |
| 85  | L5    | 4191 | G    |
| 85  | L5    | 4196 | G    |
| 85  | L5    | 4197 | G    |
| 85  | L5    | 4201 | G    |
| 85  | L5    | 4203 | A    |
| 85  | L5    | 4212 | A    |
| 85  | L5    | 4222 | G    |
| 85  | L5    | 4225 | G    |
| 85  | L5    | 4229 | U    |
| 85  | L5    | 4232 | U    |
| 85  | L5    | 4233 | A    |
| 85  | L5    | 4234 | A    |
| 85  | L5    | 4241 | C    |
| 85  | L5    | 4251 | A    |
| 85  | L5    | 4254 | G    |
| 85  | L5    | 4255 | A    |
| 85  | L5    | 4265 | U    |
| 85  | L5    | 4268 | A    |
| 85  | L5    | 4273 | A    |
| 85  | L5    | 4280 | A    |
| 85  | L5    | 4281 | A    |
| 85  | L5    | 4289 | U    |
| 85  | L5    | 4290 | U    |
| 85  | L5    | 4297 | G    |
| 85  | L5    | 4304 | A    |
| 85  | L5    | 4305 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 85  | L5    | 4306 | U    |
| 85  | L5    | 4313 | A    |
| 85  | L5    | 4314 | C    |
| 85  | L5    | 4326 | G    |
| 85  | L5    | 4329 | G    |
| 85  | L5    | 4330 | G    |
| 85  | L5    | 4332 | C    |
| 85  | L5    | 4339 | A    |
| 85  | L5    | 4349 | C    |
| 85  | L5    | 4354 | U    |
| 85  | L5    | 4373 | G    |
| 85  | L5    | 4377 | G    |
| 85  | L5    | 4378 | A    |
| 85  | L5    | 4380 | A    |
| 85  | L5    | 4387 | C    |
| 85  | L5    | 4393 | G    |
| 85  | L5    | 4394 | A    |
| 85  | L5    | 4421 | C    |
| 85  | L5    | 4422 | A    |
| 85  | L5    | 4426 | C    |
| 85  | L5    | 4438 | U    |
| 85  | L5    | 4444 | C    |
| 85  | L5    | 4448 | G    |
| 85  | L5    | 4449 | A    |
| 85  | L5    | 4453 | C    |
| 85  | L5    | 4464 | A    |
| 85  | L5    | 4466 | C    |
| 85  | L5    | 4475 | G    |
| 85  | L5    | 4477 | A    |
| 85  | L5    | 4488 | A    |
| 85  | L5    | 4500 | U    |
| 85  | L5    | 4512 | U    |
| 85  | L5    | 4513 | A    |
| 85  | L5    | 4518 | A    |
| 85  | L5    | 4522 | G    |
| 85  | L5    | 4524 | G    |
| 85  | L5    | 4545 | G    |
| 85  | L5    | 4548 | A    |
| 85  | L5    | 4549 | G    |
| 85  | L5    | 4557 | U    |
| 85  | L5    | 4560 | C    |
| 85  | L5    | 4567 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 85  | L5    | 4572 | U    |
| 85  | L5    | 4573 | G    |
| 85  | L5    | 4575 | G    |
| 85  | L5    | 4581 | G    |
| 85  | L5    | 4584 | A    |
| 85  | L5    | 4589 | A    |
| 85  | L5    | 4590 | A    |
| 85  | L5    | 4600 | G    |
| 85  | L5    | 4601 | U    |
| 85  | L5    | 4617 | G    |
| 85  | L5    | 4627 | U    |
| 85  | L5    | 4635 | A    |
| 85  | L5    | 4636 | U    |
| 85  | L5    | 4637 | G    |
| 85  | L5    | 4652 | G    |
| 85  | L5    | 4656 | A    |
| 85  | L5    | 4659 | G    |
| 85  | L5    | 4670 | C    |
| 85  | L5    | 4672 | A    |
| 85  | L5    | 4687 | A    |
| 85  | L5    | 4694 | G    |
| 85  | L5    | 4695 | C    |
| 85  | L5    | 4700 | A    |
| 85  | L5    | 4707 | A    |
| 85  | L5    | 4708 | A    |
| 85  | L5    | 4709 | U    |
| 85  | L5    | 4719 | G    |
| 85  | L5    | 4721 | G    |
| 85  | L5    | 4732 | G    |
| 85  | L5    | 4733 | C    |
| 85  | L5    | 4734 | A    |
| 85  | L5    | 4740 | G    |
| 85  | L5    | 4741 | C    |
| 85  | L5    | 4742 | G    |
| 85  | L5    | 4745 | G    |
| 85  | L5    | 4747 | C    |
| 85  | L5    | 4750 | G    |
| 85  | L5    | 4754 | G    |
| 85  | L5    | 4757 | C    |
| 85  | L5    | 4759 | C    |
| 85  | L5    | 4761 | G    |
| 85  | L5    | 4764 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 85  | L5    | 4765 | G    |
| 85  | L5    | 4771 | C    |
| 85  | L5    | 4772 | C    |
| 85  | L5    | 4773 | C    |
| 85  | L5    | 4775 | C    |
| 85  | L5    | 4776 | G    |
| 85  | L5    | 4859 | C    |
| 85  | L5    | 4860 | G    |
| 85  | L5    | 4862 | G    |
| 85  | L5    | 4863 | G    |
| 85  | L5    | 4865 | C    |
| 85  | L5    | 4867 | G    |
| 85  | L5    | 4870 | G    |
| 85  | L5    | 4871 | C    |
| 85  | L5    | 4875 | G    |
| 85  | L5    | 4877 | G    |
| 85  | L5    | 4880 | C    |
| 85  | L5    | 4881 | U    |
| 85  | L5    | 4882 | U    |
| 85  | L5    | 4883 | C    |
| 85  | L5    | 4889 | G    |
| 85  | L5    | 4895 | C    |
| 85  | L5    | 4896 | G    |
| 85  | L5    | 4900 | C    |
| 85  | L5    | 4901 | G    |
| 85  | L5    | 4902 | C    |
| 85  | L5    | 4910 | G    |
| 85  | L5    | 4912 | G    |
| 85  | L5    | 4913 | G    |
| 85  | L5    | 4914 | C    |
| 85  | L5    | 4918 | C    |
| 85  | L5    | 4922 | C    |
| 85  | L5    | 4923 | C    |
| 85  | L5    | 4925 | U    |
| 85  | L5    | 4926 | C    |
| 85  | L5    | 4927 | G    |
| 85  | L5    | 4928 | C    |
| 85  | L5    | 4931 | G    |
| 85  | L5    | 4937 | C    |
| 85  | L5    | 4940 | C    |
| 85  | L5    | 4941 | G    |
| 85  | L5    | 4943 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 85  | L5    | 4944 | C    |
| 85  | L5    | 4947 | U    |
| 85  | L5    | 4951 | G    |
| 85  | L5    | 4960 | G    |
| 85  | L5    | 4976 | U    |
| 85  | L5    | 4985 | U    |
| 85  | L5    | 4988 | U    |
| 85  | L5    | 4989 | U    |
| 85  | L5    | 4990 | C    |
| 85  | L5    | 4991 | U    |
| 85  | L5    | 4995 | U    |
| 85  | L5    | 5006 | U    |
| 85  | L5    | 5009 | G    |
| 85  | L5    | 5014 | A    |
| 85  | L5    | 5017 | G    |
| 85  | L5    | 5020 | G    |
| 85  | L5    | 5024 | C    |
| 85  | L5    | 5026 | U    |
| 85  | L5    | 5027 | C    |
| 85  | L5    | 5028 | G    |
| 85  | L5    | 5029 | C    |
| 85  | L5    | 5030 | U    |
| 85  | L5    | 5034 | A    |
| 85  | L5    | 5041 | G    |
| 85  | L5    | 5050 | C    |
| 85  | L5    | 5054 | C    |
| 85  | L5    | 5055 | G    |
| 85  | L5    | 5061 | A    |
| 85  | L5    | 5062 | G    |
| 85  | L5    | 5069 | U    |
| 20  | L7    | 2    | U    |
| 20  | L7    | 4    | U    |
| 20  | L7    | 5    | A    |
| 20  | L7    | 22   | A    |
| 20  | L7    | 24   | C    |
| 20  | L7    | 33   | U    |
| 20  | L7    | 38   | U    |
| 20  | L7    | 53   | U    |
| 20  | L7    | 54   | A    |
| 20  | L7    | 63   | C    |
| 20  | L7    | 64   | G    |
| 20  | L7    | 91   | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 20  | L7    | 97  | G    |
| 20  | L7    | 100 | A    |
| 20  | L7    | 111 | C    |
| 21  | L8    | 2   | G    |
| 21  | L8    | 34  | U    |
| 21  | L8    | 35  | C    |
| 21  | L8    | 48  | A    |
| 21  | L8    | 59  | A    |
| 21  | L8    | 62  | A    |
| 21  | L8    | 63  | U    |
| 21  | L8    | 80  | A    |
| 21  | L8    | 82  | A    |
| 21  | L8    | 83  | C    |
| 21  | L8    | 84  | A    |
| 21  | L8    | 85  | U    |
| 21  | L8    | 86  | U    |
| 21  | L8    | 87  | G    |
| 21  | L8    | 94  | G    |
| 21  | L8    | 103 | A    |
| 21  | L8    | 105 | C    |
| 21  | L8    | 110 | U    |
| 21  | L8    | 111 | U    |
| 21  | L8    | 112 | G    |
| 21  | L8    | 114 | G    |
| 21  | L8    | 123 | U    |
| 21  | L8    | 124 | U    |
| 21  | L8    | 125 | C    |
| 21  | L8    | 126 | C    |
| 21  | L8    | 127 | U    |
| 21  | L8    | 151 | G    |
| 21  | L8    | 156 | U    |
| 79  | S2    | 2   | A    |
| 79  | S2    | 4   | C    |
| 79  | S2    | 13  | C    |
| 79  | S2    | 25  | A    |
| 79  | S2    | 33  | G    |
| 79  | S2    | 41  | G    |
| 79  | S2    | 42  | A    |
| 79  | S2    | 44  | U    |
| 79  | S2    | 45  | A    |
| 79  | S2    | 46  | A    |
| 79  | S2    | 56  | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 79  | S2    | 59  | U    |
| 79  | S2    | 62  | G    |
| 79  | S2    | 64  | A    |
| 79  | S2    | 65  | C    |
| 79  | S2    | 66  | G    |
| 79  | S2    | 67  | C    |
| 79  | S2    | 68  | A    |
| 79  | S2    | 72  | C    |
| 79  | S2    | 73  | C    |
| 79  | S2    | 74  | G    |
| 79  | S2    | 76  | U    |
| 79  | S2    | 92  | A    |
| 79  | S2    | 103 | A    |
| 79  | S2    | 113 | G    |
| 79  | S2    | 114 | G    |
| 79  | S2    | 115 | U    |
| 79  | S2    | 116 | U    |
| 79  | S2    | 126 | G    |
| 79  | S2    | 129 | C    |
| 79  | S2    | 130 | G    |
| 79  | S2    | 143 | U    |
| 79  | S2    | 147 | A    |
| 79  | S2    | 149 | A    |
| 79  | S2    | 158 | A    |
| 79  | S2    | 160 | U    |
| 79  | S2    | 162 | C    |
| 79  | S2    | 163 | U    |
| 79  | S2    | 170 | A    |
| 79  | S2    | 175 | A    |
| 79  | S2    | 179 | C    |
| 79  | S2    | 182 | C    |
| 79  | S2    | 188 | C    |
| 79  | S2    | 190 | G    |
| 79  | S2    | 192 | C    |
| 79  | S2    | 196 | C    |
| 79  | S2    | 197 | U    |
| 79  | S2    | 198 | U    |
| 79  | S2    | 200 | G    |
| 79  | S2    | 202 | G    |
| 79  | S2    | 203 | G    |
| 79  | S2    | 204 | G    |
| 79  | S2    | 206 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 79  | S2    | 207 | G    |
| 79  | S2    | 208 | G    |
| 79  | S2    | 209 | A    |
| 79  | S2    | 211 | G    |
| 79  | S2    | 212 | C    |
| 79  | S2    | 213 | G    |
| 79  | S2    | 214 | U    |
| 79  | S2    | 220 | U    |
| 79  | S2    | 291 | G    |
| 79  | S2    | 292 | A    |
| 79  | S2    | 294 | U    |
| 79  | S2    | 295 | C    |
| 79  | S2    | 298 | G    |
| 79  | S2    | 301 | A    |
| 79  | S2    | 303 | C    |
| 79  | S2    | 305 | U    |
| 79  | S2    | 306 | C    |
| 79  | S2    | 307 | G    |
| 79  | S2    | 308 | G    |
| 79  | S2    | 309 | G    |
| 79  | S2    | 310 | C    |
| 79  | S2    | 311 | C    |
| 79  | S2    | 312 | G    |
| 79  | S2    | 318 | A    |
| 79  | S2    | 319 | C    |
| 79  | S2    | 322 | C    |
| 79  | S2    | 323 | C    |
| 79  | S2    | 324 | C    |
| 79  | S2    | 325 | C    |
| 79  | S2    | 326 | C    |
| 79  | S2    | 328 | U    |
| 79  | S2    | 329 | G    |
| 79  | S2    | 332 | G    |
| 79  | S2    | 338 | G    |
| 79  | S2    | 339 | A    |
| 79  | S2    | 340 | C    |
| 79  | S2    | 347 | G    |
| 79  | S2    | 360 | A    |
| 79  | S2    | 361 | U    |
| 79  | S2    | 362 | C    |
| 79  | S2    | 364 | A    |
| 79  | S2    | 368 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 79  | S2    | 369 | C    |
| 79  | S2    | 370 | G    |
| 79  | S2    | 374 | G    |
| 79  | S2    | 375 | U    |
| 79  | S2    | 377 | G    |
| 79  | S2    | 385 | G    |
| 79  | S2    | 386 | C    |
| 79  | S2    | 407 | G    |
| 79  | S2    | 408 | A    |
| 79  | S2    | 409 | C    |
| 79  | S2    | 421 | G    |
| 79  | S2    | 423 | U    |
| 79  | S2    | 426 | A    |
| 79  | S2    | 428 | U    |
| 79  | S2    | 437 | G    |
| 79  | S2    | 448 | A    |
| 79  | S2    | 449 | A    |
| 79  | S2    | 450 | C    |
| 79  | S2    | 452 | G    |
| 79  | S2    | 464 | A    |
| 79  | S2    | 465 | A    |
| 79  | S2    | 471 | G    |
| 79  | S2    | 472 | C    |
| 79  | S2    | 473 | A    |
| 79  | S2    | 474 | G    |
| 79  | S2    | 476 | A    |
| 79  | S2    | 478 | G    |
| 79  | S2    | 483 | C    |
| 79  | S2    | 485 | A    |
| 79  | S2    | 487 | U    |
| 79  | S2    | 488 | U    |
| 79  | S2    | 492 | C    |
| 79  | S2    | 493 | A    |
| 79  | S2    | 496 | C    |
| 79  | S2    | 502 | C    |
| 79  | S2    | 516 | A    |
| 79  | S2    | 517 | C    |
| 79  | S2    | 529 | A    |
| 79  | S2    | 530 | U    |
| 79  | S2    | 532 | C    |
| 79  | S2    | 537 | C    |
| 79  | S2    | 538 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 79  | S2    | 543 | C    |
| 79  | S2    | 544 | G    |
| 79  | S2    | 546 | G    |
| 79  | S2    | 547 | G    |
| 79  | S2    | 548 | C    |
| 79  | S2    | 550 | C    |
| 79  | S2    | 552 | G    |
| 79  | S2    | 553 | U    |
| 79  | S2    | 554 | A    |
| 79  | S2    | 555 | A    |
| 79  | S2    | 556 | U    |
| 79  | S2    | 557 | U    |
| 79  | S2    | 558 | G    |
| 79  | S2    | 559 | G    |
| 79  | S2    | 560 | A    |
| 79  | S2    | 563 | G    |
| 79  | S2    | 564 | A    |
| 79  | S2    | 566 | U    |
| 79  | S2    | 569 | A    |
| 79  | S2    | 576 | A    |
| 79  | S2    | 582 | U    |
| 79  | S2    | 583 | A    |
| 79  | S2    | 587 | A    |
| 79  | S2    | 589 | G    |
| 79  | S2    | 590 | A    |
| 79  | S2    | 591 | U    |
| 79  | S2    | 593 | C    |
| 79  | S2    | 594 | A    |
| 79  | S2    | 604 | A    |
| 79  | S2    | 606 | G    |
| 79  | S2    | 607 | U    |
| 79  | S2    | 608 | C    |
| 79  | S2    | 613 | G    |
| 79  | S2    | 614 | C    |
| 79  | S2    | 617 | G    |
| 79  | S2    | 622 | C    |
| 79  | S2    | 623 | G    |
| 79  | S2    | 628 | A    |
| 79  | S2    | 629 | A    |
| 79  | S2    | 631 | U    |
| 79  | S2    | 632 | C    |
| 79  | S2    | 638 | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 79  | S2    | 643 | A    |
| 79  | S2    | 644 | G    |
| 79  | S2    | 660 | C    |
| 79  | S2    | 664 | A    |
| 79  | S2    | 668 | A    |
| 79  | S2    | 669 | A    |
| 79  | S2    | 671 | A    |
| 79  | S2    | 672 | A    |
| 79  | S2    | 673 | G    |
| 79  | S2    | 683 | G    |
| 79  | S2    | 684 | G    |
| 79  | S2    | 688 | U    |
| 79  | S2    | 689 | U    |
| 79  | S2    | 692 | G    |
| 79  | S2    | 693 | A    |
| 79  | S2    | 695 | C    |
| 79  | S2    | 696 | G    |
| 79  | S2    | 697 | G    |
| 79  | S2    | 698 | G    |
| 79  | S2    | 732 | U    |
| 79  | S2    | 733 | C    |
| 79  | S2    | 734 | C    |
| 79  | S2    | 736 | C    |
| 79  | S2    | 738 | C    |
| 79  | S2    | 749 | U    |
| 79  | S2    | 750 | C    |
| 79  | S2    | 751 | G    |
| 79  | S2    | 752 | G    |
| 79  | S2    | 753 | C    |
| 79  | S2    | 788 | G    |
| 79  | S2    | 789 | G    |
| 79  | S2    | 791 | C    |
| 79  | S2    | 792 | C    |
| 79  | S2    | 794 | A    |
| 79  | S2    | 798 | G    |
| 79  | S2    | 799 | U    |
| 79  | S2    | 809 | A    |
| 79  | S2    | 821 | G    |
| 79  | S2    | 822 | U    |
| 79  | S2    | 823 | U    |
| 79  | S2    | 824 | C    |
| 79  | S2    | 830 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 79  | S2    | 833 | C    |
| 79  | S2    | 834 | C    |
| 79  | S2    | 835 | C    |
| 79  | S2    | 836 | G    |
| 79  | S2    | 837 | A    |
| 79  | S2    | 838 | G    |
| 79  | S2    | 839 | C    |
| 79  | S2    | 842 | C    |
| 79  | S2    | 847 | A    |
| 79  | S2    | 859 | G    |
| 79  | S2    | 861 | A    |
| 79  | S2    | 869 | A    |
| 79  | S2    | 870 | A    |
| 79  | S2    | 873 | G    |
| 79  | S2    | 874 | G    |
| 79  | S2    | 877 | C    |
| 79  | S2    | 878 | G    |
| 79  | S2    | 882 | U    |
| 79  | S2    | 888 | U    |
| 79  | S2    | 889 | U    |
| 79  | S2    | 890 | U    |
| 79  | S2    | 891 | G    |
| 79  | S2    | 894 | G    |
| 79  | S2    | 896 | U    |
| 79  | S2    | 897 | U    |
| 79  | S2    | 898 | U    |
| 79  | S2    | 899 | U    |
| 79  | S2    | 900 | C    |
| 79  | S2    | 901 | G    |
| 79  | S2    | 903 | A    |
| 79  | S2    | 905 | C    |
| 79  | S2    | 913 | A    |
| 79  | S2    | 917 | U    |
| 79  | S2    | 919 | A    |
| 79  | S2    | 920 | A    |
| 79  | S2    | 933 | G    |
| 79  | S2    | 934 | G    |
| 79  | S2    | 949 | G    |
| 79  | S2    | 954 | U    |
| 79  | S2    | 955 | A    |
| 79  | S2    | 956 | G    |
| 79  | S2    | 963 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 79  | S2    | 969  | U    |
| 79  | S2    | 971  | G    |
| 79  | S2    | 972  | A    |
| 79  | S2    | 978  | G    |
| 79  | S2    | 984  | C    |
| 79  | S2    | 988  | C    |
| 79  | S2    | 989  | C    |
| 79  | S2    | 990  | A    |
| 79  | S2    | 992  | A    |
| 79  | S2    | 999  | G    |
| 79  | S2    | 1001 | A    |
| 79  | S2    | 1002 | U    |
| 79  | S2    | 1008 | A    |
| 79  | S2    | 1017 | U    |
| 79  | S2    | 1023 | A    |
| 79  | S2    | 1027 | A    |
| 79  | S2    | 1045 | U    |
| 79  | S2    | 1047 | C    |
| 79  | S2    | 1060 | A    |
| 79  | S2    | 1061 | U    |
| 79  | S2    | 1062 | A    |
| 79  | S2    | 1067 | C    |
| 79  | S2    | 1083 | A    |
| 79  | S2    | 1085 | C    |
| 79  | S2    | 1088 | U    |
| 79  | S2    | 1107 | G    |
| 79  | S2    | 1108 | G    |
| 79  | S2    | 1109 | C    |
| 79  | S2    | 1110 | G    |
| 79  | S2    | 1113 | A    |
| 79  | S2    | 1114 | U    |
| 79  | S2    | 1115 | U    |
| 79  | S2    | 1116 | C    |
| 79  | S2    | 1118 | C    |
| 79  | S2    | 1119 | A    |
| 79  | S2    | 1121 | G    |
| 79  | S2    | 1126 | G    |
| 79  | S2    | 1133 | A    |
| 79  | S2    | 1138 | C    |
| 79  | S2    | 1139 | C    |
| 79  | S2    | 1148 | A    |
| 79  | S2    | 1153 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 79  | S2    | 1154 | U    |
| 79  | S2    | 1155 | U    |
| 79  | S2    | 1162 | C    |
| 79  | S2    | 1170 | A    |
| 79  | S2    | 1195 | A    |
| 79  | S2    | 1200 | A    |
| 79  | S2    | 1207 | G    |
| 79  | S2    | 1208 | A    |
| 79  | S2    | 1210 | G    |
| 79  | S2    | 1215 | C    |
| 79  | S2    | 1216 | C    |
| 79  | S2    | 1217 | A    |
| 79  | S2    | 1220 | A    |
| 79  | S2    | 1224 | G    |
| 79  | S2    | 1227 | G    |
| 79  | S2    | 1237 | C    |
| 79  | S2    | 1240 | A    |
| 79  | S2    | 1242 | U    |
| 79  | S2    | 1243 | U    |
| 79  | S2    | 1251 | A    |
| 79  | S2    | 1253 | A    |
| 79  | S2    | 1256 | G    |
| 79  | S2    | 1257 | G    |
| 79  | S2    | 1259 | A    |
| 79  | S2    | 1264 | C    |
| 79  | S2    | 1274 | G    |
| 79  | S2    | 1275 | G    |
| 79  | S2    | 1282 | A    |
| 79  | S2    | 1283 | C    |
| 79  | S2    | 1284 | A    |
| 79  | S2    | 1286 | G    |
| 79  | S2    | 1287 | A    |
| 79  | S2    | 1290 | G    |
| 79  | S2    | 1294 | G    |
| 79  | S2    | 1295 | A    |
| 79  | S2    | 1301 | A    |
| 79  | S2    | 1302 | G    |
| 79  | S2    | 1303 | C    |
| 79  | S2    | 1306 | U    |
| 79  | S2    | 1308 | U    |
| 79  | S2    | 1322 | G    |
| 79  | S2    | 1333 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 79  | S2    | 1342 | U    |
| 79  | S2    | 1351 | G    |
| 79  | S2    | 1352 | G    |
| 79  | S2    | 1358 | U    |
| 79  | S2    | 1363 | C    |
| 79  | S2    | 1364 | U    |
| 79  | S2    | 1371 | U    |
| 79  | S2    | 1372 | U    |
| 79  | S2    | 1376 | A    |
| 79  | S2    | 1378 | A    |
| 79  | S2    | 1398 | G    |
| 79  | S2    | 1401 | A    |
| 79  | S2    | 1402 | A    |
| 79  | S2    | 1406 | G    |
| 79  | S2    | 1407 | U    |
| 79  | S2    | 1408 | U    |
| 79  | S2    | 1411 | G    |
| 79  | S2    | 1414 | A    |
| 79  | S2    | 1415 | C    |
| 79  | S2    | 1419 | C    |
| 79  | S2    | 1420 | G    |
| 79  | S2    | 1421 | A    |
| 79  | S2    | 1422 | G    |
| 79  | S2    | 1423 | C    |
| 79  | S2    | 1426 | U    |
| 79  | S2    | 1433 | C    |
| 79  | S2    | 1434 | C    |
| 79  | S2    | 1435 | C    |
| 79  | S2    | 1436 | C    |
| 79  | S2    | 1438 | A    |
| 79  | S2    | 1442 | U    |
| 79  | S2    | 1449 | G    |
| 79  | S2    | 1452 | A    |
| 79  | S2    | 1454 | A    |
| 79  | S2    | 1463 | U    |
| 79  | S2    | 1466 | G    |
| 79  | S2    | 1474 | A    |
| 79  | S2    | 1476 | A    |
| 79  | S2    | 1478 | U    |
| 79  | S2    | 1480 | A    |
| 79  | S2    | 1484 | A    |
| 79  | S2    | 1489 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 79  | S2    | 1490 | G    |
| 79  | S2    | 1494 | U    |
| 79  | S2    | 1495 | G    |
| 79  | S2    | 1497 | G    |
| 79  | S2    | 1498 | A    |
| 79  | S2    | 1501 | C    |
| 79  | S2    | 1507 | G    |
| 79  | S2    | 1508 | A    |
| 79  | S2    | 1520 | G    |
| 79  | S2    | 1521 | C    |
| 79  | S2    | 1522 | A    |
| 79  | S2    | 1533 | A    |
| 79  | S2    | 1535 | U    |
| 79  | S2    | 1536 | G    |
| 79  | S2    | 1537 | A    |
| 79  | S2    | 1544 | C    |
| 79  | S2    | 1552 | G    |
| 79  | S2    | 1556 | A    |
| 79  | S2    | 1570 | G    |
| 79  | S2    | 1572 | C    |
| 79  | S2    | 1574 | C    |
| 79  | S2    | 1579 | A    |
| 79  | S2    | 1580 | A    |
| 79  | S2    | 1581 | C    |
| 79  | S2    | 1584 | G    |
| 79  | S2    | 1585 | U    |
| 79  | S2    | 1586 | U    |
| 79  | S2    | 1587 | G    |
| 79  | S2    | 1588 | A    |
| 79  | S2    | 1594 | A    |
| 79  | S2    | 1598 | G    |
| 79  | S2    | 1599 | U    |
| 79  | S2    | 1600 | G    |
| 79  | S2    | 1601 | A    |
| 79  | S2    | 1604 | G    |
| 79  | S2    | 1606 | G    |
| 79  | S2    | 1621 | U    |
| 79  | S2    | 1623 | A    |
| 79  | S2    | 1630 | A    |
| 79  | S2    | 1633 | A    |
| 79  | S2    | 1634 | A    |
| 79  | S2    | 1637 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 79  | S2    | 1638 | G    |
| 79  | S2    | 1639 | G    |
| 79  | S2    | 1640 | A    |
| 79  | S2    | 1646 | C    |
| 79  | S2    | 1648 | G    |
| 79  | S2    | 1654 | G    |
| 79  | S2    | 1657 | G    |
| 79  | S2    | 1663 | A    |
| 79  | S2    | 1665 | G    |
| 79  | S2    | 1680 | G    |
| 79  | S2    | 1683 | C    |
| 79  | S2    | 1694 | U    |
| 79  | S2    | 1696 | C    |
| 79  | S2    | 1699 | A    |
| 79  | S2    | 1706 | G    |
| 79  | S2    | 1712 | A    |
| 79  | S2    | 1715 | A    |
| 79  | S2    | 1722 | G    |
| 79  | S2    | 1726 | G    |
| 79  | S2    | 1729 | U    |
| 79  | S2    | 1742 | C    |
| 79  | S2    | 1743 | G    |
| 79  | S2    | 1744 | G    |
| 79  | S2    | 1745 | A    |
| 79  | S2    | 1752 | C    |
| 79  | S2    | 1753 | C    |
| 79  | S2    | 1754 | G    |
| 79  | S2    | 1755 | C    |
| 79  | S2    | 1756 | C    |
| 79  | S2    | 1757 | G    |
| 79  | S2    | 1758 | G    |
| 79  | S2    | 1759 | G    |
| 79  | S2    | 1761 | U    |
| 79  | S2    | 1772 | C    |
| 79  | S2    | 1773 | C    |
| 79  | S2    | 1774 | C    |
| 79  | S2    | 1777 | G    |
| 79  | S2    | 1780 | G    |
| 79  | S2    | 1782 | G    |
| 79  | S2    | 1783 | C    |
| 79  | S2    | 1784 | G    |
| 79  | S2    | 1785 | C    |

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| Mol | Chain | Res   | Type |
|-----|-------|-------|------|
| 79  | S2    | 1787  | G    |
| 79  | S2    | 1798  | C    |
| 79  | S2    | 1809  | A    |
| 79  | S2    | 1810  | U    |
| 79  | S2    | 1812  | U    |
| 79  | S2    | 1813  | A    |
| 79  | S2    | 1819  | A    |
| 79  | S2    | 1820  | G    |
| 79  | S2    | 1822  | A    |
| 79  | S2    | 1823  | A    |
| 79  | S2    | 1824  | A    |
| 79  | S2    | 1829  | G    |
| 79  | S2    | 1835  | A    |
| 79  | S2    | 1838  | U    |
| 79  | S2    | 1849  | G    |
| 79  | S2    | 1851  | A    |
| 79  | S2    | 1852  | C    |
| 79  | S2    | 1861  | G    |
| 79  | S2    | 1862  | G    |
| 79  | S2    | 1863  | A    |
| 79  | S2    | 1864  | U    |
| 79  | S2    | 1865  | C    |
| 81  | AP    | 7     | G    |
| 81  | AP    | 8     | U    |
| 81  | AP    | 9     | A    |
| 81  | AP    | 10    | G    |
| 81  | AP    | 11    | U    |
| 81  | AP    | 13    | U    |
| 81  | AP    | 14    | A    |
| 81  | AP    | 20(A) | U    |
| 81  | AP    | 21    | A    |
| 81  | AP    | 25    | C    |
| 81  | AP    | 26    | G    |
| 81  | AP    | 47    | U    |
| 81  | AP    | 48    | C    |
| 81  | AP    | 49    | C    |
| 81  | AP    | 55    | U    |
| 81  | AP    | 56    | C    |
| 81  | AP    | 58    | A    |
| 81  | AP    | 61    | C    |
| 81  | AP    | 63    | G    |
| 81  | AP    | 64    | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 81  | AP    | 65  | G    |
| 81  | AP    | 67  | G    |
| 81  | AP    | 69  | A    |
| 81  | AP    | 70  | A    |
| 81  | AP    | 71  | A    |
| 82  | PE    | 4   | C    |
| 82  | PE    | 5   | G    |
| 82  | PE    | 7   | A    |
| 82  | PE    | 8   | U    |
| 82  | PE    | 9   | A    |
| 82  | PE    | 10  | G    |
| 82  | PE    | 11  | C    |
| 82  | PE    | 13  | C    |
| 82  | PE    | 15  | G    |
| 82  | PE    | 19  | G    |
| 82  | PE    | 20  | U    |
| 82  | PE    | 21  | A    |
| 82  | PE    | 25  | C    |
| 82  | PE    | 26  | A    |
| 82  | PE    | 27  | U    |
| 82  | PE    | 31  | A    |
| 82  | PE    | 32  | C    |
| 82  | PE    | 33  | U    |
| 82  | PE    | 34  | U    |
| 82  | PE    | 35  | U    |
| 82  | PE    | 36  | U    |
| 82  | PE    | 38  | A    |
| 82  | PE    | 46  | G    |
| 82  | PE    | 47  | U    |
| 82  | PE    | 48  | C    |
| 82  | PE    | 49  | C    |
| 82  | PE    | 50  | A    |
| 82  | PE    | 52  | G    |
| 82  | PE    | 54  | U    |
| 82  | PE    | 55  | U    |
| 82  | PE    | 56  | C    |
| 82  | PE    | 58  | A    |
| 82  | PE    | 60  | U    |
| 82  | PE    | 61  | C    |
| 82  | PE    | 64  | U    |
| 82  | PE    | 65  | G    |
| 82  | PE    | 67  | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 82  | PE    | 69  | G    |
| 82  | PE    | 70  | G    |
| 82  | PE    | 76  | A    |

All (50) RNA pucker outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 85  | L5    | 265  | C    |
| 85  | L5    | 406  | C    |
| 85  | L5    | 493  | G    |
| 85  | L5    | 509  | A    |
| 85  | L5    | 912  | G    |
| 85  | L5    | 914  | U    |
| 85  | L5    | 935  | A    |
| 85  | L5    | 1082 | C    |
| 85  | L5    | 1324 | A    |
| 85  | L5    | 1633 | G    |
| 85  | L5    | 1977 | C    |
| 85  | L5    | 2033 | A    |
| 85  | L5    | 2416 | G    |
| 85  | L5    | 2485 | U    |
| 85  | L5    | 2675 | G    |
| 85  | L5    | 2760 | G    |
| 85  | L5    | 2786 | C    |
| 85  | L5    | 3614 | G    |
| 85  | L5    | 3673 | C    |
| 85  | L5    | 3948 | C    |
| 85  | L5    | 4055 | U    |
| 85  | L5    | 4061 | G    |
| 85  | L5    | 4101 | C    |
| 85  | L5    | 4102 | C    |
| 85  | L5    | 4106 | G    |
| 85  | L5    | 4107 | G    |
| 85  | L5    | 4108 | G    |
| 85  | L5    | 4110 | C    |
| 85  | L5    | 4111 | U    |
| 85  | L5    | 4112 | C    |
| 85  | L5    | 4114 | C    |
| 85  | L5    | 4600 | G    |
| 85  | L5    | 4699 | U    |
| 85  | L5    | 4913 | G    |
| 79  | S2    | 291  | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 79  | S2    | 307  | G    |
| 79  | S2    | 420  | G    |
| 79  | S2    | 531  | A    |
| 79  | S2    | 557  | U    |
| 79  | S2    | 563  | G    |
| 79  | S2    | 688  | U    |
| 79  | S2    | 1355 | C    |
| 79  | S2    | 1434 | C    |
| 79  | S2    | 1521 | C    |
| 79  | S2    | 1693 | G    |
| 79  | S2    | 1781 | A    |
| 81  | AP    | 9    | A    |
| 82  | PE    | 18   | U    |
| 82  | PE    | 33   | U    |
| 82  | PE    | 34   | U    |

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 522 ligands modelled in this entry, 522 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 85  | L5    | 10               |
| 85  | l5    | 10               |
| 79  | s2    | 7                |
| 79  | S2    | 5                |
| 84  | Lt    | 1                |
| 84  | lt    | 1                |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | S2    | 753:C     | O3'    | 785:C     | P      | 27.80        |
| 1     | s2    | 753:C     | O3'    | 785:C     | P      | 27.36        |
| 1     | L5    | 2910:G    | O3'    | 3584:C    | P      | 20.89        |
| 1     | l5    | 2910:G    | O3'    | 3584:C    | P      | 20.75        |
| 1     | l5    | 760:G     | O3'    | 903:C     | P      | 17.11        |
| 1     | L5    | 760:G     | O3'    | 903:C     | P      | 16.89        |
| 1     | l5    | 519:C     | O3'    | 642:G     | P      | 16.44        |
| 1     | L5    | 519:C     | O3'    | 642:G     | P      | 16.09        |
| 1     | l5    | 4776:G    | O3'    | 4858:C    | P      | 16.06        |
| 1     | S2    | 698:G     | O3'    | 730:C     | P      | 16.04        |
| 1     | L5    | 4776:G    | O3'    | 4858:C    | P      | 15.73        |
| 1     | s2    | 698:G     | O3'    | 730:C     | P      | 15.29        |
| 1     | l5    | 996:G     | O3'    | 1047:C    | P      | 14.03        |
| 1     | L5    | 996:G     | O3'    | 1047:C    | P      | 13.71        |
| 1     | S2    | 739:C     | O3'    | 746:C     | P      | 13.70        |
| 1     | l5    | 2112:G    | O3'    | 2249:C    | P      | 13.56        |
| 1     | L5    | 2112:G    | O3'    | 2249:C    | P      | 13.45        |
| 1     | s2    | 739:C     | O3'    | 746:C     | P      | 13.16        |
| 1     | l5    | 1222:A    | O3'    | 1234:G    | P      | 11.54        |
| 1     | L5    | 1222:A    | O3'    | 1234:G    | P      | 11.34        |
| 1     | Lt    | 87:GLU    | C      | 104:ILE   | N      | 11.05        |
| 1     | lt    | 87:GLU    | C      | 104:ILE   | N      | 9.67         |
| 1     | s2    | 553:U     | O3'    | 554:A     | P      | 9.47         |
| 1     | l5    | 1051:G    | O3'    | 1064:G    | P      | 8.75         |
| 1     | s2    | 530:U     | O3'    | 531:A     | P      | 8.59         |
| 1     | L5    | 1051:G    | O3'    | 1064:G    | P      | 8.51         |
| 1     | s2    | 225:G     | O3'    | 287:U     | P      | 7.98         |
| 1     | S2    | 225:G     | O3'    | 287:U     | P      | 6.68         |
| 1     | L5    | 1100:U    | O3'    | 1167:C    | P      | 6.64         |
| 1     | l5    | 1100:U    | O3'    | 1167:C    | P      | 6.41         |

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| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | L5    | 1709:C    | O3'    | 1714:C    | P      | 5.51         |
| 1     | l5    | 1709:C    | O3'    | 1714:C    | P      | 5.38         |
| 1     | s2    | 1210:G    | O3'    | 1211:G    | P      | 3.70         |
| 1     | S2    | 1210:G    | O3'    | 1211:G    | P      | 3.50         |

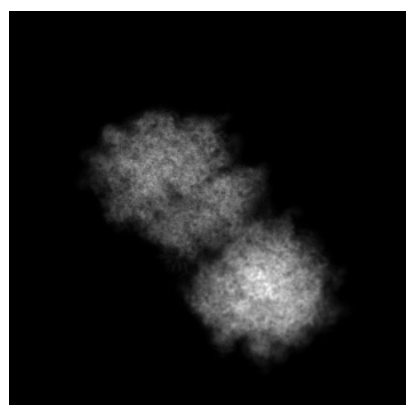
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44050. These allow visual inspection of the internal detail of the map and identification of artifacts.

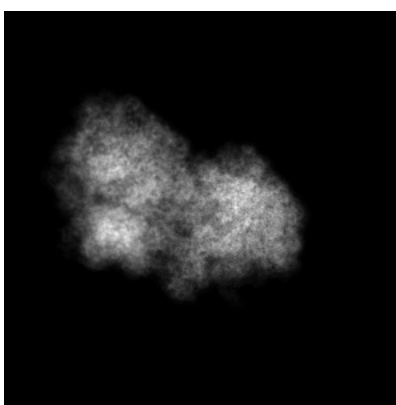
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

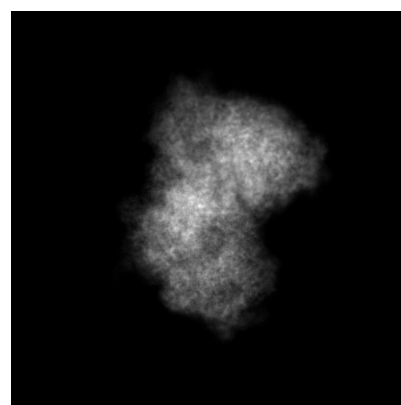
#### 6.1.1 Primary map



X



Y

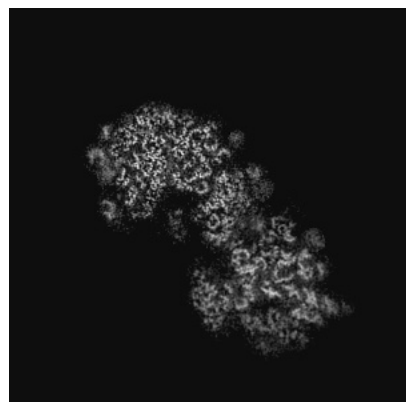


Z

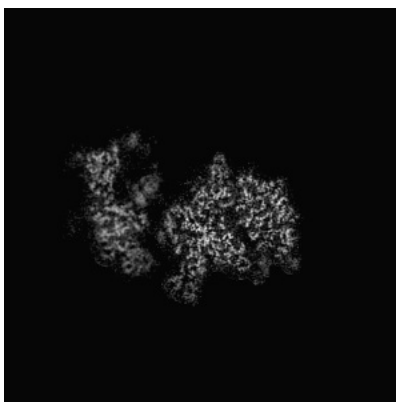
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

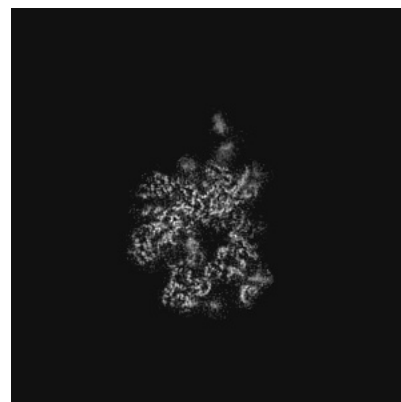
#### 6.2.1 Primary map



X Index: 300



Y Index: 300

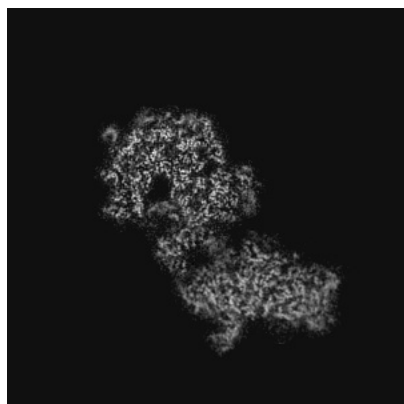


Z Index: 300

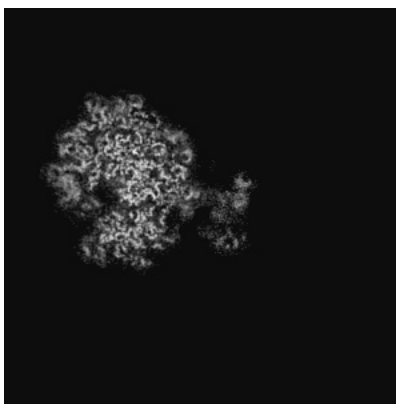
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

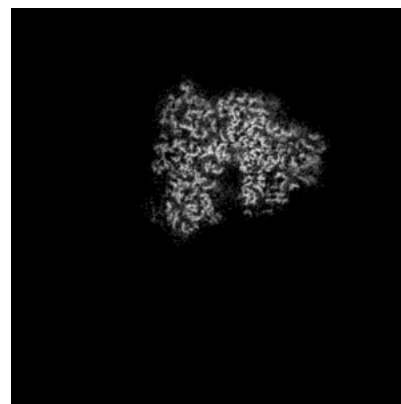
### 6.3.1 Primary map



X Index: 266



Y Index: 375

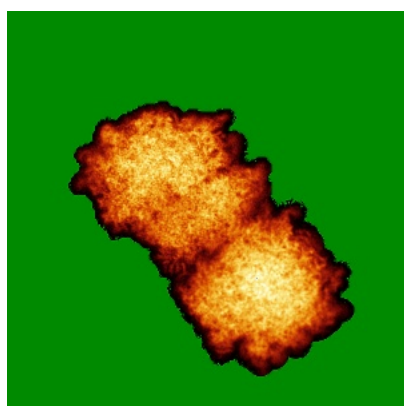


Z Index: 176

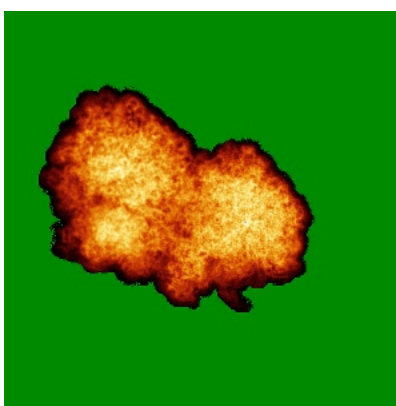
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

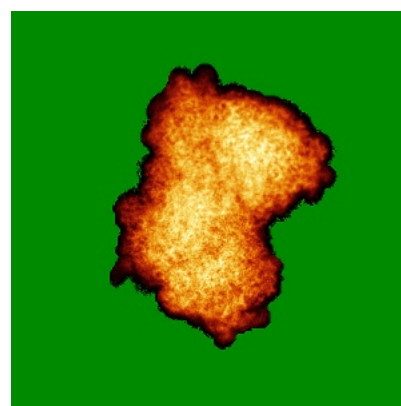
### 6.4.1 Primary map



X



Y

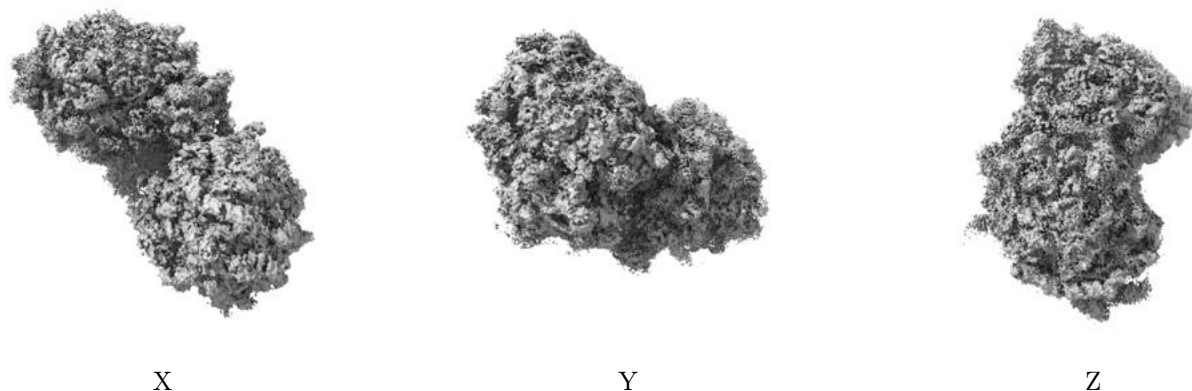


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.096. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

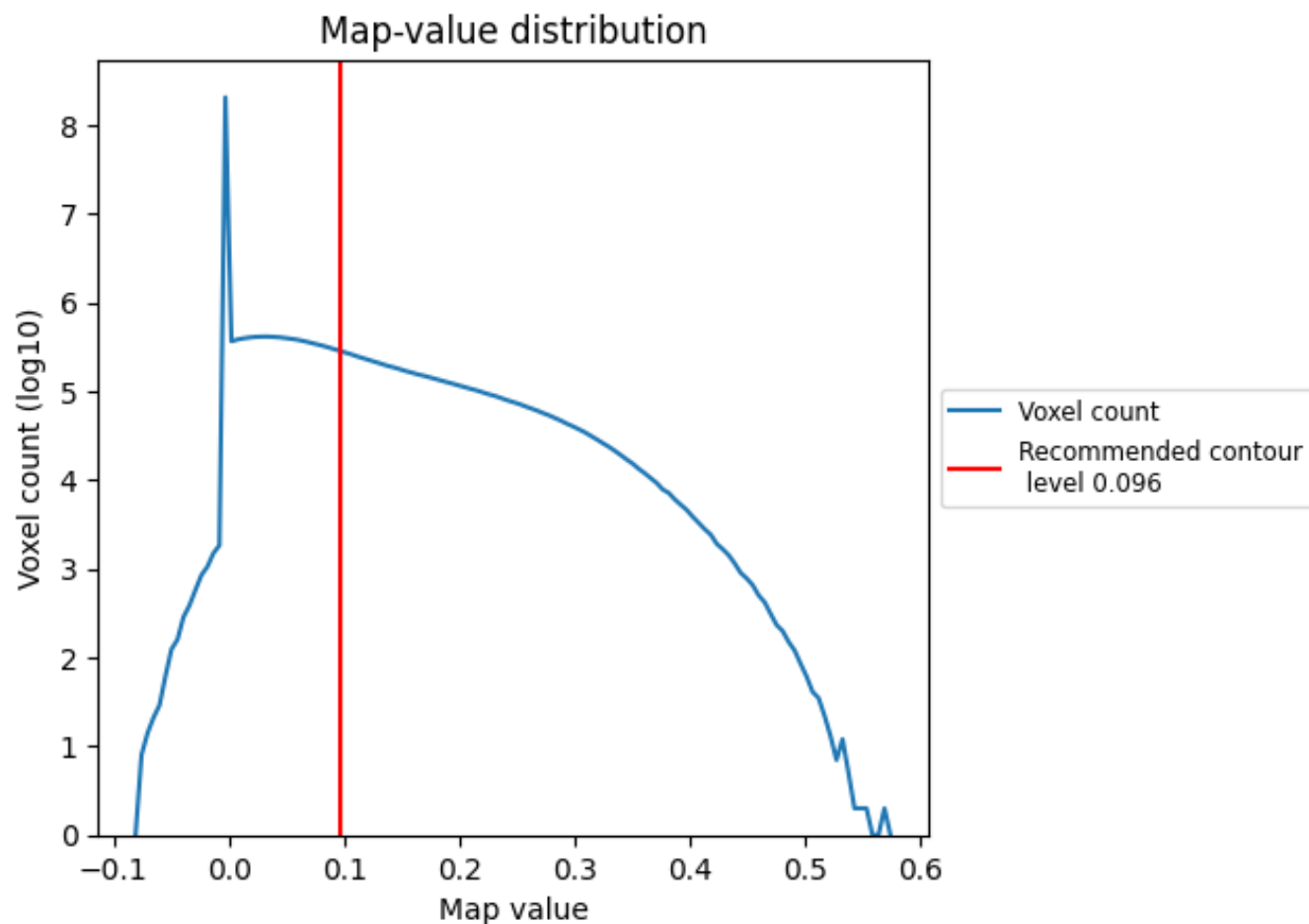
## 6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

## 7 Map analysis [i](#)

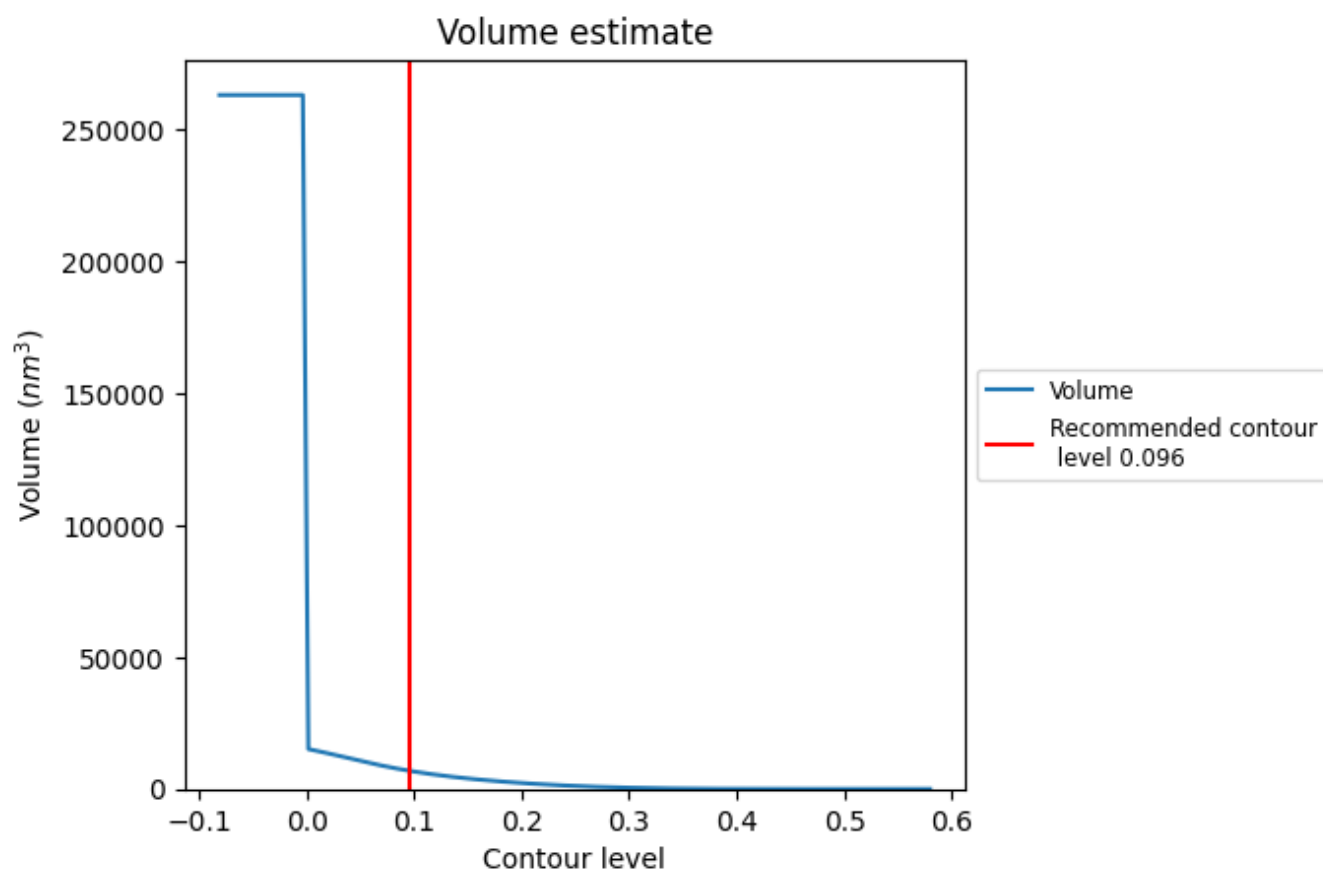
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

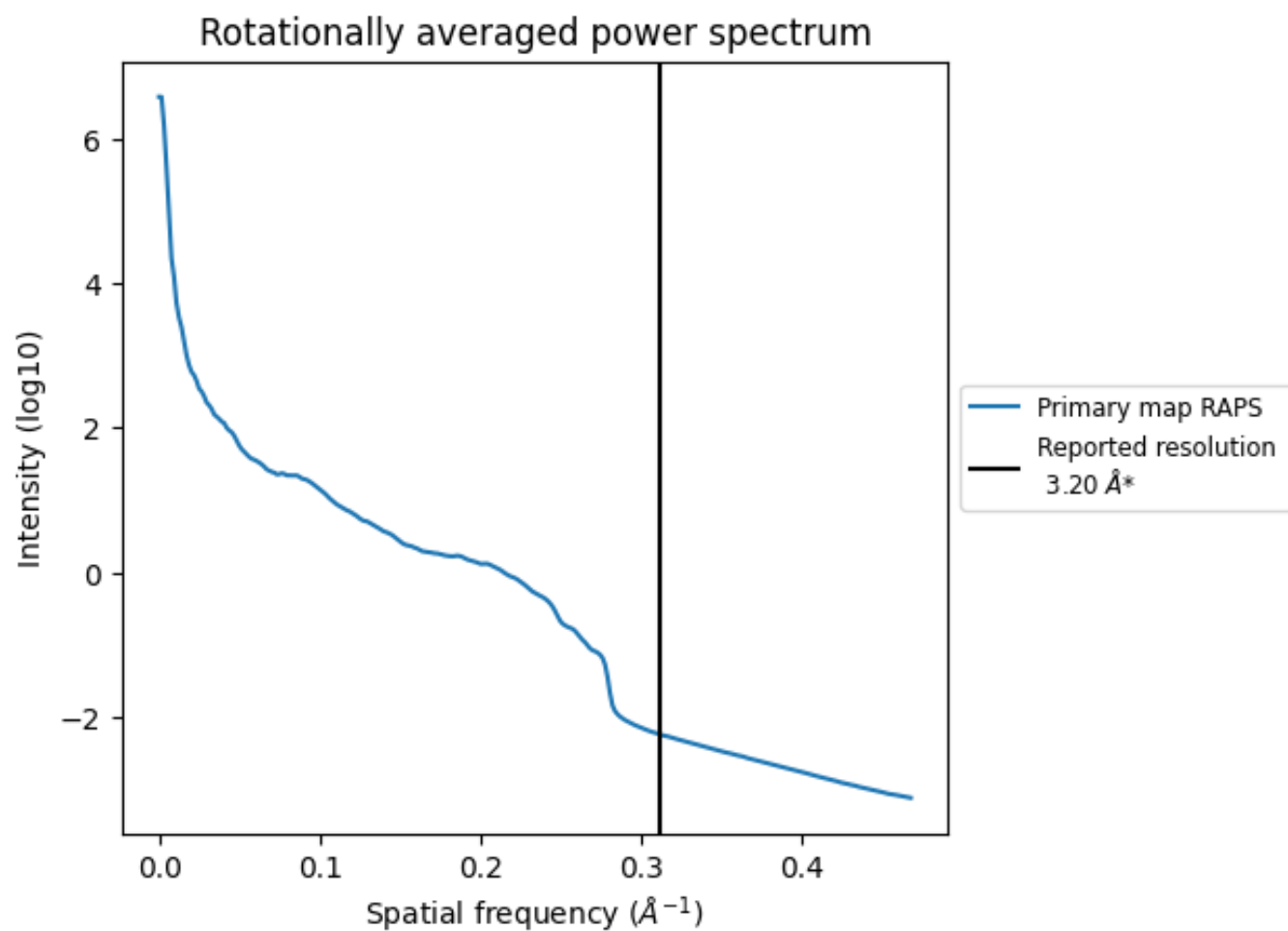
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 6868  $\text{nm}^3$ ; this corresponds to an approximate mass of 6204 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ



\*Reported resolution corresponds to spatial frequency of 0.312 Å<sup>-1</sup>



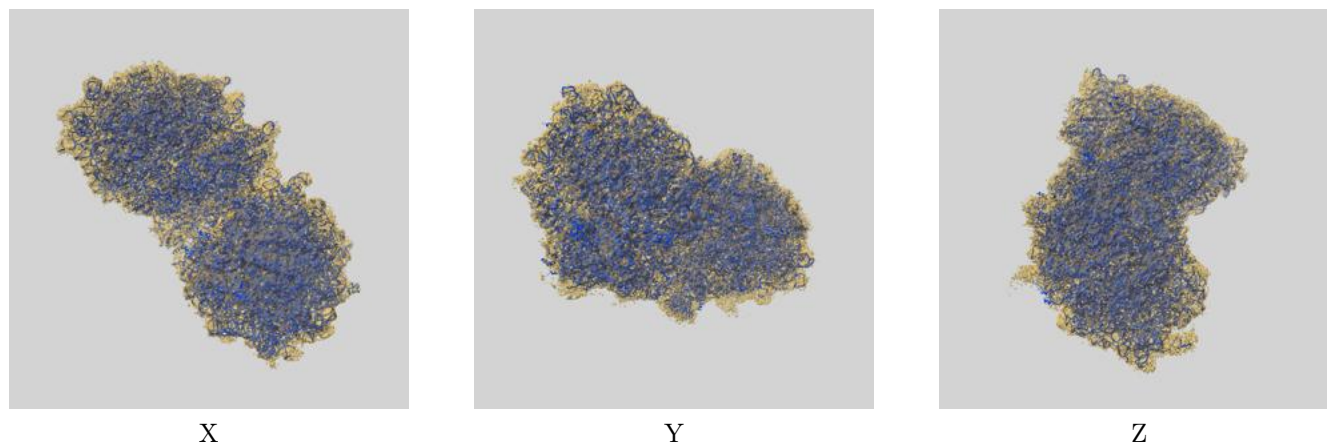
## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

## 9 Map-model fit [i](#)

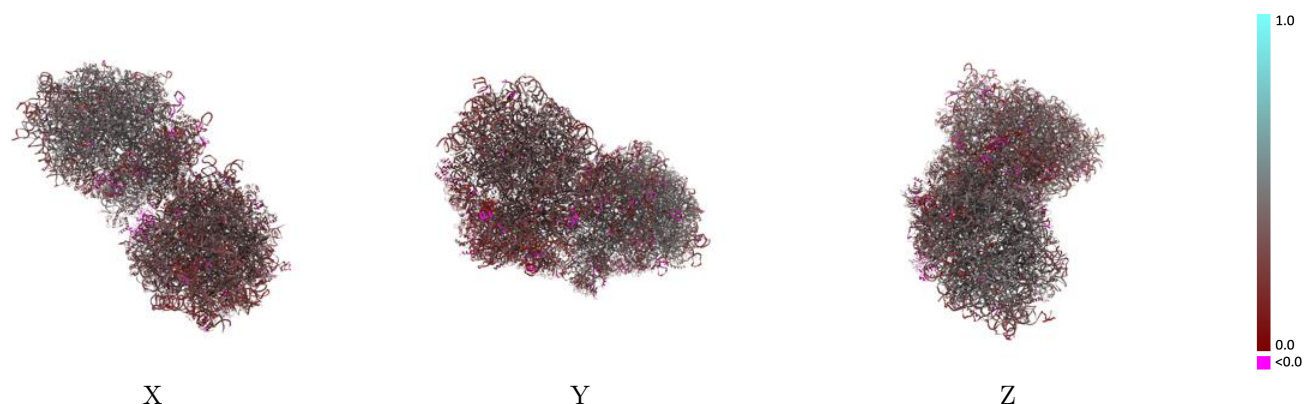
This section contains information regarding the fit between EMDB map EMD-44050 and PDB model 9B0Q. Per-residue inclusion information can be found in section [3](#) on page [29](#).

### 9.1 Map-model overlay [i](#)



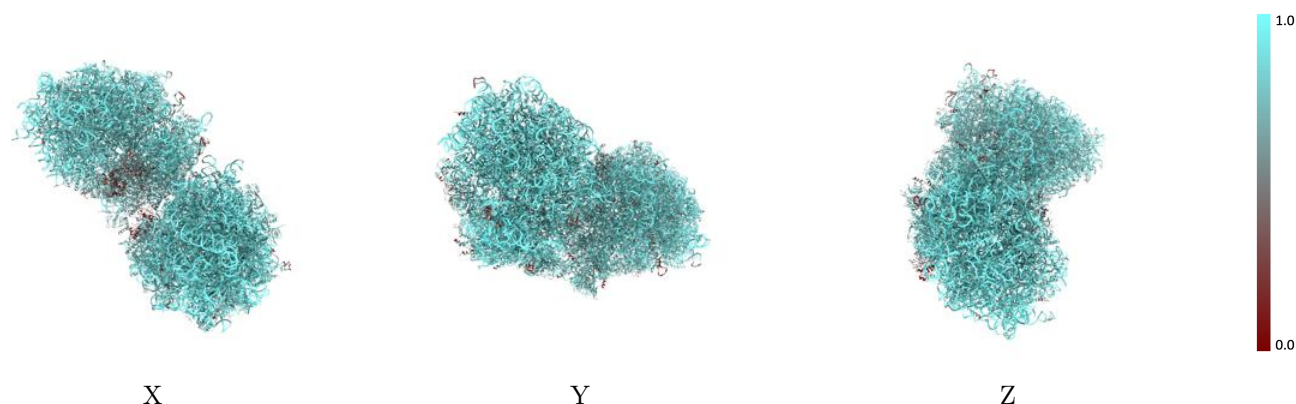
The images above show the 3D surface view of the map at the recommended contour level 0.096 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)



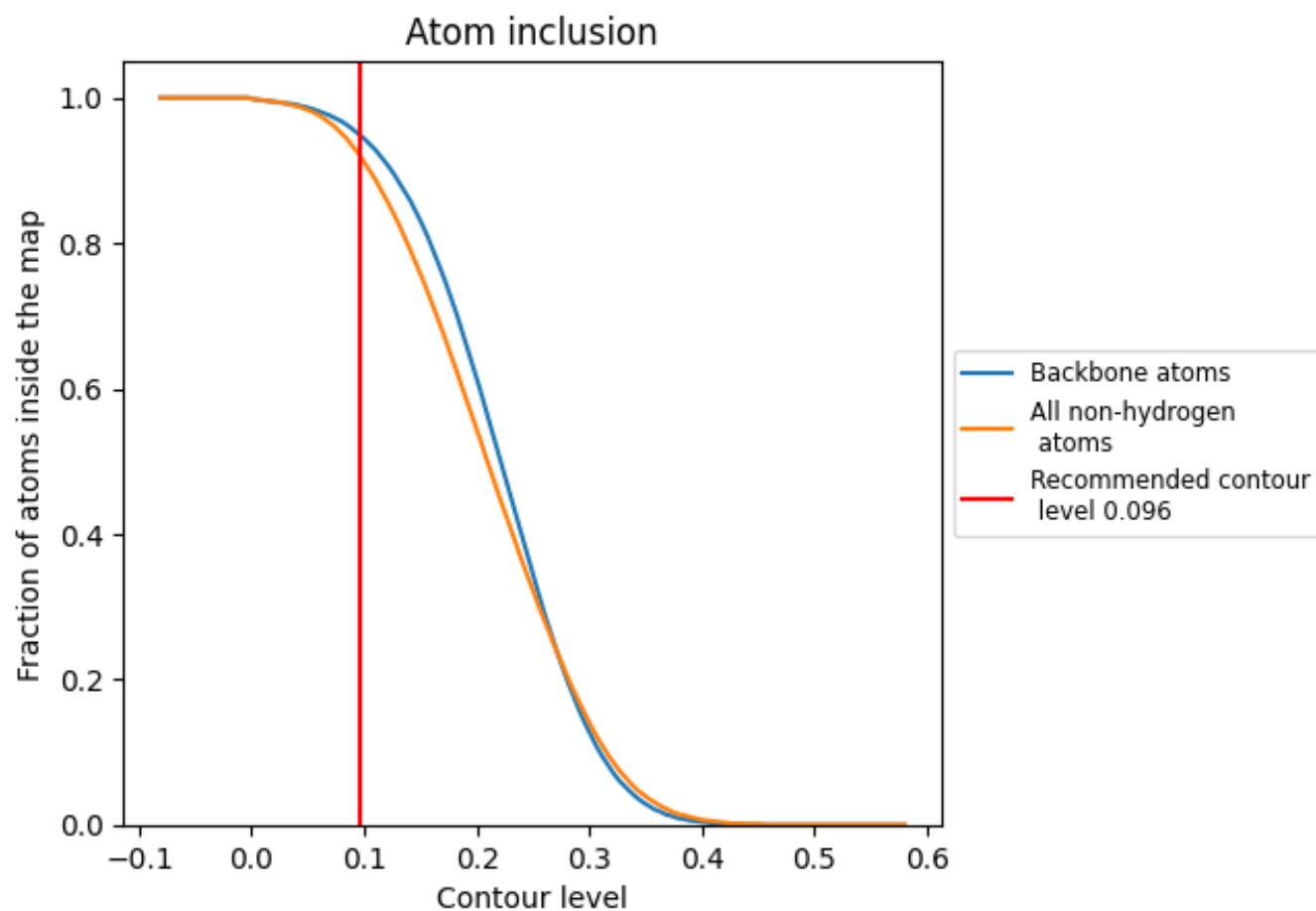
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.096).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 92% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.096) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.9210   |  0.3380   |
| AP    |  0.9890   |  0.2490   |
| CB    |  0.7800   |  0.2340   |
| CH    |  0.8100   |  0.2630   |
| L5    |  0.9770   |  0.3260   |
| L7    |  0.9940   |  0.3480   |
| L8    |  0.9890   |  0.3380   |
| LA    |  0.9430   |  0.3620   |
| LB    |  0.9500   |  0.3260   |
| LC    |  0.9170   |  0.3350   |
| LD    |  0.8620   |  0.3050   |
| LE    |  0.8910   |  0.2770   |
| LF    |  0.9420   |  0.3060   |
| LG    |  0.8550   |  0.3020   |
| LH    |  0.9460  |  0.2980  |
| LI    |  0.9600 |  0.3440 |
| LJ    |  0.8400 |  0.2860 |
| LL    |  0.8590 |  0.3240 |
| LM    |  0.9390 |  0.2950 |
| LN    |  0.9520 |  0.3440 |
| LO    |  0.9490 |  0.3060 |
| LP    |  0.9710 |  0.3410 |
| LQ    |  0.9360 |  0.3500 |
| LR    |  0.8780 |  0.2920 |
| LS    |  0.9630 |  0.3360 |
| LT    |  0.9420 |  0.3450 |
| LU    |  0.8790 |  0.2710 |
| LV    |  0.9800 |  0.3660 |
| LW    |  0.8630 |  0.2550 |
| LX    |  0.9060 |  0.3360 |
| LY    |  0.9390 |  0.3400 |
| LZ    |  0.8370 |  0.3300 |
| La    |  0.9270 |  0.3560 |
| Lb    |  0.8700 |  0.3000 |
| Lc    |  0.8180 |  0.3150 |



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| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| Ld    |  0.9580   |  0.3460   |
| Le    |  0.9750   |  0.3560   |
| Lf    |  0.9830   |  0.3420   |
| Lg    |  0.9210   |  0.3380   |
| Lh    |  0.8980   |  0.3140   |
| Li    |  0.8760   |  0.3220   |
| Lj    |  0.9760   |  0.3360   |
| Lk    |  0.8350   |  0.3020   |
| Ll    |  0.9860   |  0.3620   |
| Lm    |  0.9660   |  0.3330   |
| Ln    |  1.0000   |  0.3110   |
| Lo    |  0.9250   |  0.3720   |
| Lp    |  0.9450   |  0.3520   |
| Lr    |  0.9200   |  0.3330   |
| Ls    |  0.6150   |  0.1490   |
| Lt    |  0.6780   |  0.1520   |
| Lz    |  0.2280   |  0.0220   |
| PE    |  0.9750   |  0.2490   |
| S2    |  0.9770   |  0.3130   |
| SA    |  0.7830  |  0.2940  |
| SB    |  0.8680 |  0.3190 |
| SC    |  0.8790 |  0.3120 |
| SD    |  0.8310 |  0.2850 |
| SE    |  0.9030 |  0.2810 |
| SF    |  0.8540 |  0.2690 |
| SG    |  0.8750 |  0.2410 |
| SH    |  0.7460 |  0.2620 |
| SI    |  0.8770 |  0.2800 |
| SJ    |  0.8770 |  0.2650 |
| SK    |  0.8680 |  0.2670 |
| SL    |  0.8780 |  0.3170 |
| SM    |  0.6840 |  0.2260 |
| SN    |  0.8540 |  0.3050 |
| SO    |  0.8680 |  0.3130 |
| SP    |  0.9020 |  0.2970 |
| SQ    |  0.8740 |  0.2650 |
| SR    |  0.7730 |  0.2640 |
| SS    |  0.8410 |  0.2900 |
| ST    |  0.8760 |  0.2640 |
| SU    |  0.8450 |  0.2660 |
| SV    |  0.8390 |  0.2970 |
| SW    |  0.9210 |  0.3140 |

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| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| SX    |  0.9570   |  0.3270   |
| SY    |  0.8950   |  0.2280   |
| SZ    |  0.7920   |  0.2820   |
| Sa    |  0.9240   |  0.3510   |
| Sb    |  0.7920   |  0.3030   |
| Sc    |  0.7690   |  0.2130   |
| Sd    |  0.9910   |  0.2900   |
| Se    |  0.9280   |  0.2890   |
| Sf    |  0.7800   |  0.2520   |
| Sg    |  0.7610   |  0.2190   |
| aP    |  0.9410   |  0.2670   |
| cB    |  0.4910   |  0.2650   |
| cH    |  0.7590   |  0.2850   |
| l5    |  0.9720   |  0.3850   |
| l7    |  0.9900   |  0.4140   |
| l8    |  0.9840   |  0.3920   |
| lA    |  0.9490   |  0.4410   |
| lB    |  0.9010   |  0.4250   |
| lC    |  0.9370  |  0.4300  |
| lD    |  0.9060 |  0.3910 |
| lE    |  0.8760 |  0.3780 |
| lF    |  0.9490 |  0.4230 |
| lG    |  0.8750 |  0.3660 |
| lH    |  0.8760 |  0.4080 |
| lI    |  0.9190 |  0.4380 |
| lJ    |  0.8060 |  0.3410 |
| lL    |  0.9140 |  0.4000 |
| lM    |  0.9010 |  0.4050 |
| lN    |  0.9620 |  0.4360 |
| lO    |  0.9270 |  0.4220 |
| lP    |  0.9510 |  0.4590 |
| lQ    |  0.9600 |  0.4480 |
| lR    |  0.8850 |  0.3770 |
| lS    |  0.9360 |  0.4390 |
| lT    |  0.9530 |  0.4330 |
| lU    |  0.8650 |  0.3410 |
| lV    |  0.9000 |  0.4350 |
| lW    |  0.8700 |  0.3470 |
| lX    |  0.9200 |  0.4110 |
| lY    |  0.9520 |  0.4120 |
| lZ    |  0.8750 |  0.3880 |
| la    |  0.9630 |  0.4400 |

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| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| lb    |  0.9070   |  0.3700   |
| lc    |  0.8720   |  0.3740   |
| ld    |  0.9290   |  0.4230   |
| le    |  0.9600   |  0.4530   |
| lf    |  0.9570   |  0.4440   |
| lg    |  0.9400   |  0.4310   |
| lh    |  0.9380   |  0.3960   |
| li    |  0.9010   |  0.3950   |
| lj    |  0.9910   |  0.4490   |
| lk    |  0.8740   |  0.3870   |
| ll    |  0.9740   |  0.4330   |
| lm    |  0.9210   |  0.4170   |
| ln    |  0.9670   |  0.4230   |
| lo    |  0.9200   |  0.4420   |
| lp    |  0.9300   |  0.4150   |
| lr    |  0.9490   |  0.4310   |
| ls    |  0.5370   |  0.1750   |
| lt    |  0.4830   |  0.1610   |
| lz    |  0.2500   |  0.0520   |
| pE    |  0.9460  |  0.2340  |
| s2    |  0.9720 |  0.3540 |
| sA    |  0.8050 |  0.3430 |
| sB    |  0.8870 |  0.3690 |
| sC    |  0.8850 |  0.3830 |
| sD    |  0.8530 |  0.3680 |
| sE    |  0.9170 |  0.3530 |
| sF    |  0.8590 |  0.3310 |
| sG    |  0.8450 |  0.2910 |
| sH    |  0.7730 |  0.3100 |
| sI    |  0.8830 |  0.3390 |
| sJ    |  0.8870 |  0.3260 |
| sK    |  0.8550 |  0.3460 |
| sL    |  0.8900 |  0.3770 |
| sM    |  0.6750 |  0.2310 |
| sN    |  0.9180 |  0.3770 |
| sO    |  0.8750 |  0.3800 |
| sP    |  0.8440 |  0.3730 |
| sQ    |  0.8870 |  0.3290 |
| sR    |  0.6810 |  0.1450 |
| sS    |  0.8760 |  0.3500 |
| sT    |  0.8650 |  0.3330 |
| sU    |  0.8590 |  0.3370 |

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| Chain | Atom inclusion                                                                           | Q-score                                                                                  |
|-------|------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------|
| sV    |  0.8180 |  0.3410 |
| sW    |  0.9360 |  0.4060 |
| sX    |  0.8980 |  0.3890 |
| sY    |  0.8750 |  0.2830 |
| sZ    |  0.8340 |  0.3240 |
| sa    |  0.9020 |  0.3880 |
| sb    |  0.8700 |  0.3570 |
| sc    |  0.7570 |  0.2720 |
| sd    |  0.9410 |  0.3860 |
| se    |  0.7370 |  0.2490 |
| sf    |  0.7320 |  0.2540 |
| sg    |  0.7940 |  0.2850 |