



## Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 04:32 AM UTC

PDB ID : 8P8V / pdb\_00008p8v  
EMDB ID : EMD-17145  
Title : Mycoplasma pneumoniae di-ribosome in chloramphenicol-treated cells (leading 70S)  
Authors : Schacherl, M.; Xue, L.; Spahn, C.M.T.; Mahamid, J.  
Deposited on : 2023-06-02  
Resolution : 8.70 Å (reported)  
Based on initial models : 7OOD, 7OOC

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:

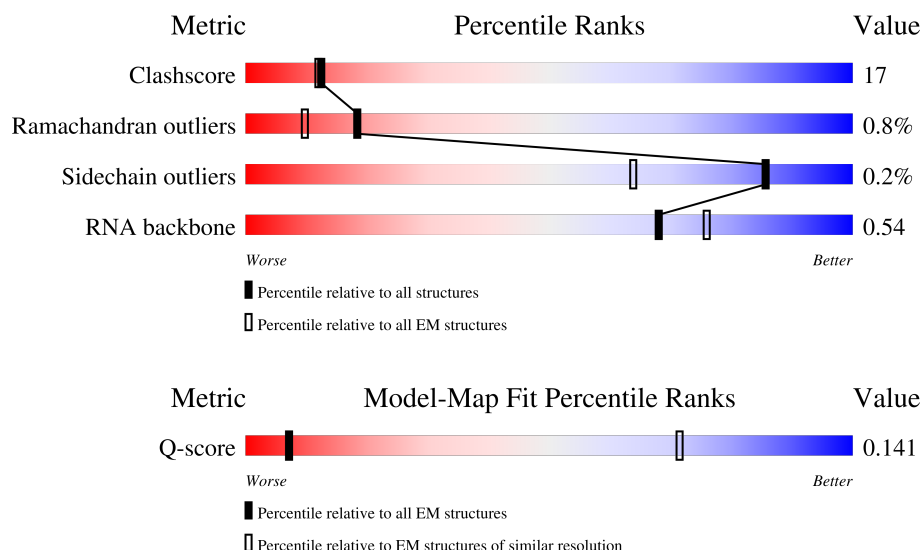
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (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 8.70 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                       | 282 ( 8.20 - 9.20 )                                      |

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   | 0     | 48     |                  |
| 2   | 1     | 59     |                  |
| 3   | 2     | 37     |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 4   | 3     | 2907   |                  |
| 5   | 4     | 108    |                  |
| 6   | 5     | 1520   |                  |
| 7   | 6     | 76     |                  |
| 8   | 7     | 75     |                  |
| 9   | 8     | 76     |                  |
| 10  | 9     | 226    |                  |
| 11  | A     | 294    |                  |
| 12  | B     | 273    |                  |
| 13  | C     | 205    |                  |
| 14  | D     | 219    |                  |
| 15  | E     | 215    |                  |
| 16  | F     | 155    |                  |
| 17  | G     | 142    |                  |
| 18  | H     | 132    |                  |
| 19  | I     | 108    |                  |
| 20  | J     | 121    |                  |
| 21  | K     | 139    |                  |
| 22  | L     | 124    |                  |
| 23  | M     | 61     |                  |
| 24  | N     | 86     |                  |
| 25  | O     | 94     |                  |
| 26  | P     | 85     |                  |
| 27  | Q     | 104    |                  |
| 28  | R     | 87     |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 29  | S     | 87     |                  |
| 30  | T     | 60     |                  |
| 31  | X     | 444    |                  |
| 32  | Y     | 40     |                  |
| 33  | Z     | 36     |                  |
| 34  | a     | 287    |                  |
| 35  | b     | 287    |                  |
| 36  | c     | 212    |                  |
| 37  | d     | 180    |                  |
| 38  | e     | 184    |                  |
| 39  | f     | 149    |                  |
| 40  | g     | 161    |                  |
| 41  | h     | 137    |                  |
| 42  | i     | 146    |                  |
| 43  | j     | 122    |                  |
| 44  | k     | 151    |                  |
| 45  | l     | 139    |                  |
| 46  | m     | 124    |                  |
| 47  | n     | 116    |                  |
| 48  | o     | 119    |                  |
| 49  | p     | 127    |                  |
| 50  | q     | 100    |                  |
| 51  | r     | 159    |                  |
| 52  | s     | 237    |                  |
| 53  | t     | 111    |                  |

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| Mol | Chain | Length | Quality of chain                                                         |
|-----|-------|--------|--------------------------------------------------------------------------|
| 54  | u     | 104    | <div> <div>12%</div> <div>51%</div> <div>34%</div> <div>15%</div> </div> |
| 55  | v     | 65     | <div> <div>12%</div> <div>52%</div> <div>46%</div> <div>•</div> </div>   |
| 56  | w     | 111    | <div> <div>17%</div> <div>56%</div> <div>43%</div> <div>•</div> </div>   |
| 57  | x     | 97     | <div> <div>38%</div> <div>54%</div> <div>38%</div> <div>8%</div> </div>  |
| 58  | y     | 57     | <div> <div>9%</div> <div>47%</div> <div>49%</div> <div>••</div> </div>   |
| 59  | z     | 53     | <div> <div>6%</div> <div>62%</div> <div>32%</div> <div>6%</div> </div>   |

## 2 Entry composition

There are 64 unique types of molecules in this entry. The entry contains 153622 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 50S ribosomal protein L34.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 1   | 0     | 47       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 380   | 236 | 81 | 61 | 2 |         |       |

- Molecule 2 is a protein called 50S ribosomal protein L35.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 2   | 1     | 59       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 477   | 300 | 99 | 77 | 1 |         |       |

- Molecule 3 is a protein called 50S ribosomal protein L36.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 3   | 2     | 37       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 304   | 189 | 65 | 46 | 4 |         |       |

- Molecule 4 is a RNA chain called 23S ribosomal RNA.

| Mol | Chain | Residues | Atoms |       |       |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|-------|
| 4   | 3     | 2893     | Total | C     | N     | O     | P    | 0       | 0     |
|     |       |          | 61995 | 27704 | 11293 | 20105 | 2893 |         |       |

- Molecule 5 is a RNA chain called 5S ribosomal RNA.

| Mol | Chain | Residues | Atoms |      |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|-------|
| 5   | 4     | 108      | Total | C    | N   | O   | P   | 0       | 0     |
|     |       |          | 2305  | 1030 | 415 | 752 | 108 |         |       |

- Molecule 6 is a RNA chain called 16S ribosomal RNA.

| Mol | Chain | Residues | Atoms |       |      |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|-------|
| 6   | 5     | 1506     | Total | C     | N    | O     | P    | 0       | 0     |
|     |       |          | 32238 | 14411 | 5844 | 10477 | 1506 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference   |
|-------|---------|----------|--------|----------|-------------|
| 5     | 1003    | A        | G      | conflict | GB 26117688 |

- Molecule 7 is a RNA chain called tRNA-Ala (E-site).

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 7   | 6     | 76       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 1620  | 723 | 287 | 534 | 76 |         |       |

- Molecule 8 is a RNA chain called tRNA-Asp (P-site).

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 8   | 7     | 75       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 1599  | 712 | 279 | 533 | 75 |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment   | Reference   |
|-------|---------|----------|--------|-----------|-------------|
| 7     | 17      | G        | -      | insertion | GB 26117688 |
| 7     | 55      | C        | U      | conflict  | GB 26117688 |

- Molecule 9 is a RNA chain called tRNA-Lys (A-site).

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 9   | 8     | 76       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 1615  | 722 | 284 | 533 | 76 |         |       |

- Molecule 10 is a protein called 50S ribosomal protein L1.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 10  | 9     | 226      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1711  | 1095 | 292 | 318 | 6 |         |       |

- Molecule 11 is a protein called 30S ribosomal protein S2.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 11  | A     | 268      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2152  | 1368 | 379 | 396 | 9 |         |       |

- Molecule 12 is a protein called 30S ribosomal protein S3.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 12  | B     | 224      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1764  | 1116 | 326 | 317 | 5 |         |       |

- Molecule 13 is a protein called 30S ribosomal protein S4.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 13  | C     | 204      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1669  | 1057 | 316 | 292 | 4 |         |       |

- Molecule 14 is a protein called 30S ribosomal protein S5.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 14  | D     | 158      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1217  | 771 | 232 | 211 | 3 |         |       |

- Molecule 15 is a protein called 30S ribosomal protein S6.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 15  | E     | 215      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1793  | 1111 | 341 | 339 | 2 |         |       |

- Molecule 16 is a protein called 30S ribosomal protein S7.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 16  | F     | 155      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1254  | 790 | 240 | 217 | 7 |         |       |

- Molecule 17 is a protein called 30S ribosomal protein S8.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 17  | G     | 142      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1118  | 728 | 194 | 193 | 3 |         |       |

- Molecule 18 is a protein called 30S ribosomal protein S9.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 18  | H     | 129      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1040  | 661 | 195 | 183 | 1 |         |       |

- Molecule 19 is a protein called 30S ribosomal protein S10.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 19  | I     | 104      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 832   | 536 | 147 | 148 | 1 |         |       |

- Molecule 20 is a protein called 30S ribosomal protein S11.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 20  | J     | 120      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 878   | 547 | 163 | 162 | 6 |         |       |

- Molecule 21 is a protein called 30S ribosomal protein S12.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 21  | K     | 135      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1071  | 677 | 212 | 180 | 2 |         |       |

- Molecule 22 is a protein called 30S ribosomal protein S13.

| Mol | Chain | Residues | Atoms |     |     |     |  | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|-------|
| 22  | L     | 121      | Total | C   | N   | O   |  | 0       | 0     |
|     |       |          | 975   | 609 | 197 | 169 |  |         |       |

- Molecule 23 is a protein called 30S ribosomal protein S14 type Z.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 23  | M     | 60       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 474   | 302 | 96 | 72 | 4 |         |       |

- Molecule 24 is a protein called 30S ribosomal protein S15.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 24  | N     | 86       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 697   | 441 | 131 | 124 | 1 |         |       |

- Molecule 25 is a protein called 30S ribosomal protein S16.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 25  | O     | 87       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 705   | 453 | 130 | 118 | 4 |         |       |

- Molecule 26 is a protein called 30S ribosomal protein S17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 26  | P     | 85       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 693   | 436 | 138 | 118 | 1 |         |       |

- Molecule 27 is a protein called 30S ribosomal protein S18.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 27  | Q     | 73       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 605   | 389 | 117 | 95 | 4 |         |       |

- Molecule 28 is a protein called 30S ribosomal protein S19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 28  | R     | 86       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 700   | 444 | 132 | 122 | 2 |         |       |

- Molecule 29 is a protein called 30S ribosomal protein S20.

| Mol | Chain | Residues | Atoms |     |     |     |  | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|-------|
| 29  | S     | 79       | Total | C   | N   | O   |  | 0       | 0     |
|     |       |          | 643   | 391 | 138 | 114 |  |         |       |

- Molecule 30 is a protein called 30S ribosomal protein S21.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 30  | T     | 59       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 519   | 326 | 111 | 80 | 2 |         |       |

- Molecule 31 is a protein called Trigger factor.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 31  | X     | 30       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 242   | 155 | 43 | 43 | 1 |         |       |

- Molecule 32 is a RNA chain called mRNA.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 32  | Y     | 40       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 862   | 388 | 170 | 264 | 40 |         |       |

- Molecule 33 is a protein called Nascent chain.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 33  | Z     | 36       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 187   | 112 | 37 | 38 |         |       |

- Molecule 34 is a protein called 50S ribosomal protein L2.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 34  | a     | 285      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2225  | 1385 | 437 | 397 | 6 |         |       |

- Molecule 35 is a protein called 50S ribosomal protein L3.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 35  | b     | 229      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1762  | 1119 | 318 | 318 | 7 |         |       |

- Molecule 36 is a protein called 50S ribosomal protein L4.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 36  | c     | 211      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1654  | 1053 | 299 | 299 | 3 |         |       |

- Molecule 37 is a protein called 50S ribosomal protein L5.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 37  | d     | 179      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1416  | 910 | 251 | 251 | 4 |         |       |

- Molecule 38 is a protein called 50S ribosomal protein L6.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 38  | e     | 176      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 1396  | 899 | 247 | 250 |         |       |

- Molecule 39 is a protein called 50S ribosomal protein L9.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 39  | f     | 149      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1210  | 780 | 212 | 215 | 3 |         |       |

- Molecule 40 is a protein called 50S ribosomal protein L10.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 40  | g     | 125      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 951   | 606 | 165 | 177 | 3 |         |       |

- Molecule 41 is a protein called 50S ribosomal protein L11.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 41  | h     | 128      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 959   | 616 | 160 | 177 | 6 |         |       |

- Molecule 42 is a protein called 50S ribosomal protein L13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 42  | i     | 144      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1164  | 737 | 213 | 209 | 5 |         |       |

- Molecule 43 is a protein called 50S ribosomal protein L14.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 43  | j     | 122      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 944   | 595 | 178 | 167 | 4 |         |       |

- Molecule 44 is a protein called 50S ribosomal protein L15.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 44  | k     | 150      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1170  | 741 | 228 | 200 | 1 |         |       |

- Molecule 45 is a protein called 50S ribosomal protein L16.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 45  | l     | 136      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1079  | 694 | 196 | 182 | 7 |         |       |

- Molecule 46 is a protein called 50S ribosomal protein L17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 46  | m     | 119      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 958   | 609 | 175 | 171 | 3 |         |       |

- Molecule 47 is a protein called 50S ribosomal protein L18.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 47  | n     | 116      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 918   | 573 | 181 | 162 | 2 |         |       |

- Molecule 48 is a protein called 50S ribosomal protein L19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 48  | o     | 118      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 966   | 609 | 186 | 170 | 1 |         |       |

- Molecule 49 is a protein called 50S ribosomal protein L20.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 49  | p     | 118      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 981   | 624 | 194 | 161 | 2 |         |       |

- Molecule 50 is a protein called 50S ribosomal protein L21.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 50  | q     | 99       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 811   | 525 | 148 | 134 | 4 |         |       |

- Molecule 51 is a protein called 50S ribosomal protein L22.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 51  | r     | 142      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1091  | 677 | 212 | 195 | 7 |         |       |

- Molecule 52 is a protein called 50S ribosomal protein L23.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 52  | s     | 95       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 740   | 486 | 125 | 128 | 1 |         |       |

- Molecule 53 is a protein called 50S ribosomal protein L24.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 53  | t     | 111      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 871   | 550 | 166 | 152 | 3 |         |       |

- Molecule 54 is a protein called 50S ribosomal protein L27.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 54  | u     | 88       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 670   | 416 | 132 | 121 | 1 |         |       |

- Molecule 55 is a protein called 50S ribosomal protein L28.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 55  | v     | 64       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 520   | 320 | 109 | 90 | 1 |         |       |

- Molecule 56 is a protein called 50S ribosomal protein L29.

| Mol | Chain | Residues | Atoms |     |     |     |  | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|-------|
| 56  | w     | 110      | Total | C   | N   | O   |  | 0       | 0     |
|     |       |          | 906   | 576 | 168 | 162 |  |         |       |

- Molecule 57 is a protein called 50S ribosomal protein L31.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 57  | x     | 89       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 708   | 449 | 124 | 131 | 4 |         |       |

- Molecule 58 is a protein called 50S ribosomal protein L32.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 58  | y     | 56       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 452   | 274 | 98 | 75 | 5 |         |       |

- Molecule 59 is a protein called 50S ribosomal protein L33 1.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 59  | z     | 50       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 408   | 255 | 81 | 68 | 4 |         |       |

- Molecule 60 is ZINC ION (CCD ID: ZN) (formula: Zn).

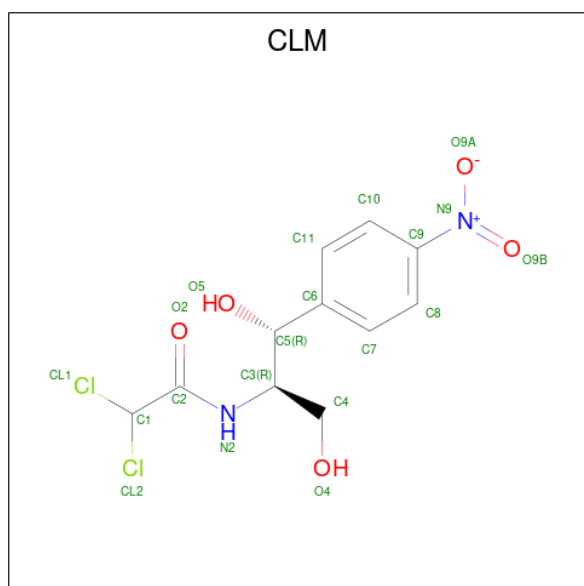
| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 60  | 2     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 60  | M     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 60  | Q     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |

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| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 60  | x     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 60  | y     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 60  | z     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 61 is CHLORAMPHENICOL (CCD ID: CLM) (formula:  $C_{11}H_{12}Cl_2N_2O_5$ ) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 61  | 3     | 1        | Total | C  | Cl | N | O | 0       |
|     |       |          | 20    | 11 | 2  | 2 | 5 |         |

- Molecule 62 is POTASSIUM ION (CCD ID: K) (formula: K).

| Mol | Chain | Residues | Atoms |   | AltConf |
|-----|-------|----------|-------|---|---------|
| 62  | 3     | 1        | Total | K | 0       |
|     |       |          | 1     | 1 |         |

- Molecule 63 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

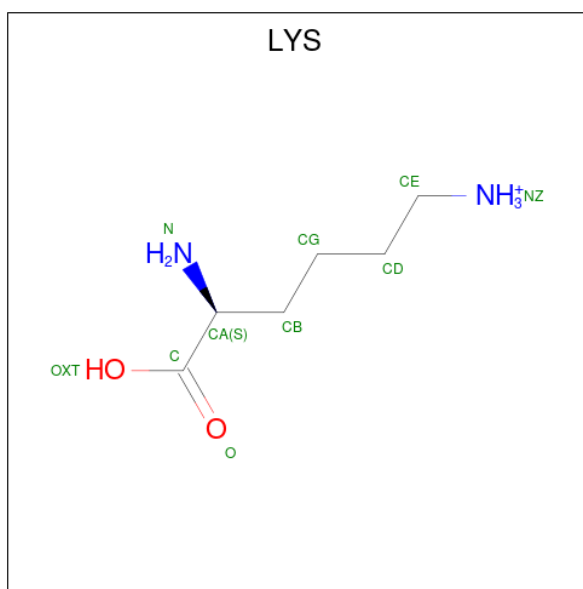
| Mol | Chain | Residues | Atoms |     | AltConf |
|-----|-------|----------|-------|-----|---------|
| 63  | 3     | 209      | Total | Mg  | 0       |
|     |       |          | 209   | 209 |         |

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| Mol | Chain | Residues | Atoms       |          | AltConf |
|-----|-------|----------|-------------|----------|---------|
| 63  | 4     | 1        | Total<br>1  | Mg<br>1  | 0       |
| 63  | 5     | 87       | Total<br>87 | Mg<br>87 | 0       |
| 63  | 6     | 1        | Total<br>1  | Mg<br>1  | 0       |
| 63  | 8     | 1        | Total<br>1  | Mg<br>1  | 0       |
| 63  | E     | 1        | Total<br>1  | Mg<br>1  | 0       |
| 63  | K     | 1        | Total<br>1  | Mg<br>1  | 0       |
| 63  | L     | 1        | Total<br>1  | Mg<br>1  | 0       |
| 63  | P     | 1        | Total<br>1  | Mg<br>1  | 0       |
| 63  | Y     | 2        | Total<br>2  | Mg<br>2  | 0       |
| 63  | a     | 1        | Total<br>1  | Mg<br>1  | 0       |
| 63  | b     | 1        | Total<br>1  | Mg<br>1  | 0       |
| 63  | f     | 12       | Total<br>12 | Mg<br>12 | 0       |
| 63  | i     | 1        | Total<br>1  | Mg<br>1  | 0       |
| 63  | y     | 2        | Total<br>2  | Mg<br>2  | 0       |

- Molecule 64 is LYSINE (CCD ID: LYS) (formula:  $C_6H_{15}N_2O_2$ ).



| Mol | Chain | Residues | Atoms |   |   |   | AltConf |
|-----|-------|----------|-------|---|---|---|---------|
|     |       |          | Total | C | N | O |         |
| 64  | 8     | 1        | 9     | 6 | 2 | 1 | 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.

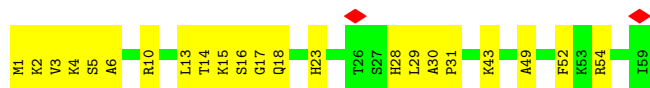
#### • Molecule 1: 50S ribosomal protein L34

Chain 0: 



#### • Molecule 2: 50S ribosomal protein L35

Chain 1: 



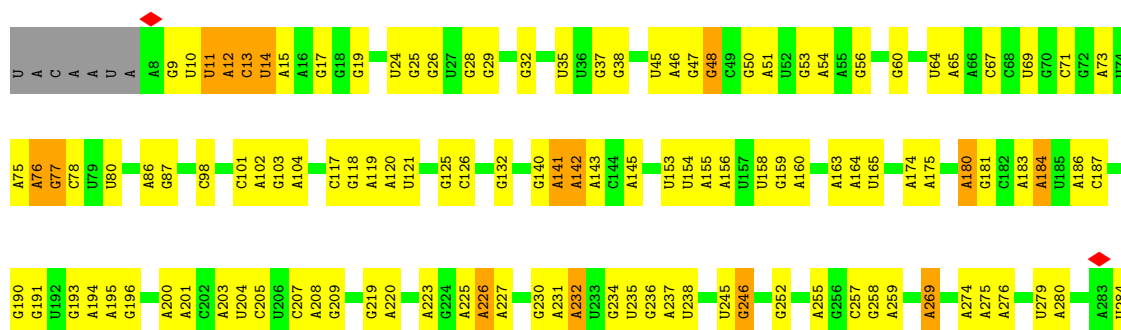
#### • Molecule 3: 50S ribosomal protein L36

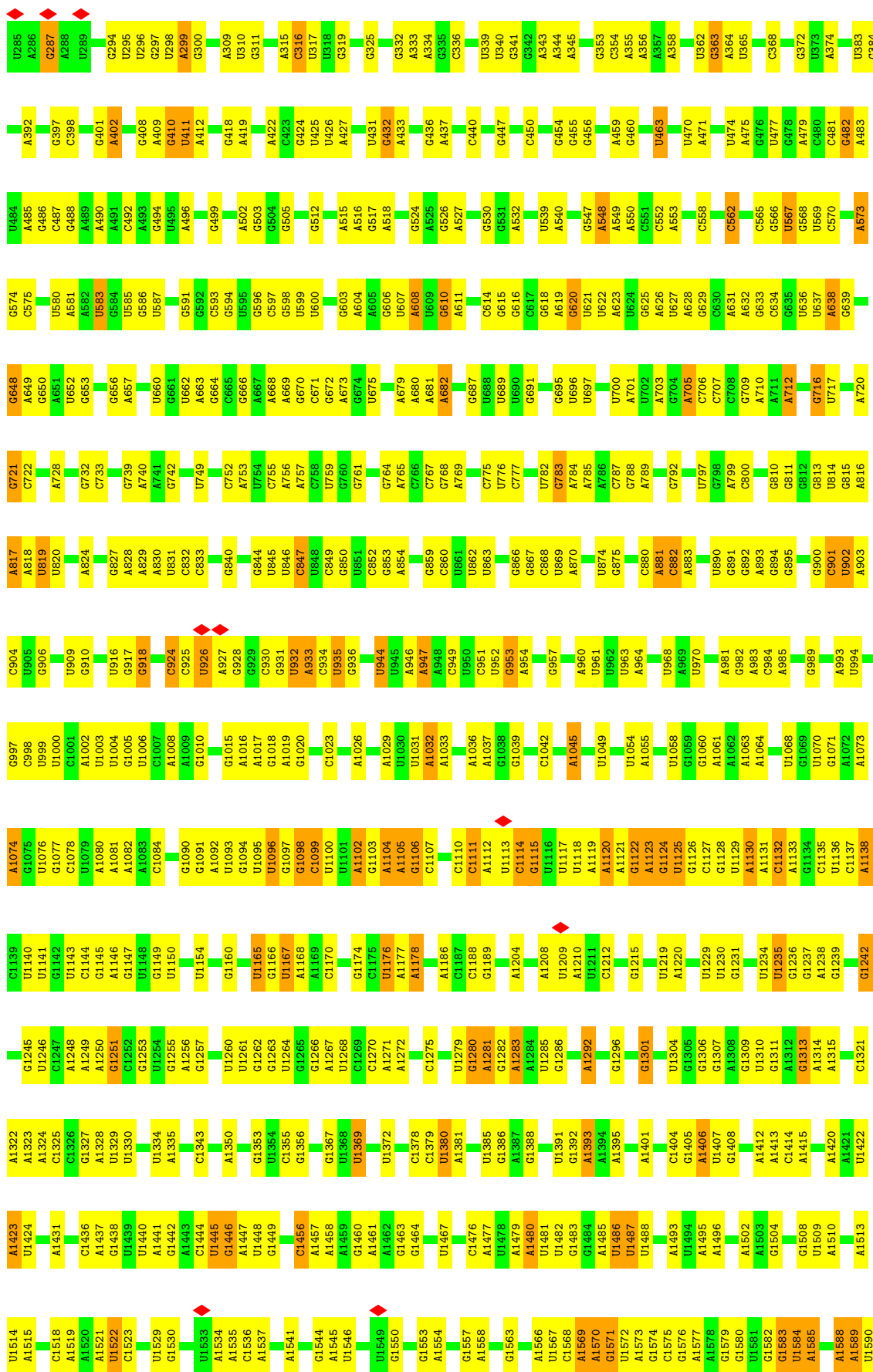
Chain 2: 



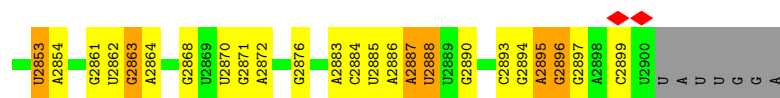
#### • Molecule 4: 23S ribosomal RNA

Chain 3: 

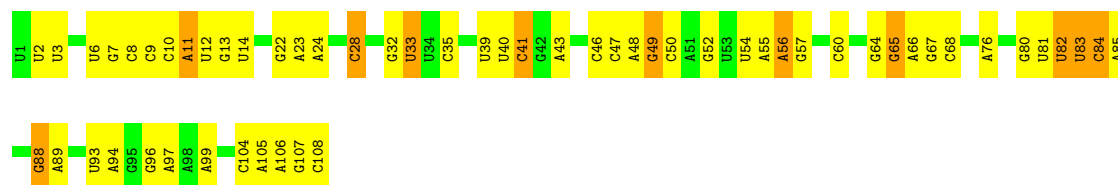




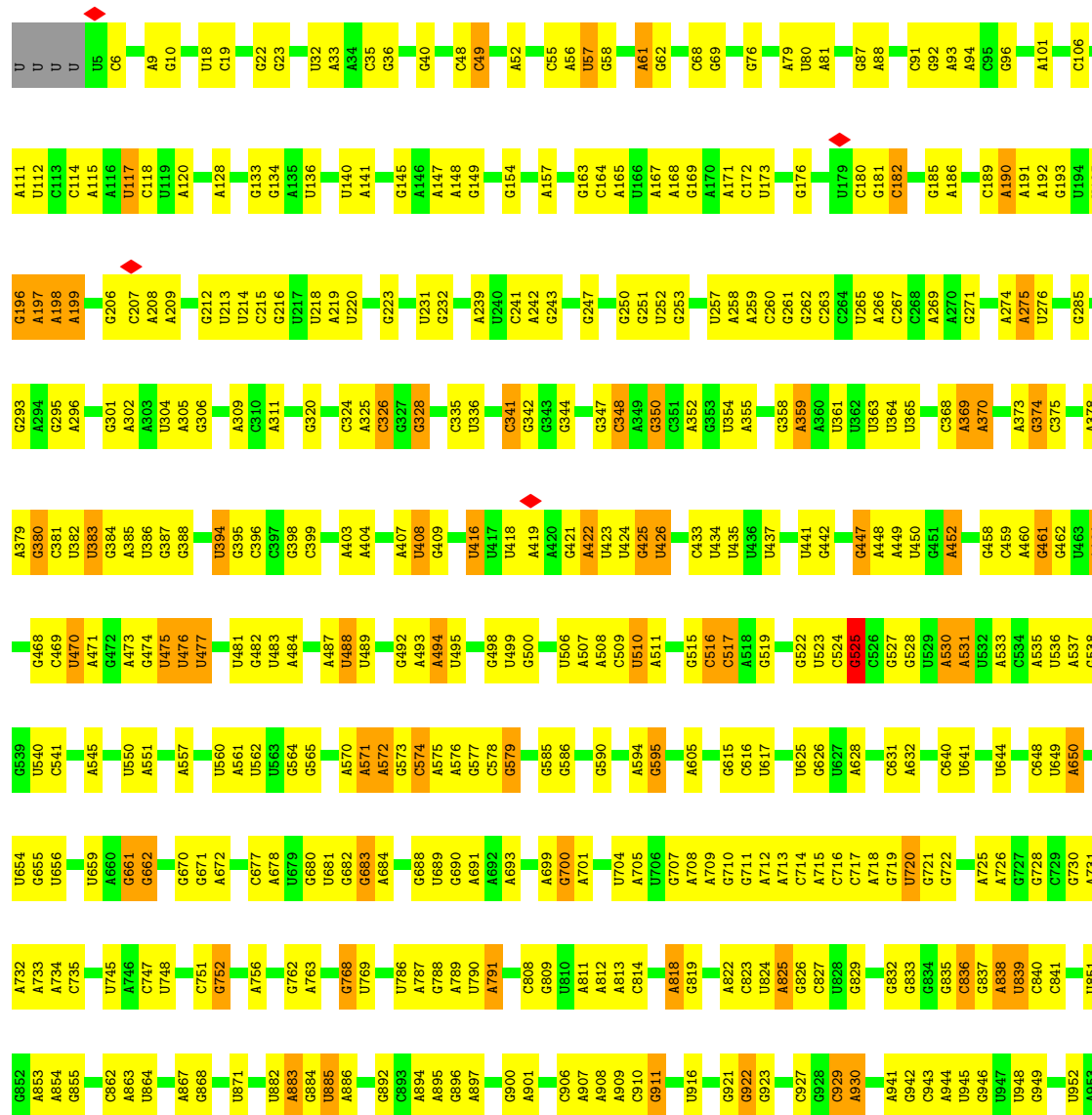


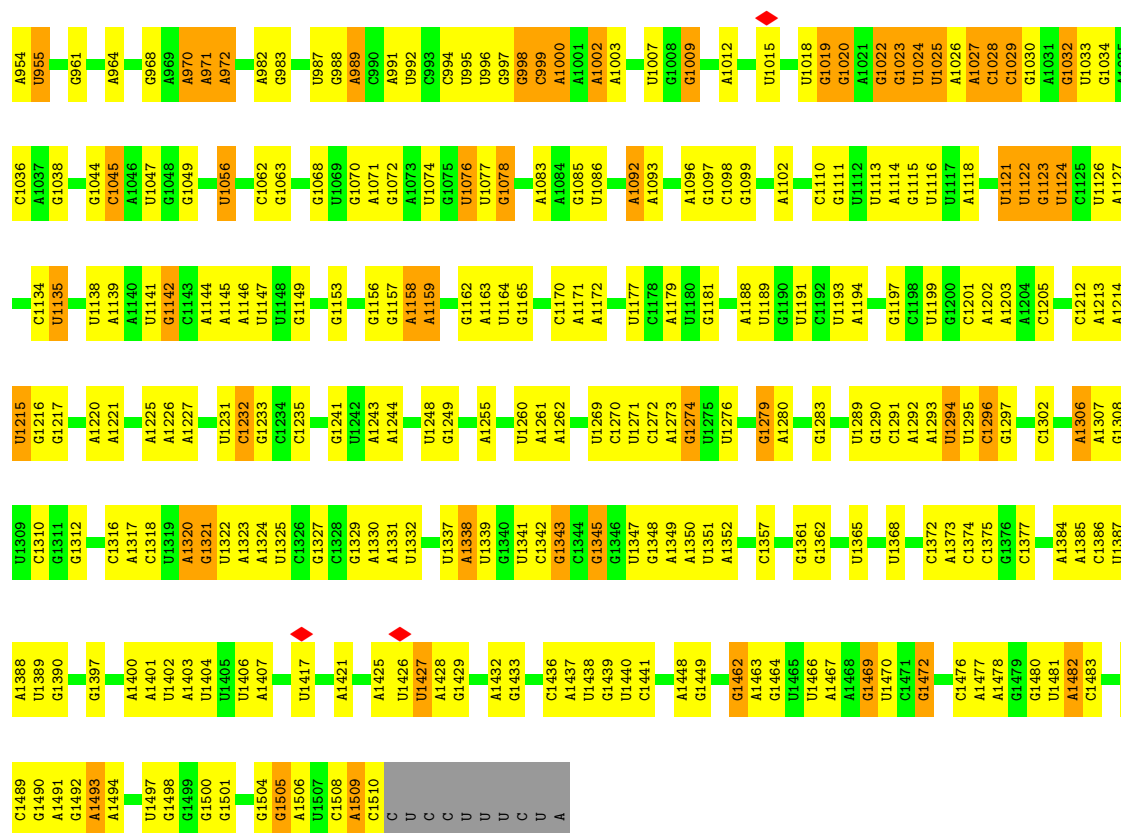


• Molecule 5: 5S ribosomal RNA



• Molecule 6: 16S ribosomal RNA





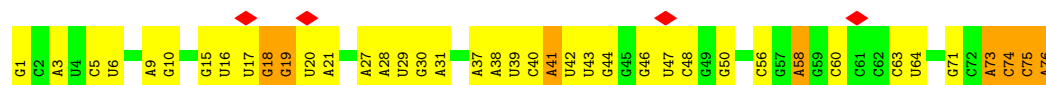
• Molecule 7: tRNA-Ala (E-site)



• Molecule 8: tRNA-Asp (P-site)

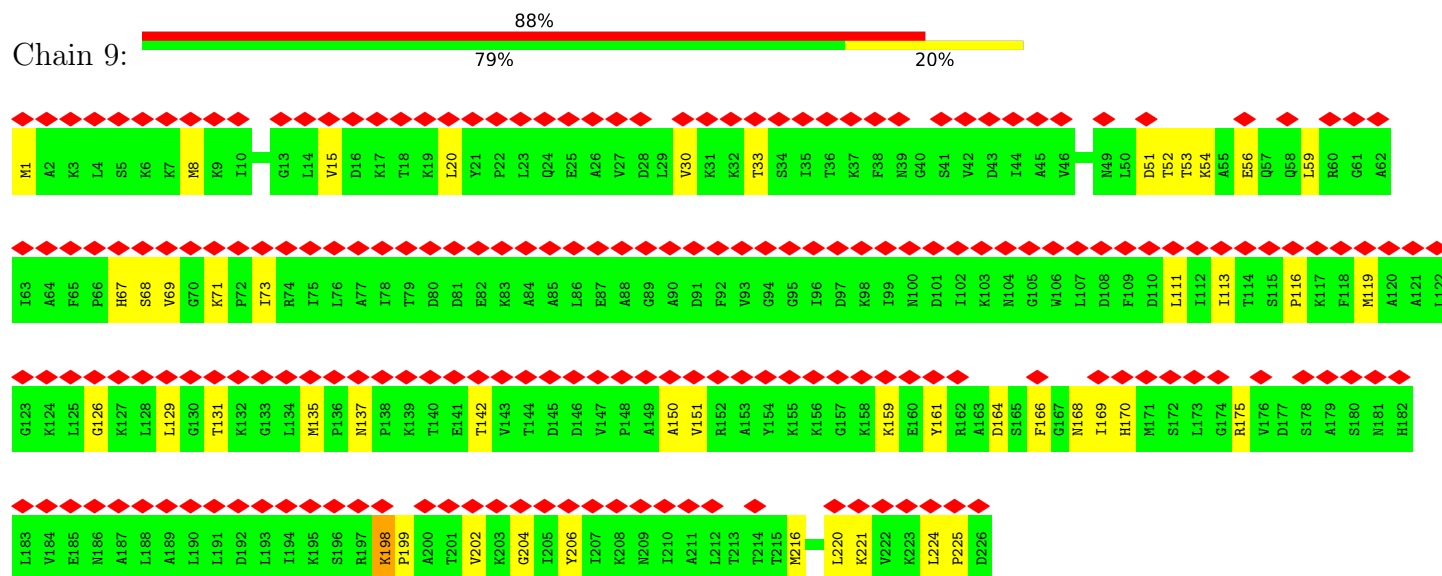


• Molecule 9: tRNA-Lys (A-site)



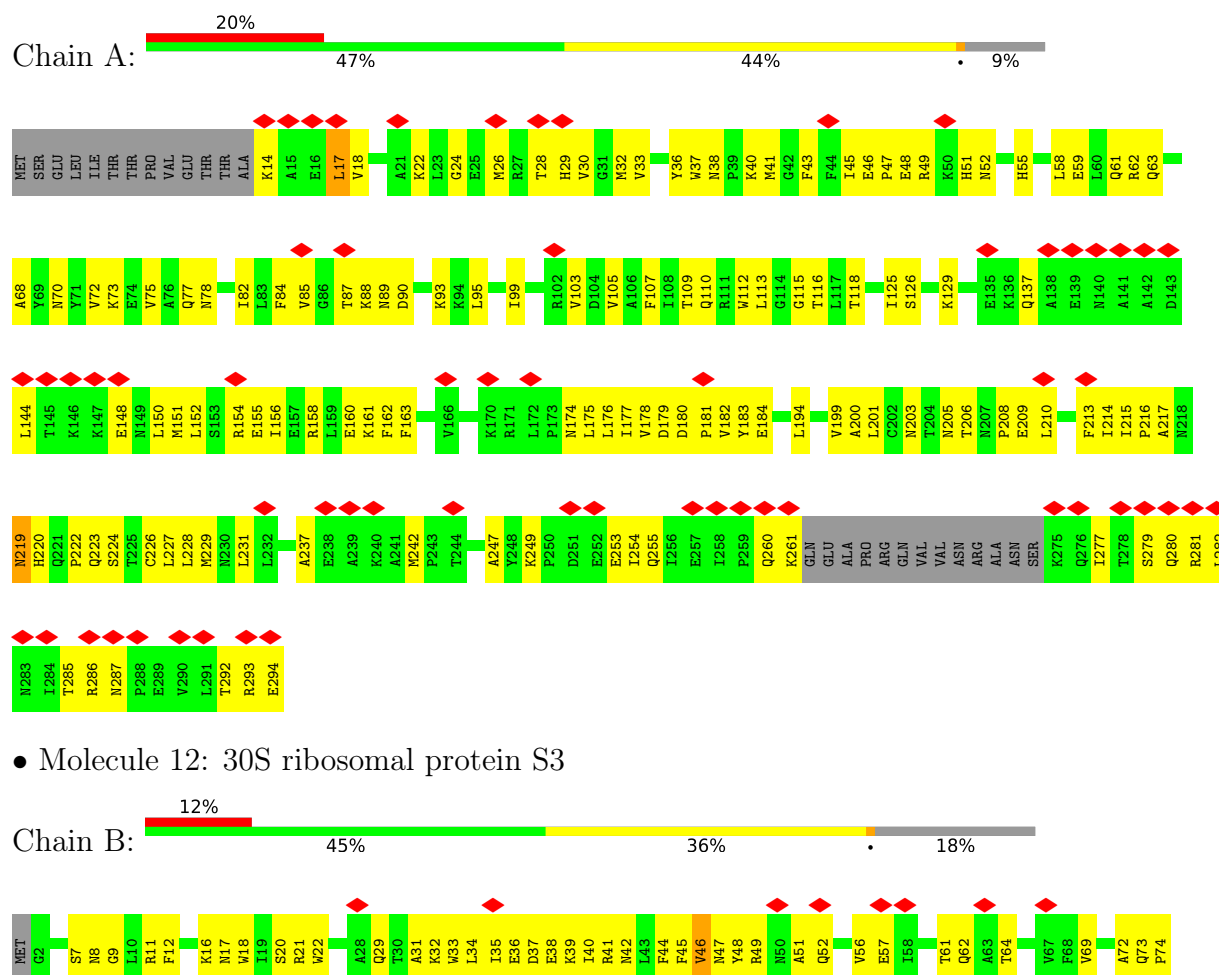
- Molecule 10: 50S ribosomal protein L1

Chain 9:



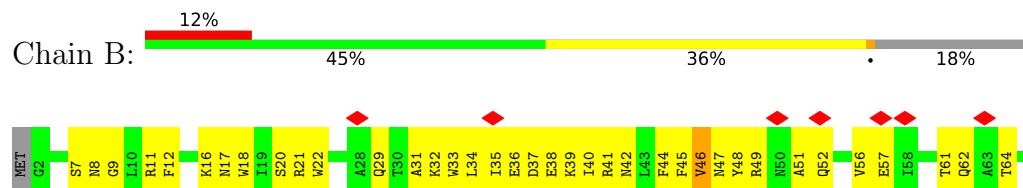
- Molecule 11: 30S ribosomal protein S2

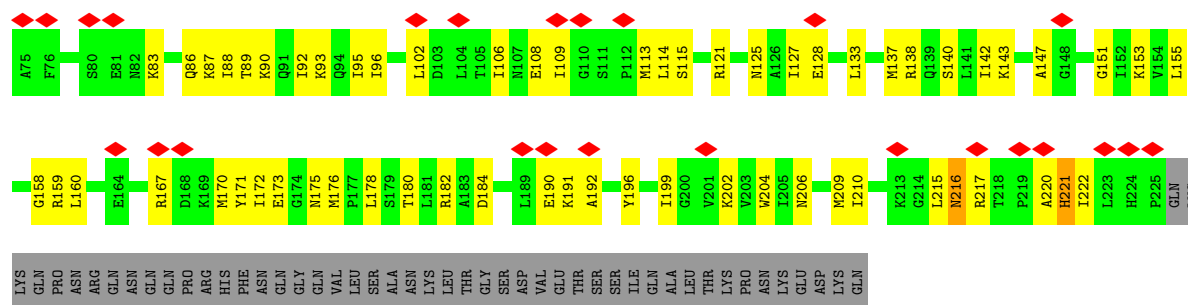
Chain A:



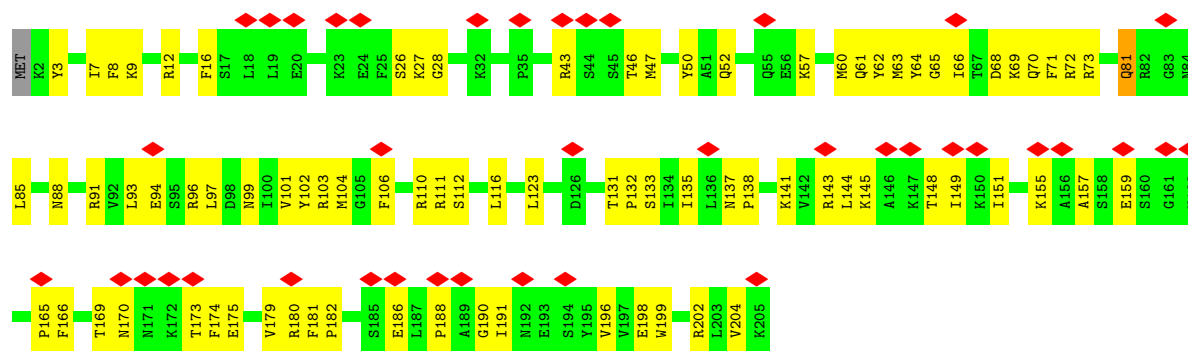
- Molecule 12: 30S ribosomal protein S3

Chain B:

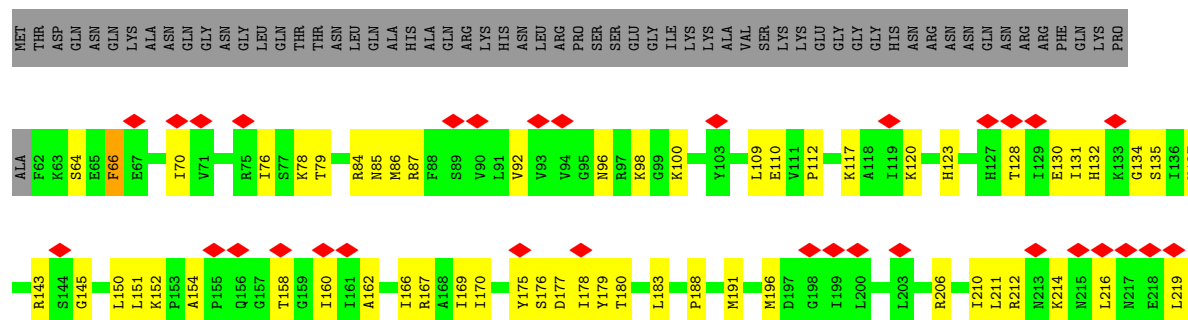




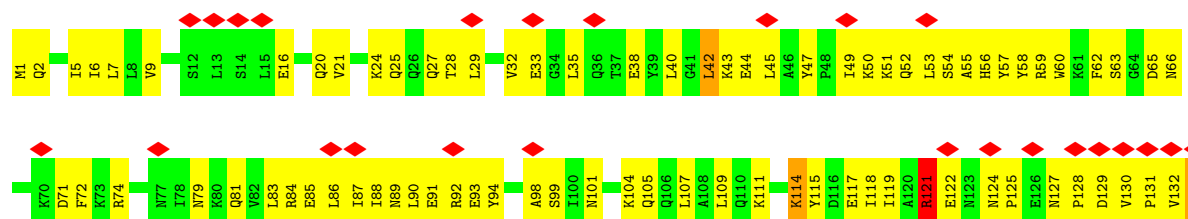
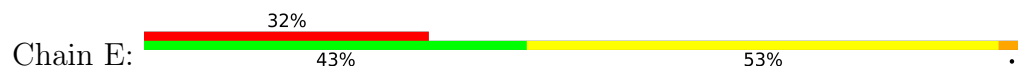
• Molecule 13: 30S ribosomal protein S4

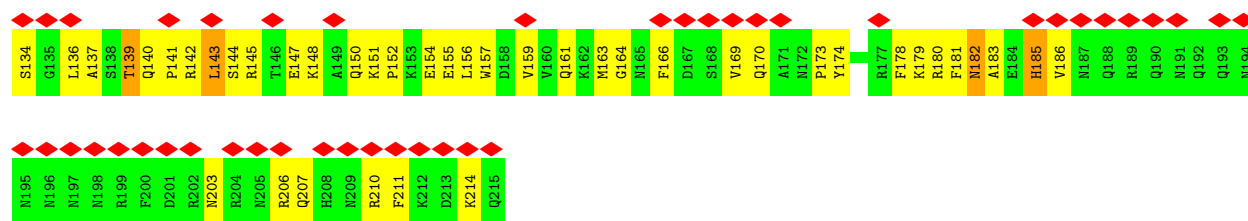


• Molecule 14: 30S ribosomal protein S5

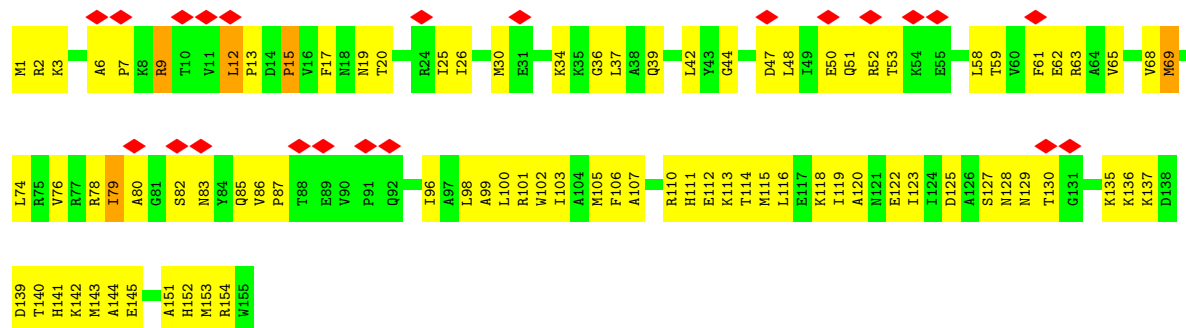
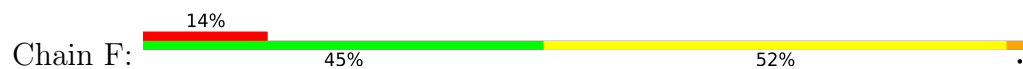


• Molecule 15: 30S ribosomal protein S6

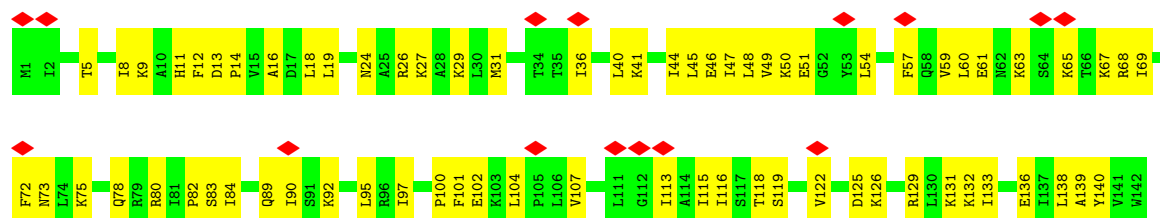




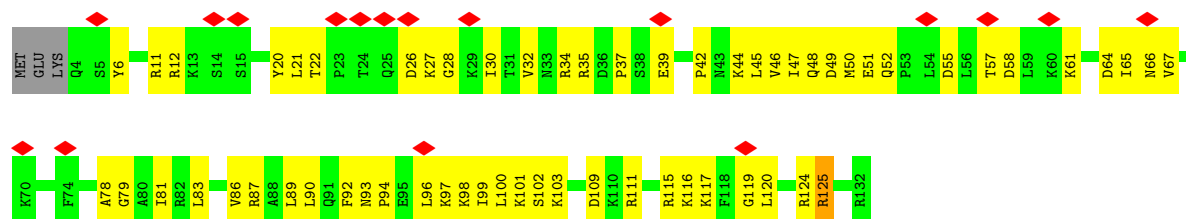
• Molecule 16: 30S ribosomal protein S7



• Molecule 17: 30S ribosomal protein S8

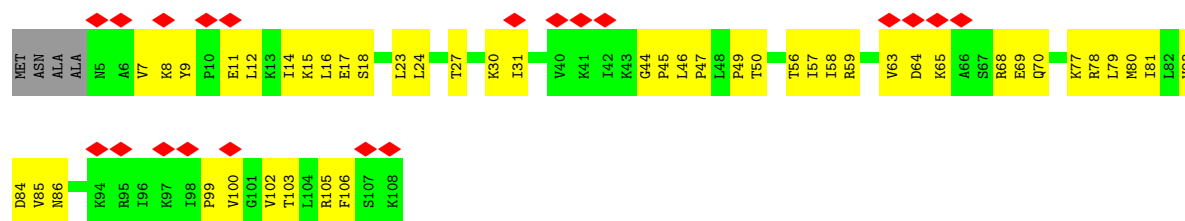


• Molecule 18: 30S ribosomal protein S9

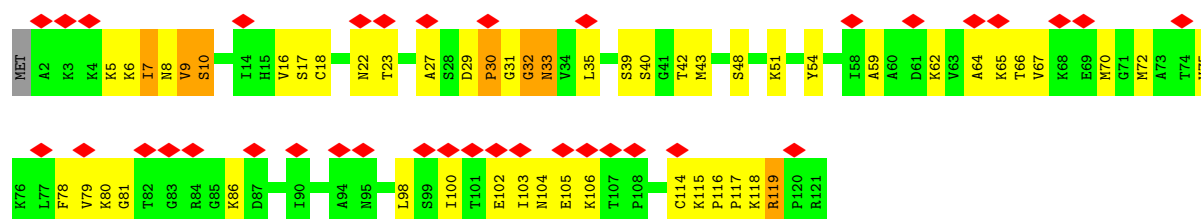


• Molecule 19: 30S ribosomal protein S10

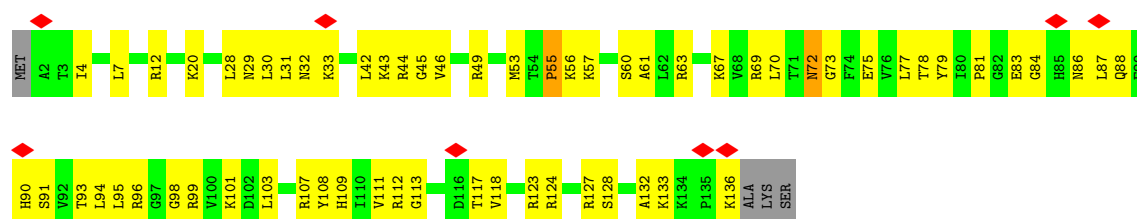




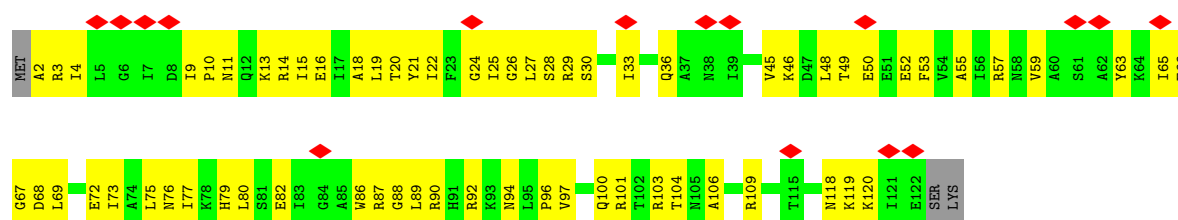
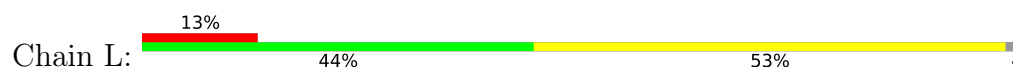
- Molecule 20: 30S ribosomal protein S11



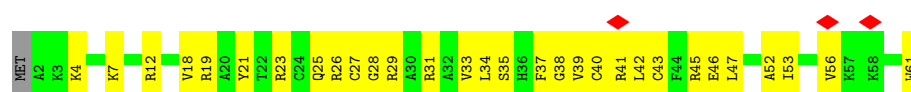
- Molecule 21: 30S ribosomal protein S12



- Molecule 22: 30S ribosomal protein S13



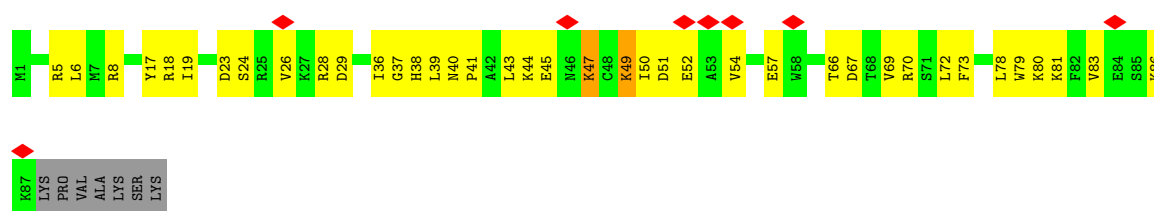
- Molecule 23: 30S ribosomal protein S14 type Z



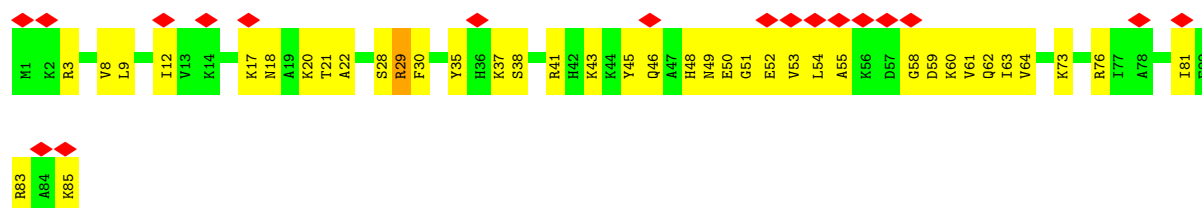
- Molecule 24: 30S ribosomal protein S15



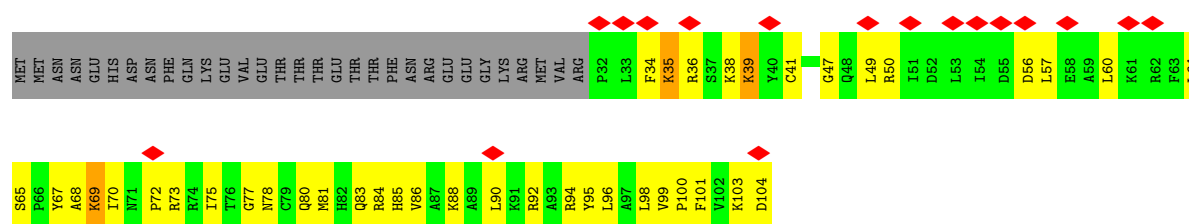
• Molecule 25: 30S ribosomal protein S16



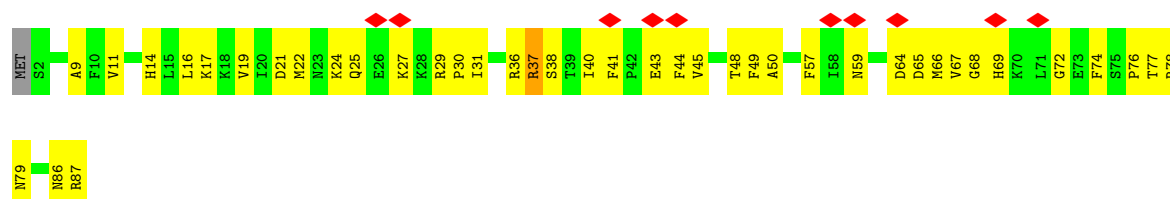
• Molecule 26: 30S ribosomal protein S17



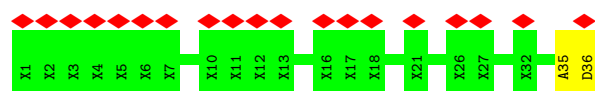
• Molecule 27: 30S ribosomal protein S18



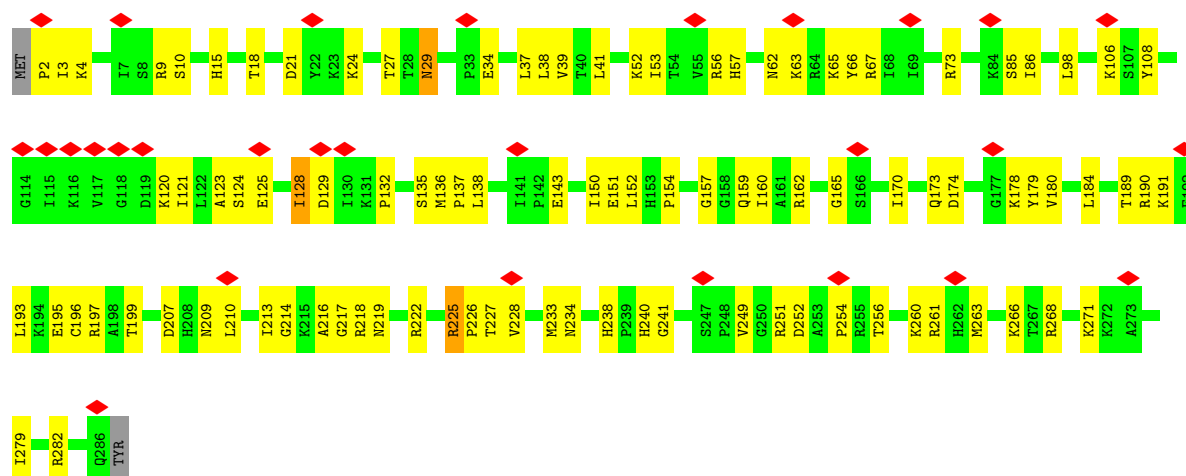
• Molecule 28: 30S ribosomal protein S19



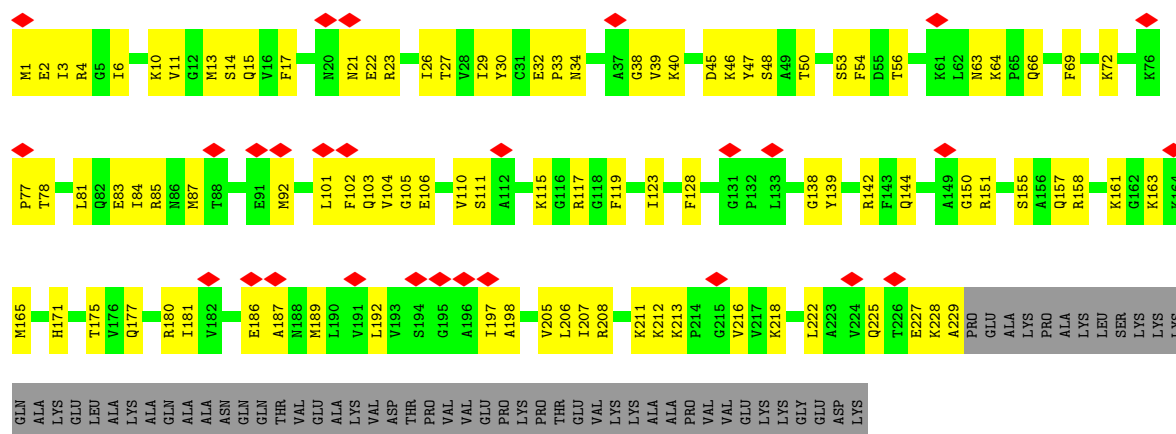




• Molecule 34: 50S ribosomal protein L2

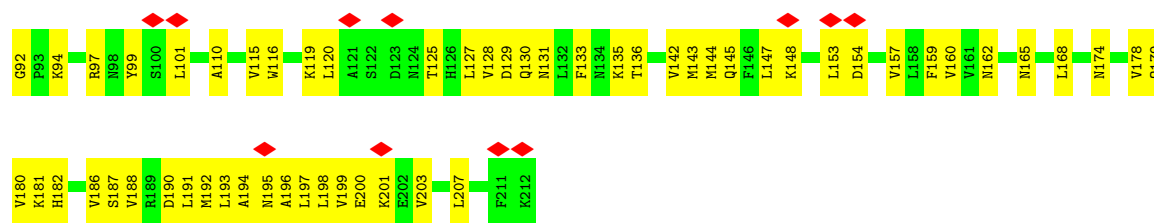


• Molecule 35: 50S ribosomal protein L3

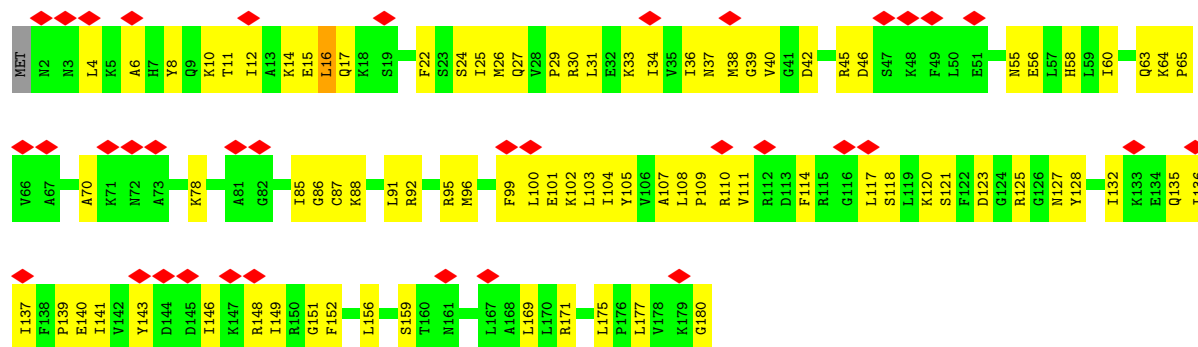


• Molecule 36: 50S ribosomal protein L4

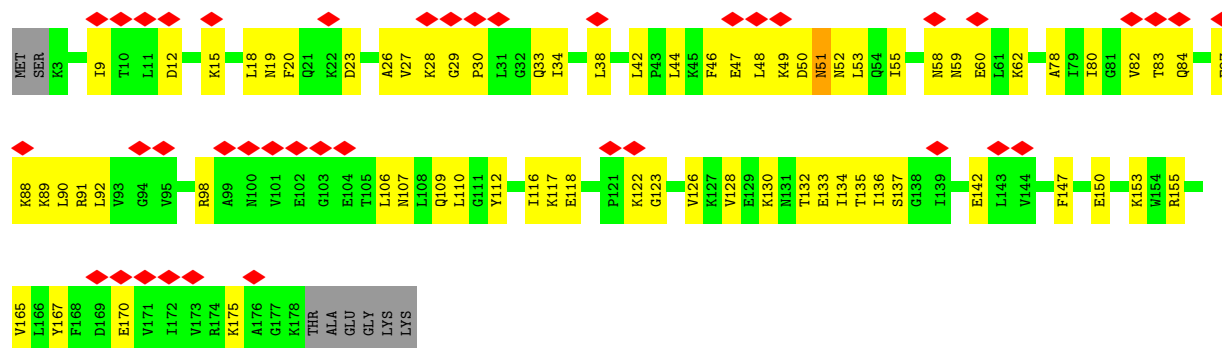




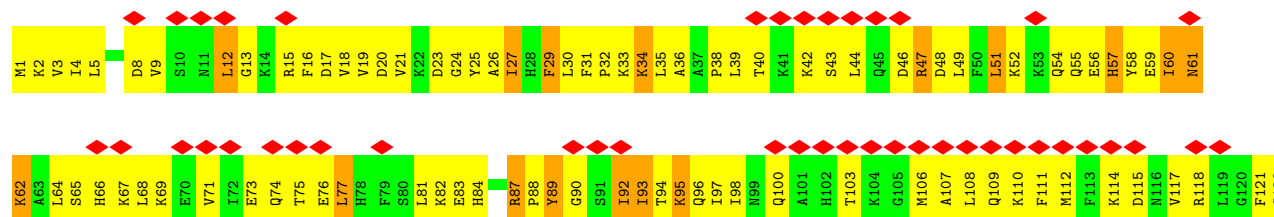
• Molecule 37: 50S ribosomal protein L5

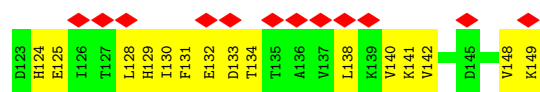


• Molecule 38: 50S ribosomal protein L6

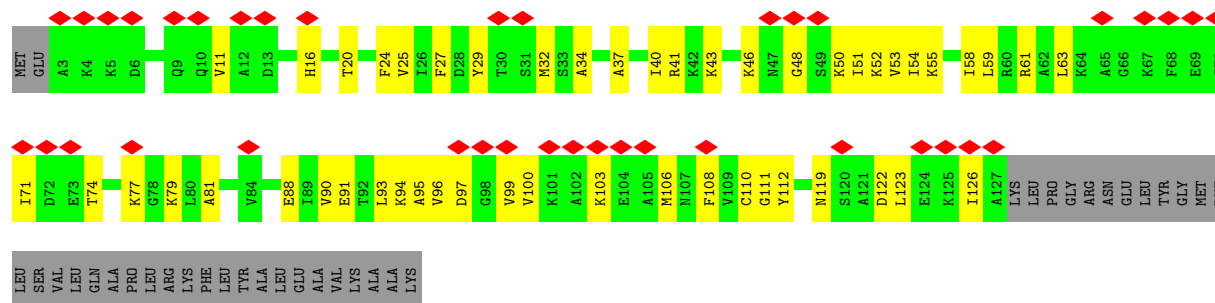


• Molecule 39: 50S ribosomal protein L9

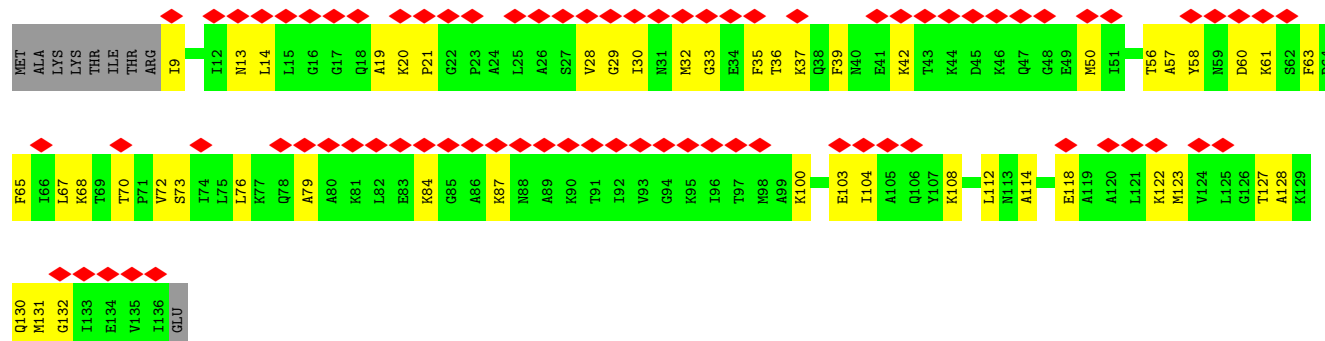




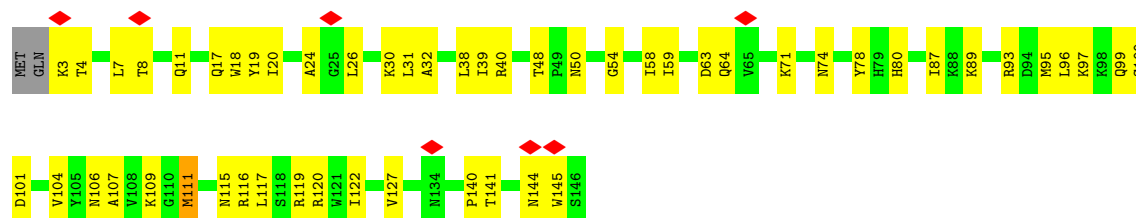
• Molecule 40: 50S ribosomal protein L10



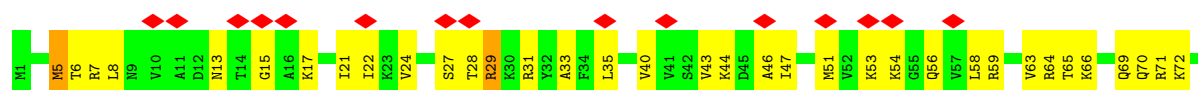
• Molecule 41: 50S ribosomal protein L11



• Molecule 42: 50S ribosomal protein L13

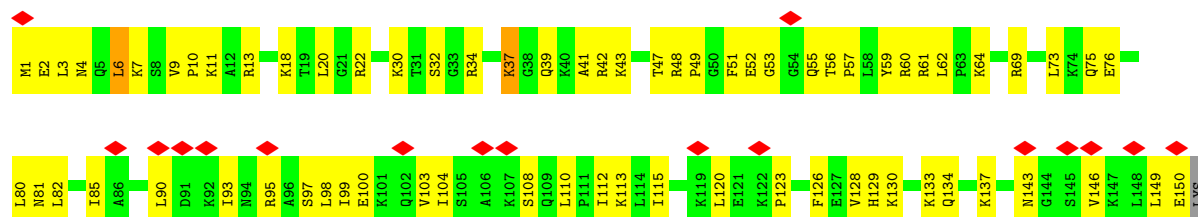


• Molecule 43: 50S ribosomal protein L14

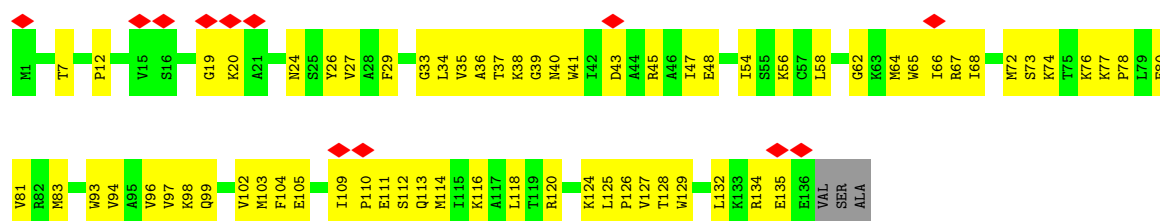




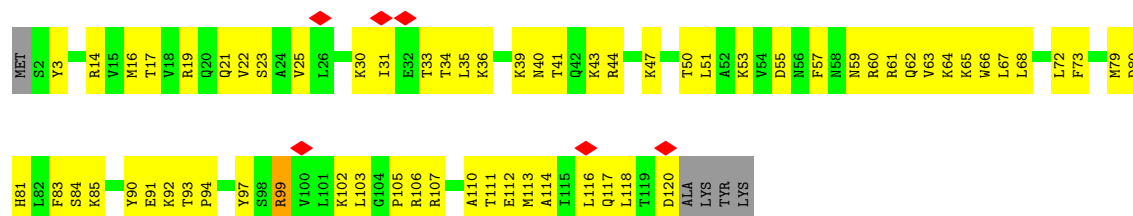
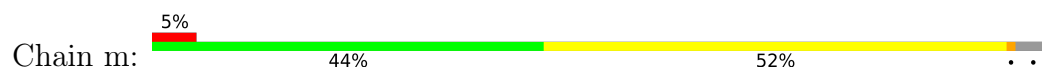
• Molecule 44: 50S ribosomal protein L15



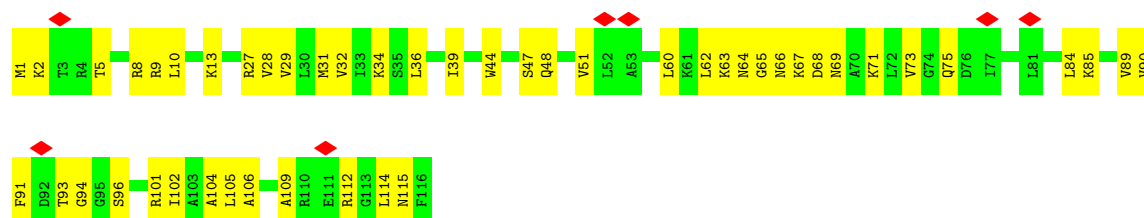
• Molecule 45: 50S ribosomal protein L16



• Molecule 46: 50S ribosomal protein L17



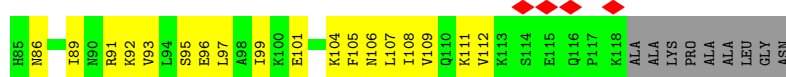
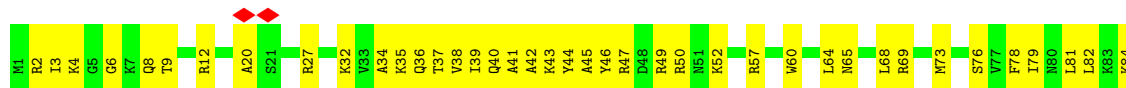
• Molecule 47: 50S ribosomal protein L18



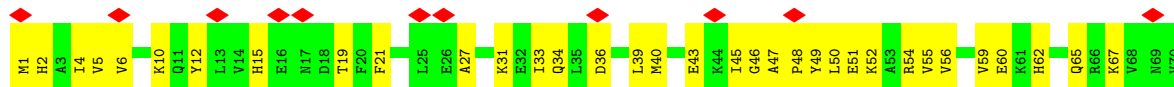
• Molecule 48: 50S ribosomal protein L19



• Molecule 49: 50S ribosomal protein L20



• Molecule 50: 50S ribosomal protein L21



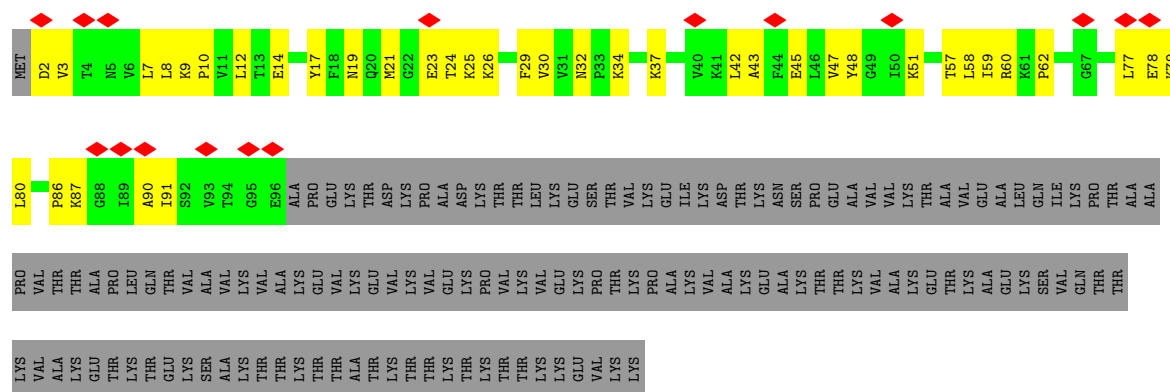
• Molecule 51: 50S ribosomal protein L22



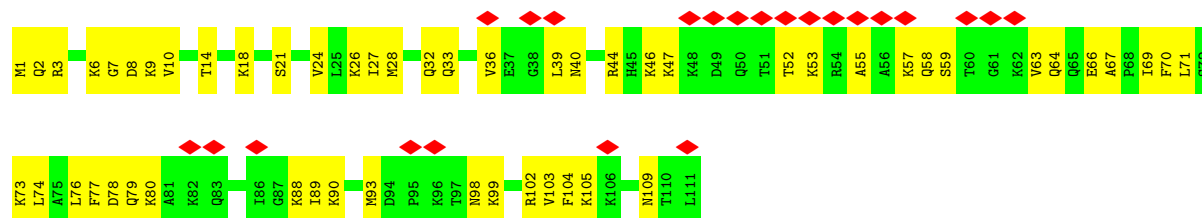
LYS

• Molecule 52: 50S ribosomal protein L23

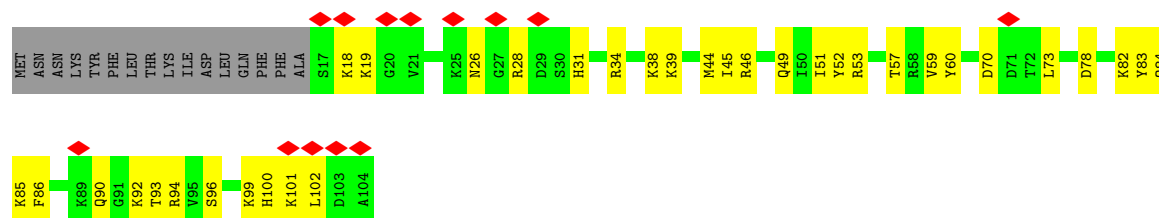




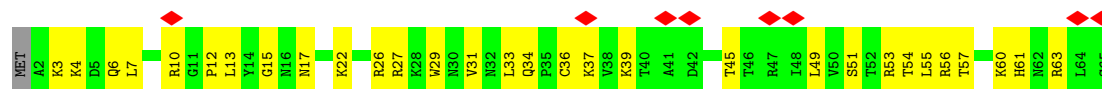
- Molecule 53: 50S ribosomal protein L24



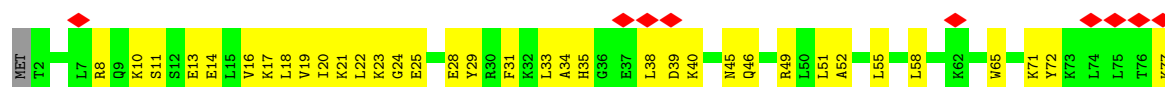
- Molecule 54: 50S ribosomal protein L27

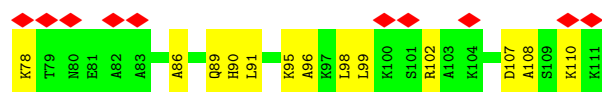


- Molecule 55: 50S ribosomal protein L28

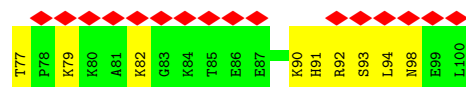
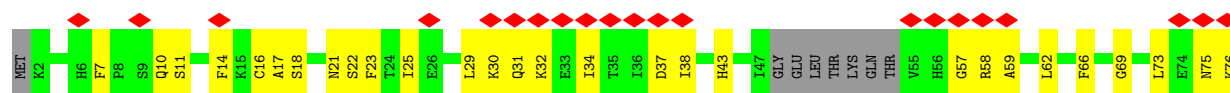
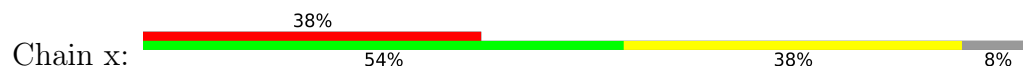


- Molecule 56: 50S ribosomal protein L29

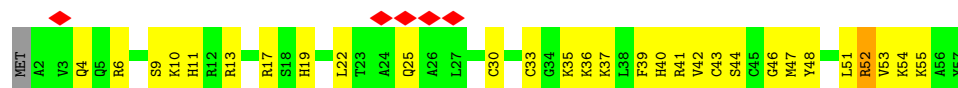




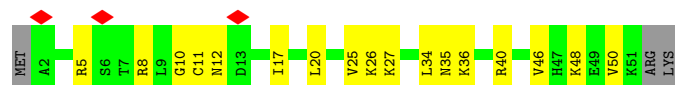
- Molecule 57: 50S ribosomal protein L31



- Molecule 58: 50S ribosomal protein L32



- Molecule 59: 50S ribosomal protein L33 1



## 4 Experimental information

| Property                             | Value                                                                                          | Source    |
|--------------------------------------|------------------------------------------------------------------------------------------------|-----------|
| EM reconstruction method             | SUBTOMOGRAM AVERAGING                                                                          | Depositor |
| Imposed symmetry                     | POINT, C1                                                                                      | Depositor |
| Number of subtomograms used          | 963                                                                                            | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                                                                              | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION; CTF estimation and 3D CTF correction are done in Warp | Depositor |
| Microscope                           | FEI TITAN KRIOS                                                                                | Depositor |
| Voltage (kV)                         | 300                                                                                            | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 137                                                                                            | Depositor |
| Minimum defocus (nm)                 | 1000                                                                                           | Depositor |
| Maximum defocus (nm)                 | 3250                                                                                           | Depositor |
| Magnification                        | 64000                                                                                          | Depositor |
| Image detector                       | GATAN K3 BIOQUANTUM (6k x 4k)                                                                  | Depositor |
| Maximum map value                    | 5.477                                                                                          | Depositor |
| Minimum map value                    | -2.425                                                                                         | Depositor |
| Average map value                    | 0.022                                                                                          | Depositor |
| Map value standard deviation         | 0.237                                                                                          | Depositor |
| Recommended contour level            | 1.2                                                                                            | Depositor |
| Map size ( $\text{\AA}$ )            | 793.6, 793.6, 793.6                                                                            | wwPDB     |
| Map dimensions                       | 256, 256, 256                                                                                  | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0                                                                               | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 3.1, 3.1, 3.1                                                                                  | Depositor |

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: OMG, B8T, MA6, K, CLM, 7MG, 1MG, ZN, 2MA, MG, 5MC

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   | 0     | 0.15         | 0/383          | 0.53        | 0/504           |
| 2   | 1     | 0.18         | 0/484          | 0.52        | 0/637           |
| 3   | 2     | 0.18         | 0/306          | 0.56        | 0/401           |
| 4   | 3     | 0.12         | 1/69363 (0.0%) | 0.25        | 1/108161 (0.0%) |
| 5   | 4     | 0.09         | 0/2578         | 0.21        | 0/4016          |
| 6   | 5     | 0.11         | 0/35970        | 0.24        | 0/56077         |
| 7   | 6     | 0.16         | 0/1810         | 0.48        | 2/2817 (0.1%)   |
| 8   | 7     | 0.19         | 0/1785         | 0.35        | 0/2779          |
| 9   | 8     | 0.22         | 1/1804 (0.1%)  | 0.30        | 0/2807          |
| 10  | 9     | 0.19         | 0/1735         | 0.56        | 1/2337 (0.0%)   |
| 11  | A     | 0.24         | 0/2186         | 0.64        | 0/2952          |
| 12  | B     | 0.23         | 0/1791         | 0.55        | 0/2421          |
| 13  | C     | 0.22         | 0/1700         | 0.58        | 0/2278          |
| 14  | D     | 0.18         | 0/1233         | 0.55        | 0/1651          |
| 15  | E     | 0.34         | 0/1824         | 0.80        | 2/2454 (0.1%)   |
| 16  | F     | 0.28         | 0/1274         | 0.74        | 1/1710 (0.1%)   |
| 17  | G     | 0.24         | 0/1134         | 0.67        | 1/1527 (0.1%)   |
| 18  | H     | 0.27         | 0/1056         | 0.72        | 2/1409 (0.1%)   |
| 19  | I     | 0.19         | 0/843          | 0.57        | 0/1132          |
| 20  | J     | 0.24         | 0/893          | 0.70        | 1/1198 (0.1%)   |
| 21  | K     | 0.21         | 0/1089         | 0.58        | 0/1461          |
| 22  | L     | 0.22         | 0/986          | 0.54        | 0/1321          |
| 23  | M     | 0.18         | 0/483          | 0.52        | 0/643           |
| 24  | N     | 0.18         | 0/703          | 0.53        | 0/936           |
| 25  | O     | 0.21         | 0/718          | 0.67        | 1/962 (0.1%)    |
| 26  | P     | 0.23         | 0/702          | 0.66        | 1/934 (0.1%)    |
| 27  | Q     | 0.28         | 0/617          | 0.79        | 1/823 (0.1%)    |
| 28  | R     | 0.24         | 0/716          | 0.72        | 2/958 (0.2%)    |
| 29  | S     | 0.18         | 0/645          | 0.58        | 1/857 (0.1%)    |
| 30  | T     | 0.29         | 0/524          | 0.74        | 1/685 (0.1%)    |
| 31  | X     | 0.23         | 0/245          | 0.63        | 0/325           |
| 32  | Y     | 0.21         | 0/969          | 0.50        | 0/1508          |

| Mol | Chain | Bond lengths |                 | Bond angles |                  |
|-----|-------|--------------|-----------------|-------------|------------------|
|     |       | RMSZ         | # Z  >5         | RMSZ        | # Z  >5          |
| 33  | Z     | 0.90         | 0/26            | 1.70        | 0/33             |
| 34  | a     | 0.21         | 0/2267          | 0.57        | 2/3044 (0.1%)    |
| 35  | b     | 0.22         | 0/1795          | 0.64        | 0/2412           |
| 36  | c     | 0.19         | 0/1681          | 0.57        | 2/2257 (0.1%)    |
| 37  | d     | 0.21         | 0/1437          | 0.56        | 1/1931 (0.1%)    |
| 38  | e     | 0.18         | 0/1420          | 0.52        | 0/1912           |
| 39  | f     | 0.60         | 0/1233          | 0.96        | 5/1653 (0.3%)    |
| 40  | g     | 0.16         | 0/960           | 0.46        | 0/1284           |
| 41  | h     | 0.17         | 0/968           | 0.47        | 0/1298           |
| 42  | i     | 0.20         | 0/1186          | 0.51        | 1/1592 (0.1%)    |
| 43  | j     | 0.68         | 2/953 (0.2%)    | 1.26        | 8/1275 (0.6%)    |
| 44  | k     | 0.20         | 0/1187          | 0.65        | 2/1581 (0.1%)    |
| 45  | l     | 0.20         | 0/1104          | 0.57        | 0/1481           |
| 46  | m     | 0.24         | 0/973           | 0.68        | 2/1309 (0.2%)    |
| 47  | n     | 0.21         | 0/927           | 0.57        | 0/1239           |
| 48  | o     | 0.27         | 0/976           | 0.70        | 0/1296           |
| 49  | p     | 0.23         | 0/996           | 0.64        | 0/1325           |
| 50  | q     | 0.22         | 0/828           | 0.62        | 0/1111           |
| 51  | r     | 0.18         | 0/1100          | 0.59        | 0/1471           |
| 52  | s     | 0.20         | 0/752           | 0.52        | 0/1015           |
| 53  | t     | 0.24         | 0/878           | 0.51        | 0/1165           |
| 54  | u     | 0.21         | 0/678           | 0.64        | 0/902            |
| 55  | v     | 0.19         | 0/526           | 0.60        | 0/703            |
| 56  | w     | 0.20         | 0/916           | 0.64        | 0/1222           |
| 57  | x     | 0.17         | 0/722           | 0.60        | 0/959            |
| 58  | y     | 0.20         | 0/457           | 0.72        | 1/601 (0.2%)     |
| 59  | z     | 0.15         | 0/412           | 0.48        | 0/547            |
| All | All   | 0.17         | 4/165907 (0.0%) | 0.40        | 42/247299 (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 |
|-----|-------|---------------------|---------------------|
| 34  | a     | 0                   | 1                   |
| 39  | f     | 0                   | 1                   |
| 55  | v     | 0                   | 1                   |
| All | All   | 0                   | 3                   |

All (4) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 43  | j     | 93  | PRO  | CB-CG | 14.87  | 2.23        | 1.49     |
| 43  | j     | 93  | PRO  | CG-CD | -11.04 | 1.13        | 1.50     |
| 9   | 8     | 76  | A    | C6-N6 | 6.00   | 1.46        | 1.33     |
| 4   | 3     | 783 | 1MG  | O3'-P | 5.21   | 1.61        | 1.56     |

All (42) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 43  | j     | 93  | PRO  | CB-CG-CD    | -23.42 | 31.15       | 106.10   |
| 43  | j     | 93  | PRO  | CA-N-CD     | -22.36 | 80.69       | 112.00   |
| 43  | j     | 93  | PRO  | N-CD-CG     | 13.17  | 122.96      | 103.20   |
| 10  | 9     | 198 | LYS  | CB-CG-CD    | 8.51   | 130.87      | 111.30   |
| 43  | j     | 93  | PRO  | N-CA-CB     | -7.70  | 96.46       | 103.31   |
| 43  | j     | 92  | SER  | C-N-CD      | 7.67   | 156.45      | 125.00   |
| 18  | H     | 125 | ARG  | CB-CG-CD    | -7.11  | 94.95       | 111.30   |
| 15  | E     | 121 | ARG  | CA-CB-CG    | 6.97   | 128.05      | 114.10   |
| 34  | a     | 132 | PRO  | CA-N-CD     | -6.65  | 102.69      | 112.00   |
| 27  | Q     | 69  | LYS  | CA-CB-CG    | 6.65   | 127.39      | 114.10   |
| 42  | i     | 111 | MET  | CB-CG-SD    | -6.64  | 92.77       | 112.70   |
| 30  | T     | 33  | GLU  | N-CA-CB     | 6.56   | 121.58      | 110.49   |
| 20  | J     | 119 | ARG  | CA-CB-CG    | 6.55   | 127.21      | 114.10   |
| 36  | c     | 97  | ARG  | CB-CG-CD    | 6.53   | 126.32      | 111.30   |
| 16  | F     | 69  | MET  | CA-CB-CG    | 6.46   | 127.02      | 114.10   |
| 25  | O     | 41  | PRO  | CA-N-CD     | -6.39  | 103.05      | 112.00   |
| 46  | m     | 91  | GLU  | CA-CB-CG    | 6.39   | 126.89      | 114.10   |
| 39  | f     | 57  | HIS  | N-CA-C      | -6.38  | 104.33      | 111.28   |
| 39  | f     | 60  | ILE  | N-CA-C      | -6.37  | 102.91      | 111.44   |
| 15  | E     | 121 | ARG  | CB-CG-CD    | 6.30   | 125.78      | 111.30   |
| 28  | R     | 76  | PRO  | CA-N-CD     | -6.22  | 103.29      | 112.00   |
| 36  | c     | 97  | ARG  | CA-CB-CG    | 6.21   | 126.52      | 114.10   |
| 44  | k     | 6   | LEU  | CA-CB-CG    | 5.87   | 136.86      | 116.30   |
| 39  | f     | 61  | ASN  | N-CA-C      | -5.87  | 104.89      | 111.28   |
| 39  | f     | 29  | PHE  | N-CA-C      | -5.81  | 106.17      | 113.72   |
| 7   | 6     | 46  | G    | C2'-C3'-O3' | 5.79   | 118.19      | 109.50   |
| 26  | P     | 29  | ARG  | CA-CB-CG    | 5.70   | 125.50      | 114.10   |
| 29  | S     | 53  | ARG  | CA-CB-CG    | 5.68   | 125.46      | 114.10   |
| 4   | 3     | 482 | G    | P-O3'-C3'   | -5.55  | 111.87      | 120.20   |
| 44  | k     | 37  | LYS  | N-CA-C      | 5.49   | 119.27      | 112.47   |
| 28  | R     | 37  | ARG  | CB-CG-CD    | -5.38  | 98.92       | 111.30   |
| 43  | j     | 5   | MET  | CA-CB-CG    | 5.36   | 124.83      | 114.10   |
| 17  | G     | 12  | PHE  | N-CA-C      | 5.34   | 118.02      | 111.82   |
| 7   | 6     | 33  | U    | C2'-C3'-O3' | -5.30  | 105.74      | 113.70   |
| 34  | a     | 132 | PRO  | N-CD-CG     | -5.25  | 95.33       | 103.20   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 58  | y     | 52  | ARG  | CA-CB-CG | 5.24  | 124.58      | 114.10   |
| 43  | j     | 29  | ARG  | CA-CB-CG | 5.19  | 124.48      | 114.10   |
| 43  | j     | 5   | MET  | CB-CG-SD | -5.18 | 97.14       | 112.70   |
| 37  | d     | 16  | LEU  | CA-CB-CG | 5.17  | 134.41      | 116.30   |
| 18  | H     | 125 | ARG  | CD-NE-CZ | -5.16 | 117.17      | 124.40   |
| 46  | m     | 99  | ARG  | CA-CB-CG | -5.09 | 103.92      | 114.10   |
| 39  | f     | 87  | ARG  | N-CA-C   | -5.06 | 106.67      | 113.25   |

There are no chirality outliers.

All (3) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 34  | a     | 225 | ARG  | Sidechain |
| 39  | f     | 118 | ARG  | Sidechain |
| 55  | v     | 63  | ARG  | Sidechain |

## 5.2 Too-close contacts

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   | 0     | 380   | 0        | 429      | 18      | 0            |
| 2   | 1     | 477   | 0        | 530      | 35      | 0            |
| 3   | 2     | 304   | 0        | 348      | 14      | 0            |
| 4   | 3     | 61995 | 0        | 31114    | 1030    | 0            |
| 5   | 4     | 2305  | 0        | 1164     | 32      | 0            |
| 6   | 5     | 32238 | 0        | 16195    | 535     | 0            |
| 7   | 6     | 1620  | 0        | 818      | 25      | 0            |
| 8   | 7     | 1599  | 0        | 805      | 26      | 0            |
| 9   | 8     | 1615  | 0        | 816      | 20      | 0            |
| 10  | 9     | 1711  | 0        | 1829     | 34      | 0            |
| 11  | A     | 2152  | 0        | 2222     | 126     | 0            |
| 12  | B     | 1764  | 0        | 1833     | 103     | 0            |
| 13  | C     | 1669  | 0        | 1729     | 94      | 0            |
| 14  | D     | 1217  | 0        | 1311     | 47      | 0            |
| 15  | E     | 1793  | 0        | 1781     | 161     | 0            |
| 16  | F     | 1254  | 0        | 1320     | 85      | 0            |
| 17  | G     | 1118  | 0        | 1238     | 86      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 18  | H     | 1040  | 0        | 1107     | 70      | 0            |
| 19  | I     | 832   | 0        | 918      | 55      | 0            |
| 20  | J     | 878   | 0        | 923      | 56      | 0            |
| 21  | K     | 1071  | 0        | 1165     | 65      | 0            |
| 22  | L     | 975   | 0        | 1043     | 72      | 0            |
| 23  | M     | 474   | 0        | 505      | 36      | 0            |
| 24  | N     | 697   | 0        | 758      | 34      | 0            |
| 25  | O     | 705   | 0        | 755      | 39      | 0            |
| 26  | P     | 693   | 0        | 753      | 42      | 0            |
| 27  | Q     | 605   | 0        | 644      | 61      | 0            |
| 28  | R     | 700   | 0        | 709      | 43      | 0            |
| 29  | S     | 643   | 0        | 694      | 40      | 0            |
| 30  | T     | 519   | 0        | 578      | 57      | 0            |
| 31  | X     | 242   | 0        | 263      | 17      | 0            |
| 32  | Y     | 862   | 0        | 435      | 40      | 0            |
| 33  | Z     | 187   | 0        | 68       | 3       | 0            |
| 34  | a     | 2225  | 0        | 2301     | 99      | 0            |
| 35  | b     | 1762  | 0        | 1808     | 108     | 0            |
| 36  | c     | 1654  | 0        | 1744     | 79      | 0            |
| 37  | d     | 1416  | 0        | 1500     | 80      | 0            |
| 38  | e     | 1396  | 0        | 1481     | 56      | 0            |
| 39  | f     | 1210  | 0        | 1259     | 117     | 0            |
| 40  | g     | 951   | 0        | 1001     | 46      | 0            |
| 41  | h     | 959   | 0        | 1039     | 39      | 0            |
| 42  | i     | 1164  | 0        | 1192     | 48      | 0            |
| 43  | j     | 944   | 0        | 1019     | 72      | 0            |
| 44  | k     | 1170  | 0        | 1274     | 80      | 0            |
| 45  | l     | 1079  | 0        | 1134     | 71      | 0            |
| 46  | m     | 958   | 0        | 1011     | 71      | 0            |
| 47  | n     | 918   | 0        | 979      | 43      | 0            |
| 48  | o     | 966   | 0        | 1042     | 92      | 0            |
| 49  | p     | 981   | 0        | 1062     | 71      | 0            |
| 50  | q     | 811   | 0        | 858      | 53      | 0            |
| 51  | r     | 1091  | 0        | 1178     | 53      | 0            |
| 52  | s     | 740   | 0        | 819      | 43      | 0            |
| 53  | t     | 871   | 0        | 972      | 47      | 0            |
| 54  | u     | 670   | 0        | 704      | 48      | 0            |
| 55  | v     | 520   | 0        | 565      | 33      | 0            |
| 56  | w     | 906   | 0        | 981      | 46      | 0            |
| 57  | x     | 708   | 0        | 710      | 31      | 0            |
| 58  | y     | 452   | 0        | 471      | 51      | 0            |
| 59  | z     | 408   | 0        | 436      | 17      | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 60  | 2     | 1      | 0        | 0        | 0       | 0            |
| 60  | M     | 1      | 0        | 0        | 0       | 0            |
| 60  | Q     | 1      | 0        | 0        | 0       | 0            |
| 60  | x     | 1      | 0        | 0        | 0       | 0            |
| 60  | y     | 1      | 0        | 0        | 0       | 0            |
| 60  | z     | 1      | 0        | 0        | 0       | 0            |
| 61  | 3     | 20     | 0        | 11       | 1       | 0            |
| 62  | 3     | 1      | 0        | 0        | 0       | 0            |
| 63  | 3     | 209    | 0        | 0        | 0       | 0            |
| 63  | 4     | 1      | 0        | 0        | 0       | 0            |
| 63  | 5     | 87     | 0        | 0        | 0       | 0            |
| 63  | 6     | 1      | 0        | 0        | 0       | 0            |
| 63  | 8     | 1      | 0        | 0        | 0       | 0            |
| 63  | E     | 1      | 0        | 0        | 0       | 0            |
| 63  | K     | 1      | 0        | 0        | 0       | 0            |
| 63  | L     | 1      | 0        | 0        | 0       | 0            |
| 63  | P     | 1      | 0        | 0        | 0       | 0            |
| 63  | Y     | 2      | 0        | 0        | 0       | 0            |
| 63  | a     | 1      | 0        | 0        | 0       | 0            |
| 63  | b     | 1      | 0        | 0        | 0       | 0            |
| 63  | f     | 12     | 0        | 0        | 0       | 0            |
| 63  | i     | 1      | 0        | 0        | 0       | 0            |
| 63  | y     | 2      | 0        | 0        | 0       | 0            |
| 64  | 8     | 9      | 0        | 12       | 0       | 0            |
| All | All   | 153622 | 0        | 105363   | 4084    | 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 17.

All (4084) 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) |
|------------------|------------------|--------------------------|-------------------|
| 39:f:132:GLU:O   | 39:f:140:VAL:HB  | 1.52                     | 1.10              |
| 6:5:839:U:OP2    | 15:E:142:ARG:NH1 | 1.85                     | 1.08              |
| 39:f:4:ILE:HG21  | 39:f:47:ARG:HG3  | 1.41                     | 1.01              |
| 58:y:42:VAL:HG22 | 58:y:48:TYR:HB2  | 1.45                     | 0.97              |
| 6:5:1322:U:O3'   | 18:H:125:ARG:NH2 | 1.98                     | 0.96              |
| 39:f:40:THR:H    | 39:f:47:ARG:HB2  | 1.31                     | 0.95              |
| 4:3:2779:C:H5''  | 35:b:211:LYS:HD3 | 1.48                     | 0.95              |
| 16:F:115:MET:HA  | 16:F:118:LYS:HB2 | 1.48                     | 0.94              |
| 15:E:94:TYR:HB2  | 27:Q:88:LYS:HE2  | 1.49                     | 0.94              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 43:j:101:PRO:HD2  | 48:o:73:ILE:HD11  | 1.49                     | 0.94              |
| 38:e:51:ASN:O     | 38:e:51:ASN:ND2   | 2.01                     | 0.93              |
| 35:b:180:ARG:HH22 | 35:b:218:LYS:HE3  | 1.33                     | 0.93              |
| 6:5:407:A:H8      | 13:C:27:LYS:HZ1   | 1.08                     | 0.93              |
| 46:m:35:LEU:HD22  | 46:m:112:GLU:HB3  | 1.48                     | 0.93              |
| 58:y:41:ARG:HE    | 58:y:42:VAL:H     | 0.95                     | 0.92              |
| 15:E:133:THR:HA   | 27:Q:38:LYS:HD2   | 1.52                     | 0.92              |
| 11:A:199:VAL:HG12 | 11:A:213:PHE:HB2  | 1.50                     | 0.90              |
| 4:3:1262:G:N3     | 51:r:128:ARG:NH1  | 2.18                     | 0.90              |
| 6:5:954:A:N7      | 28:R:78:ARG:NH1   | 2.20                     | 0.90              |
| 37:d:171:ARG:NH2  | 37:d:175:LEU:O    | 2.05                     | 0.89              |
| 35:b:39:VAL:HG22  | 35:b:92:MET:HE2   | 1.54                     | 0.89              |
| 20:J:119:ARG:HG2  | 30:T:34:TYR:HD2   | 1.36                     | 0.88              |
| 12:B:36:GLU:HA    | 12:B:39:LYS:HE3   | 1.55                     | 0.88              |
| 32:Y:90:G:H3'     | 32:Y:91:A:H5''    | 1.56                     | 0.88              |
| 11:A:214:ILE:HG22 | 11:A:216:PRO:HD3  | 1.54                     | 0.87              |
| 6:5:1295:U:O4     | 28:R:37:ARG:NH1   | 2.05                     | 0.87              |
| 58:y:52:ARG:NH1   | 58:y:54:LYS:O     | 2.08                     | 0.87              |
| 18:H:11:ARG:HH12  | 18:H:87:ARG:HH21  | 1.21                     | 0.86              |
| 39:f:84:HIS:HB2   | 39:f:148:VAL:HG22 | 1.56                     | 0.86              |
| 11:A:32:MET:HE2   | 11:A:36:TYR:HB2   | 1.58                     | 0.86              |
| 30:T:27:ARG:HE    | 30:T:30:GLN:HE22  | 1.23                     | 0.86              |
| 6:5:1290:G:N1     | 6:5:1293:A:OP2    | 2.08                     | 0.86              |
| 58:y:41:ARG:HH21  | 58:y:42:VAL:HG23  | 1.41                     | 0.85              |
| 39:f:39:LEU:HG    | 39:f:44:LEU:HA    | 1.59                     | 0.85              |
| 34:a:179:TYR:HB3  | 34:a:191:LYS:HB3  | 1.59                     | 0.85              |
| 15:E:157:TRP:CD1  | 17:G:60:LEU:HB2   | 2.11                     | 0.85              |
| 18:H:124:ARG:H    | 18:H:125:ARG:NH1  | 1.74                     | 0.85              |
| 31:X:40:ILE:HG22  | 31:X:43:PHE:HB2   | 1.59                     | 0.85              |
| 9:8:50:G:H1       | 9:8:64:U:H3       | 1.24                     | 0.85              |
| 41:h:29:GLY:O     | 41:h:61:LYS:NZ    | 2.09                     | 0.84              |
| 6:5:9:A:N6        | 13:C:198:GLU:OE2  | 2.10                     | 0.84              |
| 16:F:110:ARG:O    | 16:F:118:LYS:NZ   | 2.10                     | 0.84              |
| 43:j:7:ARG:HH22   | 43:j:44:LYS:HB2   | 1.40                     | 0.84              |
| 48:o:27:ALA:HB3   | 48:o:96:VAL:HG21  | 1.59                     | 0.84              |
| 11:A:126:SER:HA   | 11:A:129:LYS:HE2  | 1.59                     | 0.84              |
| 4:3:432:G:H5'     | 55:v:13:LEU:HD13  | 1.58                     | 0.84              |
| 4:3:2868:G:OP1    | 48:o:117:ARG:NH2  | 2.10                     | 0.84              |
| 22:L:80:LEU:HD21  | 22:L:87:ARG:HD2   | 1.57                     | 0.84              |
| 6:5:271:G:O5'     | 26:P:17:LYS:NZ    | 2.11                     | 0.84              |
| 52:s:59:ILE:HD11  | 52:s:79:LYS:HE2   | 1.60                     | 0.83              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 16:F:12:LEU:H    | 16:F:13:PRO:HD2   | 1.43                     | 0.83              |
| 4:3:1761:C:H1'   | 48:o:103:TYR:CE2  | 2.14                     | 0.83              |
| 8:7:48:G:H1      | 8:7:64:U:H3       | 1.24                     | 0.83              |
| 31:X:29:LYS:HG3  | 31:X:30:GLN:H     | 1.43                     | 0.83              |
| 4:3:1600:A:O4'   | 34:a:222:ARG:NH2  | 2.11                     | 0.83              |
| 28:R:27:LYS:O    | 28:R:29:ARG:NH1   | 2.11                     | 0.83              |
| 43:j:58:LEU:HD22 | 43:j:94:ARG:HH12  | 1.44                     | 0.83              |
| 58:y:41:ARG:NE   | 58:y:42:VAL:H     | 1.77                     | 0.83              |
| 6:5:93:A:H5'     | 6:5:94:A:H5''     | 1.62                     | 0.82              |
| 34:a:57:HIS:HA   | 34:a:225:ARG:HB3  | 1.61                     | 0.82              |
| 35:b:229:ALA:HB2 | 48:o:20:ALA:HB1   | 1.62                     | 0.82              |
| 43:j:28:THR:O    | 43:j:29:ARG:HD3   | 1.79                     | 0.82              |
| 8:7:10:G:H1      | 8:7:25:U:H3       | 1.25                     | 0.82              |
| 4:3:1392:G:OP1   | 55:v:3:LYS:NZ     | 2.12                     | 0.82              |
| 6:5:335:C:OP2    | 43:j:97:ARG:NH1   | 2.12                     | 0.82              |
| 39:f:76:GLU:HG2  | 39:f:142:VAL:HG13 | 1.59                     | 0.82              |
| 6:5:838:A:H4'    | 15:E:114:LYS:HE2  | 1.60                     | 0.81              |
| 4:3:2788:U:OP2   | 42:i:120:ARG:NH2  | 2.12                     | 0.81              |
| 4:3:2794:U:H1'   | 35:b:69:PHE:HE1   | 1.45                     | 0.81              |
| 35:b:84:ILE:HB   | 35:b:87:MET:HE2   | 1.61                     | 0.81              |
| 39:f:2:LYS:HD2   | 39:f:18:VAL:HB    | 1.62                     | 0.81              |
| 22:L:3:ARG:HH12  | 22:L:57:ARG:HB2   | 1.44                     | 0.81              |
| 11:A:88:LYS:O    | 11:A:93:LYS:NZ    | 2.13                     | 0.81              |
| 6:5:1323:A:P     | 18:H:125:ARG:HH21 | 2.03                     | 0.81              |
| 4:3:2132:G:H22   | 4:3:2180:U:H5'    | 1.45                     | 0.81              |
| 45:l:35:VAL:HG13 | 45:l:132:LEU:HD22 | 1.63                     | 0.81              |
| 6:5:1501:G:H3'   | 30:T:37:ARG:HH22  | 1.44                     | 0.81              |
| 20:J:119:ARG:HG2 | 30:T:34:TYR:CD2   | 2.15                     | 0.80              |
| 43:j:51:MET:HE1  | 43:j:94:ARG:HB3   | 1.63                     | 0.80              |
| 36:c:130:GLN:NE2 | 36:c:200:GLU:OE2  | 2.13                     | 0.80              |
| 52:s:9:LYS:HD2   | 52:s:10:PRO:HD2   | 1.63                     | 0.80              |
| 15:E:111:LYS:HA  | 15:E:114:LYS:HE3  | 1.62                     | 0.80              |
| 16:F:74:LEU:HD22 | 16:F:85:GLN:HB3   | 1.63                     | 0.80              |
| 27:Q:35:LYS:HG3  | 27:Q:36:ARG:H     | 1.47                     | 0.80              |
| 35:b:26:ILE:HD12 | 35:b:192:LEU:HD22 | 1.62                     | 0.80              |
| 53:t:3:ARG:HH22  | 53:t:74:LEU:HB2   | 1.47                     | 0.80              |
| 6:5:716:C:O2'    | 27:Q:69:LYS:NZ    | 2.13                     | 0.80              |
| 37:d:117:LEU:H   | 37:d:177:LEU:HD12 | 1.45                     | 0.80              |
| 7:6:46:G:O2'     | 7:6:47:U:H5'      | 1.82                     | 0.80              |
| 53:t:9:LYS:NZ    | 53:t:21:SER:OG    | 2.15                     | 0.79              |
| 15:E:1:MET:HG3   | 15:E:2:GLN:H      | 1.47                     | 0.79              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:E:29:LEU:HD22  | 15:E:35:LEU:HD21  | 1.62                     | 0.79              |
| 48:o:25:PHE:HB3   | 48:o:90:LEU:HD11  | 1.65                     | 0.79              |
| 3:2:19:ARG:O      | 3:2:20:HIS:ND1    | 2.16                     | 0.79              |
| 34:a:254:PRO:HG2  | 34:a:263:MET:HG3  | 1.62                     | 0.79              |
| 4:3:47:G:H5''     | 4:3:48:G:H5'      | 1.64                     | 0.78              |
| 32:Y:60:G:H3'     | 32:Y:61:A:H5''    | 1.64                     | 0.78              |
| 39:f:23:ASP:HB2   | 39:f:27:ILE:HD11  | 1.64                     | 0.78              |
| 12:B:74:PRO:HG3   | 12:B:108:GLU:HG3  | 1.65                     | 0.78              |
| 37:d:24:SER:HB3   | 37:d:27:GLN:HG2   | 1.65                     | 0.78              |
| 4:3:2312:G:H22    | 4:3:2320:U:H3     | 1.27                     | 0.78              |
| 15:E:151:LYS:HD3  | 15:E:152:PRO:HD2  | 1.64                     | 0.78              |
| 26:P:43:LYS:HZ2   | 26:P:45:TYR:HD1   | 1.28                     | 0.78              |
| 6:5:469:C:O2'     | 25:O:80:LYS:NZ    | 2.17                     | 0.78              |
| 40:g:25:VAL:HG11  | 40:g:93:LEU:HD21  | 1.66                     | 0.78              |
| 6:5:681:U:H1'     | 20:J:33:ASN:HA    | 1.66                     | 0.78              |
| 35:b:11:VAL:HG21  | 48:o:9:LEU:HD11   | 1.66                     | 0.78              |
| 27:Q:73:ARG:HH12  | 27:Q:83:GLN:HB2   | 1.46                     | 0.78              |
| 38:e:51:ASN:HD22  | 38:e:51:ASN:C     | 1.92                     | 0.78              |
| 16:F:135:LYS:NZ   | 16:F:139:ASP:OD1  | 2.17                     | 0.78              |
| 51:r:71:VAL:HA    | 51:r:107:LEU:HG   | 1.66                     | 0.78              |
| 15:E:132:VAL:HG13 | 15:E:133:THR:H    | 1.47                     | 0.78              |
| 4:3:2793:U:O2'    | 35:b:72:LYS:NZ    | 2.16                     | 0.77              |
| 12:B:182:ARG:NH1  | 12:B:209:MET:SD   | 2.57                     | 0.77              |
| 4:3:1959:A:OP2    | 43:j:44:LYS:NZ    | 2.18                     | 0.77              |
| 39:f:39:LEU:HD12  | 39:f:47:ARG:HB3   | 1.67                     | 0.77              |
| 4:3:553:A:O2'     | 51:r:18:ARG:NH1   | 2.17                     | 0.77              |
| 15:E:1:MET:HE2    | 15:E:91:GLU:HB3   | 1.64                     | 0.77              |
| 4:3:1219:U:O3'    | 50:q:78:HIS:NE2   | 2.15                     | 0.77              |
| 39:f:77:LEU:HD11  | 39:f:107:ALA:HB2  | 1.66                     | 0.77              |
| 15:E:114:LYS:O    | 15:E:117:GLU:HG3  | 1.85                     | 0.77              |
| 4:3:1032:A:OP1    | 50:q:10:LYS:NZ    | 2.18                     | 0.77              |
| 6:5:1215:U:O2     | 16:F:34:LYS:NZ    | 2.18                     | 0.77              |
| 52:s:7:LEU:HD11   | 52:s:29:PHE:HD2   | 1.49                     | 0.77              |
| 32:Y:92:A:H2'     | 32:Y:93:A:C8      | 2.20                     | 0.77              |
| 4:3:354:C:N4      | 36:c:144:MET:SD   | 2.58                     | 0.77              |
| 4:3:573:A:H4'     | 42:i:11:GLN:OE1   | 1.85                     | 0.77              |
| 7:6:49:G:H1       | 7:6:65:U:H3       | 1.30                     | 0.77              |
| 36:c:148:LYS:HA   | 36:c:153:LEU:HD11 | 1.64                     | 0.76              |
| 4:3:1691:U:OP2    | 35:b:142:ARG:NE   | 2.18                     | 0.76              |
| 4:3:1094:G:OP1    | 41:h:68:LYS:NZ    | 2.18                     | 0.76              |
| 12:B:140:SER:HA   | 12:B:143:LYS:HE3  | 1.67                     | 0.76              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 15:E:155:GLU:OE2  | 17:G:63:LYS:NZ   | 2.15                     | 0.76              |
| 25:O:39:LEU:HD21  | 25:O:72:LEU:HD11 | 1.67                     | 0.76              |
| 39:f:12:LEU:HB3   | 39:f:19:VAL:HG11 | 1.67                     | 0.76              |
| 4:3:1282:G:O6     | 49:p:35:LYS:NZ   | 2.15                     | 0.76              |
| 38:e:44:LEU:HD12  | 38:e:55:ILE:HG21 | 1.66                     | 0.76              |
| 4:3:1367:G:N7     | 52:s:60:ARG:NH2  | 2.31                     | 0.76              |
| 4:3:2363:C:O2'    | 54:u:53:ARG:NH2  | 2.19                     | 0.76              |
| 54:u:84:GLN:HE22  | 54:u:96:SER:HB2  | 1.50                     | 0.76              |
| 55:v:10:ARG:HH12  | 55:v:53:ARG:HH21 | 1.34                     | 0.76              |
| 15:E:25:GLN:HG2   | 15:E:35:LEU:HD22 | 1.66                     | 0.76              |
| 18:H:120:LEU:HG   | 18:H:125:ARG:O   | 1.85                     | 0.76              |
| 20:J:67:VAL:HA    | 20:J:70:MET:HE2  | 1.66                     | 0.76              |
| 4:3:2278:G:O3'    | 54:u:34:ARG:NH1  | 2.18                     | 0.76              |
| 40:g:100:VAL:HB   | 40:g:106:MET:HG2 | 1.68                     | 0.76              |
| 45:l:43:ASP:HA    | 45:l:94:VAL:HA   | 1.66                     | 0.76              |
| 4:3:2032:G:OP1    | 35:b:158:ARG:NH1 | 2.19                     | 0.76              |
| 26:P:22:ALA:HB2   | 26:P:49:ASN:HD21 | 1.51                     | 0.76              |
| 2:1:10:ARG:HG2    | 44:k:64:LYS:HA   | 1.68                     | 0.76              |
| 4:3:195:A:H3'     | 4:3:196:G:H21    | 1.51                     | 0.76              |
| 6:5:1179:A:O2'    | 12:B:191:LYS:NZ  | 2.15                     | 0.76              |
| 10:9:129:LEU:HB2  | 10:9:135:MET:HE2 | 1.67                     | 0.76              |
| 35:b:111:SER:OG   | 35:b:208:ARG:NH1 | 2.19                     | 0.76              |
| 42:i:80:HIS:HD2   | 42:i:87:ILE:HB   | 1.51                     | 0.76              |
| 39:f:43:SER:HB3   | 39:f:46:ASP:HB3  | 1.68                     | 0.75              |
| 42:i:3:LYS:HG3    | 42:i:4:THR:H     | 1.52                     | 0.75              |
| 4:3:993:A:H5'     | 45:l:76:LYS:HD2  | 1.66                     | 0.75              |
| 8:7:27:U:H3       | 8:7:43:G:H1      | 1.34                     | 0.75              |
| 18:H:49:ASP:HA    | 18:H:52:GLN:HE22 | 1.51                     | 0.75              |
| 41:h:42:LYS:HE2   | 41:h:67:LEU:HG   | 1.67                     | 0.75              |
| 41:h:58:TYR:CE1   | 41:h:60:ASP:HB3  | 2.21                     | 0.75              |
| 6:5:369:A:O2'     | 6:5:448:A:N7     | 2.18                     | 0.75              |
| 4:3:77:G:O2'      | 56:w:49:ARG:NH2  | 2.19                     | 0.75              |
| 17:G:13:ASP:OD2   | 17:G:16:ALA:HB3  | 1.87                     | 0.75              |
| 39:f:15:ARG:HH11  | 39:f:16:PHE:HB2  | 1.51                     | 0.75              |
| 32:Y:59:A:H2'     | 32:Y:60:G:O4'    | 1.87                     | 0.75              |
| 35:b:165:MET:SD   | 35:b:165:MET:N   | 2.60                     | 0.75              |
| 37:d:146:ILE:HG22 | 37:d:148:ARG:H   | 1.51                     | 0.75              |
| 50:q:59:VAL:HA    | 50:q:92:LEU:HG   | 1.69                     | 0.75              |
| 19:I:58:ILE:HG12  | 19:I:68:ARG:HE   | 1.51                     | 0.75              |
| 20:J:116:PRO:HB2  | 30:T:33:GLU:O    | 1.87                     | 0.75              |
| 37:d:148:ARG:HE   | 37:d:149:ILE:H   | 1.33                     | 0.75              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 47:n:1:MET:HE2    | 47:n:2:LYS:HE3    | 1.69                     | 0.74              |
| 4:3:1446:G:O2'    | 4:3:1613:A:N6     | 2.19                     | 0.74              |
| 4:3:1600:A:N3     | 34:a:62:ASN:ND2   | 2.34                     | 0.74              |
| 51:r:50:LEU:HD12  | 51:r:103:LEU:HD23 | 1.69                     | 0.74              |
| 17:G:102:GLU:OE2  | 17:G:102:GLU:N    | 2.18                     | 0.74              |
| 39:f:96:GLN:HB3   | 39:f:100:GLN:HE22 | 1.53                     | 0.74              |
| 45:l:73:SER:C     | 45:l:74:LYS:HD3   | 2.13                     | 0.74              |
| 4:3:703:A:H2'     | 4:3:705:A:H62     | 1.53                     | 0.74              |
| 48:o:93:ARG:HE    | 48:o:118:LYS:HE2  | 1.53                     | 0.74              |
| 51:r:97:THR:O     | 51:r:99:ARG:NH1   | 2.21                     | 0.74              |
| 2:1:13:LEU:HD12   | 2:1:14:THR:H      | 1.51                     | 0.74              |
| 28:R:36:ARG:HB3   | 28:R:72:GLY:HA3   | 1.70                     | 0.74              |
| 48:o:98:ARG:NH2   | 48:o:100:TYR:OH   | 2.21                     | 0.74              |
| 53:t:57:LYS:HE3   | 53:t:59:SER:HB3   | 1.69                     | 0.74              |
| 4:3:2183:U:H3'    | 4:3:2184:A:H5''   | 1.69                     | 0.74              |
| 18:H:124:ARG:H    | 18:H:125:ARG:HH12 | 1.36                     | 0.74              |
| 11:A:32:MET:HE1   | 11:A:281:ARG:HH11 | 1.53                     | 0.74              |
| 39:f:40:THR:HB    | 39:f:47:ARG:HA    | 1.70                     | 0.74              |
| 4:3:853:G:N1      | 4:3:1219:U:OP2    | 2.17                     | 0.74              |
| 35:b:50:THR:HB    | 35:b:87:MET:HE3   | 1.70                     | 0.74              |
| 42:i:8:THR:HB     | 49:p:99:ILE:HD12  | 1.69                     | 0.74              |
| 38:e:106:LEU:HD21 | 38:e:147:PHE:HZ   | 1.51                     | 0.73              |
| 4:3:1055:A:N1     | 4:3:1176:U:O2'    | 2.21                     | 0.73              |
| 6:5:661:G:H5'     | 27:Q:84:ARG:HH12  | 1.51                     | 0.73              |
| 15:E:121:ARG:HB3  | 15:E:124:ASN:HB2  | 1.70                     | 0.73              |
| 36:c:54:THR:OG1   | 36:c:57:GLU:OE1   | 2.06                     | 0.73              |
| 16:F:6:ALA:HB1    | 16:F:7:PRO:HD2    | 1.71                     | 0.73              |
| 20:J:66:THR:HG22  | 20:J:70:MET:HE1   | 1.70                     | 0.73              |
| 11:A:253:GLU:OE2  | 11:A:254:ILE:HG13 | 1.89                     | 0.73              |
| 32:Y:89:A:H2'     | 32:Y:90:G:O4'     | 1.87                     | 0.73              |
| 45:l:27:VAL:O     | 45:l:134:ARG:NH1  | 2.21                     | 0.73              |
| 4:3:562:C:O2'     | 42:i:119:ARG:NH1  | 2.18                     | 0.73              |
| 52:s:87:LYS:HG3   | 56:w:90:HIS:CE1   | 2.23                     | 0.73              |
| 4:3:2481:U:OP1    | 4:3:2483:C:N4     | 2.21                     | 0.73              |
| 6:5:1241:G:N2     | 6:5:1244:A:OP2    | 2.20                     | 0.73              |
| 6:5:1501:G:H3'    | 30:T:37:ARG:NH2   | 2.01                     | 0.73              |
| 16:F:80:ALA:HB2   | 32:Y:66:U:H5''    | 1.70                     | 0.73              |
| 43:j:6:THR:HB     | 43:j:21:ILE:HD12  | 1.69                     | 0.73              |
| 4:3:2177:G:H3'    | 4:3:2178:A:H8     | 1.54                     | 0.72              |
| 4:3:2589:G:N2     | 4:3:2589:G:OP2    | 2.22                     | 0.72              |
| 6:5:407:A:H8      | 13:C:27:LYS:NZ    | 1.87                     | 0.72              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:3:788:G:N2      | 46:m:3:TYR:OH     | 2.22                     | 0.72              |
| 35:b:4:ARG:NH2    | 35:b:106:GLU:OE2  | 2.22                     | 0.72              |
| 39:f:100:GLN:HG2  | 39:f:112:MET:HE1  | 1.71                     | 0.72              |
| 17:G:90:ILE:HG22  | 17:G:97:ILE:HG13  | 1.71                     | 0.72              |
| 45:l:74:LYS:HZ1   | 45:l:94:VAL:HG22  | 1.54                     | 0.72              |
| 4:3:477:U:O2      | 36:c:47:GLN:NE2   | 2.22                     | 0.72              |
| 4:3:1803:U:H3     | 4:3:1830:G:H1     | 1.36                     | 0.72              |
| 6:5:9:A:N1        | 13:C:202:ARG:NH2  | 2.34                     | 0.72              |
| 6:5:731:A:O2'     | 27:Q:95:TYR:OH    | 2.06                     | 0.72              |
| 20:J:118:LYS:HA   | 30:T:34:TYR:CD1   | 2.24                     | 0.72              |
| 45:l:74:LYS:NZ    | 45:l:94:VAL:HG22  | 2.04                     | 0.72              |
| 6:5:341:C:OP1     | 48:o:44:ARG:NH1   | 2.23                     | 0.72              |
| 6:5:399:C:H5''    | 13:C:132:PRO:HD2  | 1.72                     | 0.72              |
| 4:3:2066:A:H2'    | 4:3:2511:2MA:HM22 | 1.72                     | 0.72              |
| 11:A:182:VAL:HG23 | 11:A:206:THR:HG22 | 1.72                     | 0.72              |
| 32:Y:92:A:H2'     | 32:Y:93:A:H8      | 1.53                     | 0.72              |
| 55:v:6:GLN:NE2    | 55:v:49:LEU:O     | 2.22                     | 0.72              |
| 4:3:2653:G:OP2    | 4:3:2653:G:N2     | 2.20                     | 0.72              |
| 18:H:12:ARG:HD2   | 18:H:79:GLY:HA3   | 1.70                     | 0.72              |
| 39:f:117:VAL:HG12 | 39:f:131:PHE:H    | 1.54                     | 0.72              |
| 34:a:150:ILE:O    | 34:a:159:GLN:N    | 2.16                     | 0.72              |
| 4:3:530:G:N3      | 51:r:61:ASN:ND2   | 2.37                     | 0.71              |
| 6:5:930:A:N7      | 16:F:2:ARG:NH2    | 2.38                     | 0.71              |
| 12:B:61:THR:HG22  | 12:B:62:GLN:H     | 1.53                     | 0.71              |
| 12:B:83:LYS:HD2   | 12:B:86:GLN:HE22  | 1.54                     | 0.71              |
| 4:3:2066:A:H2'    | 4:3:2511:2MA:CM2  | 2.20                     | 0.71              |
| 39:f:1:MET:N      | 39:f:21:VAL:O     | 2.21                     | 0.71              |
| 4:3:2268:C:N3     | 54:u:28:ARG:NH2   | 2.38                     | 0.71              |
| 20:J:9:VAL:HG13   | 20:J:72:MET:HB3   | 1.71                     | 0.71              |
| 4:3:1042:C:H1'    | 42:i:111:MET:CE   | 2.21                     | 0.71              |
| 6:5:1038:G:H4'    | 23:M:4:LYS:HE2    | 1.71                     | 0.71              |
| 6:5:1320:A:H62    | 6:5:1349:A:H5''   | 1.56                     | 0.71              |
| 28:R:40:ILE:HG23  | 28:R:68:GLY:H     | 1.54                     | 0.71              |
| 58:y:35:LYS:HE3   | 58:y:44:SER:HB3   | 1.69                     | 0.71              |
| 4:3:656:G:H4'     | 4:3:657:A:H5'     | 1.71                     | 0.71              |
| 4:3:1099:C:O2'    | 41:h:87:LYS:NZ    | 2.23                     | 0.71              |
| 4:3:1281:A:H5'    | 49:p:12:ARG:NH2   | 2.05                     | 0.71              |
| 53:t:3:ARG:NH2    | 53:t:71:LEU:O     | 2.23                     | 0.71              |
| 4:3:487:C:N4      | 4:3:490:A:OP2     | 2.22                     | 0.71              |
| 4:3:1690:C:OP2    | 35:b:142:ARG:NH1  | 2.24                     | 0.71              |
| 11:A:95:LEU:HG    | 11:A:229:MET:HE3  | 1.72                     | 0.71              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 45:l:36:ALA:HB1   | 45:l:127:VAL:HG11 | 1.72                     | 0.71              |
| 18:H:117:LYS:HB2  | 18:H:120:LEU:HD22 | 1.73                     | 0.71              |
| 36:c:52:ILE:HG21  | 36:c:92:GLY:HA3   | 1.73                     | 0.71              |
| 6:5:206:G:N2      | 6:5:209:A:OP2     | 2.22                     | 0.71              |
| 12:B:46:VAL:HG23  | 12:B:47:ASN:H     | 1.56                     | 0.71              |
| 25:O:18:ARG:HA    | 25:O:38:HIS:HA    | 1.73                     | 0.71              |
| 4:3:2114:C:H2'    | 4:3:2115:A:C8     | 2.26                     | 0.70              |
| 44:k:56:THR:OG1   | 44:k:61:ARG:NH1   | 2.24                     | 0.70              |
| 11:A:181:PRO:HD3  | 11:A:200:ALA:HB1  | 1.73                     | 0.70              |
| 12:B:175:ASN:O    | 12:B:176:MET:HE2  | 1.91                     | 0.70              |
| 43:j:17:LYS:NZ    | 43:j:46:ALA:O     | 2.24                     | 0.70              |
| 43:j:64:ARG:HH12  | 43:j:101:PRO:HG2  | 1.57                     | 0.70              |
| 53:t:6:LYS:HE2    | 53:t:26:LYS:HA    | 1.72                     | 0.70              |
| 6:5:408:U:OP2     | 13:C:27:LYS:NZ    | 2.24                     | 0.70              |
| 34:a:3:ILE:HD12   | 34:a:18:THR:HG21  | 1.72                     | 0.70              |
| 39:f:4:ILE:HG22   | 39:f:18:VAL:HG12  | 1.74                     | 0.70              |
| 46:m:102:LYS:O    | 58:y:41:ARG:HD2   | 1.90                     | 0.70              |
| 50:q:96:ARG:HH12  | 50:q:98:VAL:HA    | 1.56                     | 0.70              |
| 6:5:952:U:H1'     | 28:R:78:ARG:NH2   | 2.05                     | 0.70              |
| 48:o:68:LYS:HE3   | 48:o:75:ILE:HD11  | 1.73                     | 0.70              |
| 48:o:117:ARG:HD3  | 48:o:118:LYS:N    | 2.07                     | 0.70              |
| 54:u:82:LYS:HG2   | 54:u:84:GLN:NE2   | 2.06                     | 0.70              |
| 6:5:1294:U:O4     | 28:R:37:ARG:HD2   | 1.91                     | 0.70              |
| 12:B:153:LYS:HB3  | 12:B:204:TRP:HB2  | 1.74                     | 0.70              |
| 13:C:81:GLN:HB2   | 13:C:85:LEU:HD11  | 1.73                     | 0.70              |
| 15:E:7:LEU:HD21   | 15:E:9:VAL:HG13   | 1.73                     | 0.70              |
| 43:j:64:ARG:NH1   | 43:j:101:PRO:O    | 2.24                     | 0.70              |
| 16:F:115:MET:SD   | 16:F:115:MET:N    | 2.62                     | 0.70              |
| 1:0:24:THR:HG23   | 1:0:27:GLY:H      | 1.56                     | 0.70              |
| 4:3:1315:A:OP1    | 46:m:107:ARG:NH1  | 2.25                     | 0.70              |
| 4:3:2295:A:N7     | 4:3:2354:A:N6     | 2.35                     | 0.70              |
| 6:5:1322:U:O2'    | 18:H:124:ARG:NH2  | 2.25                     | 0.70              |
| 27:Q:67:TYR:HE2   | 30:T:2:PRO:HB3    | 1.56                     | 0.70              |
| 56:w:98:LEU:HD21  | 56:w:102:ARG:HH22 | 1.56                     | 0.70              |
| 4:3:470:U:O2      | 4:3:471:A:N6      | 2.22                     | 0.70              |
| 4:3:2027:G:H5'    | 58:y:9:SER:HB3    | 1.74                     | 0.70              |
| 16:F:74:LEU:HD12  | 16:F:143:MET:SD   | 2.30                     | 0.70              |
| 17:G:104:LEU:O    | 17:G:129:ARG:NH2  | 2.24                     | 0.70              |
| 43:j:104:ARG:NH1  | 43:j:122:VAL:OXT  | 2.24                     | 0.70              |
| 38:e:106:LEU:HD21 | 38:e:147:PHE:CZ   | 2.26                     | 0.70              |
| 58:y:33:CYS:SG    | 58:y:35:LYS:NZ    | 2.64                     | 0.70              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:3:2116:U:N3    | 4:3:2117:G:O6     | 2.25                     | 0.70              |
| 5:4:83:U:H5'     | 5:4:84:C:H5'      | 1.74                     | 0.70              |
| 11:A:78:ASN:HB3  | 15:E:181:PHE:CD2  | 2.26                     | 0.70              |
| 39:f:65:SER:HB2  | 39:f:134:THR:OG1  | 1.92                     | 0.70              |
| 45:l:43:ASP:HB3  | 45:l:94:VAL:HG12  | 1.74                     | 0.70              |
| 4:3:499:G:N2     | 4:3:502:A:OP2     | 2.23                     | 0.69              |
| 4:3:2688:C:H5'   | 35:b:198:ALA:HA   | 1.73                     | 0.69              |
| 30:T:19:LYS:HZ1  | 32:Y:60:G:H5'     | 1.56                     | 0.69              |
| 4:3:2641:A:O2'   | 35:b:66:GLN:NE2   | 2.18                     | 0.69              |
| 44:k:75:GLN:NE2  | 44:k:76:GLU:O     | 2.25                     | 0.69              |
| 35:b:1:MET:SD    | 35:b:2:GLU:N      | 2.66                     | 0.69              |
| 39:f:115:ASP:HA  | 39:f:132:GLU:HA   | 1.74                     | 0.69              |
| 52:s:12:LEU:HD22 | 52:s:17:TYR:HE1   | 1.57                     | 0.69              |
| 6:5:196:G:O2'    | 6:5:197:A:OP1     | 2.09                     | 0.69              |
| 13:C:199:TRP:HA  | 13:C:202:ARG:NH1  | 2.07                     | 0.69              |
| 37:d:60:ILE:HG22 | 37:d:99:PHE:HE1   | 1.58                     | 0.69              |
| 2:1:10:ARG:HD2   | 44:k:59:TYR:CE1   | 2.27                     | 0.69              |
| 4:3:1391:U:O2'   | 4:3:1816:A:N3     | 2.25                     | 0.69              |
| 4:3:2538:A:N7    | 38:e:175:LYS:NZ   | 2.41                     | 0.69              |
| 6:5:169:G:N2     | 6:5:219:A:O2'     | 2.25                     | 0.69              |
| 11:A:150:LEU:HB3 | 11:A:154:ARG:HH12 | 1.55                     | 0.69              |
| 15:E:25:GLN:HE21 | 15:E:35:LEU:HD13  | 1.58                     | 0.69              |
| 47:n:31:MET:HE1  | 47:n:94:GLY:HA2   | 1.75                     | 0.69              |
| 48:o:102:SER:HA  | 48:o:105:ARG:NH2  | 2.07                     | 0.69              |
| 24:N:41:LEU:HD12 | 24:N:44:LYS:HZ1   | 1.58                     | 0.69              |
| 30:T:4:ILE:HB    | 30:T:18:PHE:CE1   | 2.28                     | 0.69              |
| 50:q:51:GLU:O    | 50:q:52:LYS:HG3   | 1.92                     | 0.69              |
| 28:R:25:GLN:HE22 | 28:R:27:LYS:HB3   | 1.57                     | 0.69              |
| 28:R:65:ASP:O    | 57:x:58:ARG:NH1   | 2.25                     | 0.69              |
| 39:f:47:ARG:HG2  | 39:f:51:LEU:HD23  | 1.74                     | 0.69              |
| 4:3:1482:U:O2    | 46:m:60:ARG:NH1   | 2.25                     | 0.69              |
| 10:9:198:LYS:NZ  | 10:9:206:TYR:HB2  | 2.08                     | 0.69              |
| 30:T:19:LYS:NZ   | 32:Y:60:G:H5'     | 2.08                     | 0.69              |
| 44:k:150:GLU:OE1 | 44:k:150:GLU:N    | 2.25                     | 0.69              |
| 4:3:354:C:O2     | 36:c:174:ASN:ND2  | 2.25                     | 0.69              |
| 6:5:813:A:OP1    | 6:5:1501:G:O2'    | 2.08                     | 0.69              |
| 17:G:29:LYS:HG2  | 17:G:80:ARG:HH21  | 1.57                     | 0.69              |
| 50:q:19:THR:HG22 | 50:q:93:LYS:HB2   | 1.75                     | 0.69              |
| 15:E:50:LYS:HD3  | 15:E:83:LEU:HG    | 1.74                     | 0.69              |
| 15:E:99:SER:O    | 15:E:105:GLN:NE2  | 2.26                     | 0.69              |
| 43:j:28:THR:C    | 43:j:29:ARG:HD3   | 2.17                     | 0.69              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 52:s:19:ASN:HB3   | 52:s:26:LYS:HB2   | 1.74                     | 0.69              |
| 18:H:124:ARG:HD3  | 18:H:125:ARG:NH1  | 2.07                     | 0.68              |
| 19:I:63:VAL:HG12  | 19:I:64:ASP:H     | 1.58                     | 0.68              |
| 49:p:97:LEU:HD21  | 49:p:108:ILE:HD13 | 1.76                     | 0.68              |
| 6:5:661:G:H5'     | 27:Q:84:ARG:NH1   | 2.07                     | 0.68              |
| 15:E:27:GLN:HG3   | 15:E:28:THR:HG23  | 1.74                     | 0.68              |
| 16:F:79:ILE:HD11  | 16:F:153:MET:HE1  | 1.75                     | 0.68              |
| 31:X:38:MET:HE2   | 31:X:57:LEU:HD12  | 1.76                     | 0.68              |
| 46:m:103:LEU:HD23 | 58:y:41:ARG:NH1   | 2.09                     | 0.68              |
| 54:u:52:TYR:HB3   | 54:u:73:LEU:HD12  | 1.75                     | 0.68              |
| 4:3:2166:U:H3'    | 4:3:2167:G:H4'    | 1.75                     | 0.68              |
| 6:5:837:G:N3      | 15:E:111:LYS:NZ   | 2.39                     | 0.68              |
| 20:J:17:SER:HA    | 20:J:80:LYS:HB3   | 1.75                     | 0.68              |
| 34:a:218:ARG:HG3  | 34:a:222:ARG:HH12 | 1.58                     | 0.68              |
| 40:g:11:VAL:HG12  | 40:g:58:ILE:HG13  | 1.74                     | 0.68              |
| 56:w:86:ALA:O     | 56:w:90:HIS:ND1   | 2.23                     | 0.68              |
| 6:5:989:A:N1      | 23:M:4:LYS:NZ     | 2.40                     | 0.68              |
| 6:5:1009:G:N2     | 6:5:1012:A:OP2    | 2.18                     | 0.68              |
| 11:A:84:PHE:HE1   | 11:A:177:ILE:HD12 | 1.59                     | 0.68              |
| 36:c:64:LYS:NZ    | 36:c:68:GLN:OE1   | 2.27                     | 0.68              |
| 4:3:204:U:O2'     | 55:v:22:LYS:NZ    | 2.17                     | 0.68              |
| 4:3:720:A:OP1     | 4:3:721:G:N2      | 2.27                     | 0.68              |
| 4:3:2823:A:O2'    | 4:3:2825:A:N7     | 2.24                     | 0.68              |
| 4:3:2825:A:H5''   | 35:b:171:HIS:CE1  | 2.29                     | 0.68              |
| 11:A:30:VAL:HA    | 11:A:55:HIS:CD2   | 2.28                     | 0.68              |
| 4:3:518:A:O2'     | 4:3:532:A:N1      | 2.26                     | 0.68              |
| 25:O:40:ASN:HB3   | 25:O:43:LEU:HB2   | 1.75                     | 0.68              |
| 26:P:28:SER:HB3   | 26:P:41:ARG:HE    | 1.59                     | 0.68              |
| 43:j:75:THR:HG23  | 48:o:77:LYS:HZ1   | 1.59                     | 0.68              |
| 4:3:343:A:N3      | 4:3:363:G:O2'     | 2.26                     | 0.68              |
| 4:3:892:G:H2'     | 4:3:893:A:C8      | 2.29                     | 0.68              |
| 6:5:452:A:N6      | 6:5:476:U:O2      | 2.27                     | 0.68              |
| 29:S:41:LEU:HD12  | 29:S:76:LEU:HD21  | 1.76                     | 0.68              |
| 29:S:68:LEU:O     | 29:S:72:ASN:ND2   | 2.27                     | 0.68              |
| 32:Y:90:G:H3'     | 32:Y:91:A:C5'     | 2.24                     | 0.68              |
| 2:1:54:ARG:NH2    | 4:3:868:C:O2'     | 2.27                     | 0.67              |
| 4:3:2060:G:O2'    | 35:b:157:GLN:NE2  | 2.28                     | 0.67              |
| 19:I:57:ILE:HG23  | 23:M:41:ARG:HB2   | 1.76                     | 0.67              |
| 41:h:76:LEU:HD11  | 41:h:127:THR:HG23 | 1.76                     | 0.67              |
| 43:j:7:ARG:NH2    | 43:j:44:LYS:HB2   | 2.08                     | 0.67              |
| 4:3:925:C:H4'     | 4:3:926:U:O4'     | 1.93                     | 0.67              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:5:96:G:H1       | 6:5:326:C:H41     | 1.40                     | 0.67              |
| 24:N:82:LEU:HD22  | 24:N:84:LEU:HB3   | 1.76                     | 0.67              |
| 12:B:52:GLN:NE2   | 12:B:73:GLN:OE1   | 2.28                     | 0.67              |
| 13:C:50:TYR:HD1   | 13:C:199:TRP:HH2  | 1.42                     | 0.67              |
| 15:E:84:ARG:NH1   | 27:Q:95:TYR:O     | 2.27                     | 0.67              |
| 27:Q:81:MET:O     | 27:Q:85:HIS:ND1   | 2.18                     | 0.67              |
| 41:h:72:VAL:HG12  | 41:h:108:LYS:HD3  | 1.76                     | 0.67              |
| 46:m:103:LEU:HB2  | 46:m:113:MET:HB2  | 1.76                     | 0.67              |
| 48:o:42:LYS:HG2   | 48:o:43:VAL:H     | 1.58                     | 0.67              |
| 11:A:293:ARG:HH21 | 30:T:50:GLN:HG2   | 1.57                     | 0.67              |
| 21:K:98:GLY:O     | 21:K:107:ARG:NH1  | 2.27                     | 0.67              |
| 11:A:286:ARG:O    | 11:A:287:ASN:ND2  | 2.27                     | 0.67              |
| 26:P:29:ARG:HD2   | 26:P:29:ARG:O     | 1.95                     | 0.67              |
| 36:c:25:ILE:HG12  | 36:c:120:LEU:HD11 | 1.77                     | 0.67              |
| 17:G:115:ILE:HG23 | 17:G:138:LEU:HB2  | 1.76                     | 0.67              |
| 4:3:479:A:N6      | 36:c:99:TYR:OH    | 2.28                     | 0.67              |
| 4:3:2115:A:N6     | 4:3:2188:U:O4     | 2.28                     | 0.67              |
| 6:5:585:G:N2      | 6:5:751:C:OP2     | 2.22                     | 0.67              |
| 7:6:73:A:H5''     | 7:6:74:C:H5       | 1.58                     | 0.67              |
| 4:3:1096:U:H1'    | 4:3:1105:A:H1'    | 1.77                     | 0.67              |
| 6:5:1009:G:H21    | 6:5:1012:A:H2     | 1.40                     | 0.67              |
| 54:u:84:GLN:OE1   | 54:u:94:ARG:NE    | 2.26                     | 0.67              |
| 6:5:499:U:OP1     | 21:K:127:ARG:NH2  | 2.27                     | 0.67              |
| 11:A:22:LYS:HB3   | 11:A:26:MET:HE2   | 1.77                     | 0.67              |
| 15:E:1:MET:HG3    | 15:E:2:GLN:N      | 2.07                     | 0.67              |
| 36:c:115:VAL:HG21 | 36:c:188:VAL:HG23 | 1.76                     | 0.67              |
| 39:f:93:ILE:HA    | 39:f:121:PHE:CE1  | 2.29                     | 0.67              |
| 20:J:119:ARG:NH1  | 30:T:33:GLU:OE2   | 2.28                     | 0.67              |
| 34:a:29:ASN:C     | 34:a:29:ASN:HD22  | 2.02                     | 0.67              |
| 4:3:569:U:H5'     | 49:p:41:ALA:HB1   | 1.76                     | 0.66              |
| 4:3:2465:U:H3     | 4:3:2502:G:H1     | 1.43                     | 0.66              |
| 6:5:1348:G:H4'    | 16:F:30:MET:HE1   | 1.77                     | 0.66              |
| 50:q:40:MET:SD    | 50:q:45:ILE:HB    | 2.36                     | 0.66              |
| 4:3:2098:U:H3'    | 4:3:2099:U:H5''   | 1.76                     | 0.66              |
| 6:5:76:G:N2       | 6:5:79:A:OP2      | 2.27                     | 0.66              |
| 7:6:33:U:OP1      | 16:F:85:GLN:NE2   | 2.29                     | 0.66              |
| 11:A:78:ASN:HB3   | 15:E:181:PHE:HD2  | 1.59                     | 0.66              |
| 36:c:115:VAL:HG12 | 36:c:191:LEU:HD22 | 1.77                     | 0.66              |
| 44:k:80:LEU:HG    | 44:k:112:ILE:HD11 | 1.77                     | 0.66              |
| 45:l:34:LEU:HD13  | 45:l:118:LEU:HB3  | 1.77                     | 0.66              |
| 47:n:84:LEU:O     | 47:n:85:LYS:HG3   | 1.95                     | 0.66              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:5:892:G:N2      | 6:5:895:A:OP2     | 2.28                     | 0.66              |
| 34:a:135:SER:O    | 34:a:136:MET:HE2  | 1.95                     | 0.66              |
| 38:e:130:LYS:NZ   | 38:e:132:THR:OG1  | 2.28                     | 0.66              |
| 22:L:3:ARG:NH1    | 22:L:57:ARG:HB2   | 2.10                     | 0.66              |
| 35:b:45:ASP:O     | 35:b:46:LYS:HG3   | 1.94                     | 0.66              |
| 4:3:1786:U:OP2    | 4:3:1791:A:N6     | 2.21                     | 0.66              |
| 39:f:26:ALA:HB3   | 39:f:30:LEU:HB2   | 1.78                     | 0.66              |
| 4:3:2236:G:OP2    | 34:a:271:LYS:NZ   | 2.28                     | 0.66              |
| 43:j:69:GLN:NE2   | 43:j:105:GLU:OE2  | 2.28                     | 0.66              |
| 7:6:3:G:H1        | 7:6:70:U:H3       | 1.44                     | 0.66              |
| 21:K:29:ASN:HD22  | 21:K:32:ASN:CG    | 2.02                     | 0.66              |
| 50:q:31:LYS:HZ1   | 50:q:33:ILE:HD13  | 1.60                     | 0.66              |
| 51:r:65:ASN:ND2   | 51:r:67:ASP:OD1   | 2.29                     | 0.66              |
| 4:3:2696:G:N1     | 4:3:2728:U:OP2    | 2.21                     | 0.66              |
| 21:K:29:ASN:HD21  | 21:K:31:LEU:HG    | 1.61                     | 0.66              |
| 1:0:34:ARG:NH2    | 4:3:503:G:N7      | 2.42                     | 0.66              |
| 4:3:881:A:H1'     | 4:3:882:C:H5''    | 1.78                     | 0.66              |
| 6:5:1068:G:N2     | 6:5:1071:A:OP2    | 2.23                     | 0.66              |
| 4:3:2166:U:C3'    | 4:3:2167:G:H4'    | 2.26                     | 0.66              |
| 4:3:2321:C:O4'    | 37:d:37:ASN:ND2   | 2.29                     | 0.66              |
| 6:5:968:G:OP1     | 19:I:65:LYS:NZ    | 2.29                     | 0.66              |
| 40:g:100:VAL:HG21 | 40:g:106:MET:HE3  | 1.78                     | 0.66              |
| 34:a:124:SER:OG   | 34:a:128:ILE:HD11 | 1.96                     | 0.65              |
| 43:j:63:VAL:HG23  | 43:j:64:ARG:HG3   | 1.79                     | 0.65              |
| 1:0:34:ARG:HH21   | 4:3:502:A:P       | 2.18                     | 0.65              |
| 15:E:90:LEU:HA    | 15:E:93:GLU:HG2   | 1.77                     | 0.65              |
| 15:E:161:GLN:HG3  | 17:G:59:VAL:HG12  | 1.78                     | 0.65              |
| 4:3:2060:G:H4'    | 35:b:157:GLN:HG2  | 1.79                     | 0.65              |
| 6:5:386:U:H4'     | 25:O:28:ARG:HH21  | 1.62                     | 0.65              |
| 17:G:8:ILE:HG21   | 17:G:69:ILE:HG21  | 1.78                     | 0.65              |
| 45:l:54:ILE:HG21  | 45:l:64:MET:HG3   | 1.78                     | 0.65              |
| 45:l:78:PRO:HG2   | 45:l:81:VAL:HG21  | 1.78                     | 0.65              |
| 4:3:1292:A:H61    | 4:3:2024:C:H42    | 1.44                     | 0.65              |
| 4:3:2797:C:O2     | 4:3:2895:A:O2'    | 2.13                     | 0.65              |
| 6:5:1343:G:H5''   | 18:H:116:LYS:HB3  | 1.78                     | 0.65              |
| 35:b:21:ASN:O     | 43:j:72:LYS:NZ    | 2.24                     | 0.65              |
| 58:y:52:ARG:NH2   | 58:y:55:LYS:HA    | 2.12                     | 0.65              |
| 4:3:2853:U:O2'    | 4:3:2870:U:O2     | 2.13                     | 0.65              |
| 12:B:138:ARG:HH21 | 12:B:142:ILE:HG21 | 1.61                     | 0.65              |
| 15:E:156:LEU:HB3  | 17:G:63:LYS:HZ2   | 1.61                     | 0.65              |
| 19:I:23:LEU:HD21  | 19:I:99:PRO:HB2   | 1.77                     | 0.65              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 30:T:16:LYS:HA    | 30:T:19:LYS:HE3   | 1.78                     | 0.65              |
| 37:d:123:ASP:OD2  | 37:d:127:ASN:ND2  | 2.30                     | 0.65              |
| 39:f:15:ARG:HD2   | 39:f:16:PHE:N     | 2.11                     | 0.65              |
| 39:f:93:ILE:HA    | 39:f:121:PHE:HE1  | 1.62                     | 0.65              |
| 4:3:341:G:N1      | 4:3:344:A:OP2     | 2.26                     | 0.65              |
| 4:3:1137:C:H2'    | 4:3:1138:A:H8     | 1.61                     | 0.65              |
| 4:3:1849:G:O2'    | 34:a:261:ARG:NH2  | 2.29                     | 0.65              |
| 4:3:2355:C:OP1    | 59:z:36:LYS:NZ    | 2.29                     | 0.65              |
| 6:5:1432:A:H5''   | 29:S:26:THR:HG22  | 1.79                     | 0.65              |
| 21:K:69:ARG:NH1   | 21:K:73:GLY:HA2   | 2.11                     | 0.65              |
| 29:S:67:ARG:HB3   | 29:S:71:ARG:NH1   | 2.11                     | 0.65              |
| 6:5:435:U:O2'     | 6:5:437:U:O4      | 2.14                     | 0.65              |
| 6:5:1323:A:OP1    | 18:H:125:ARG:NE   | 2.29                     | 0.65              |
| 31:X:40:ILE:CG2   | 31:X:43:PHE:HB2   | 2.25                     | 0.65              |
| 42:i:59:ILE:HB    | 42:i:127:VAL:HG23 | 1.78                     | 0.65              |
| 51:r:124:LEU:O    | 51:r:127:LYS:HG2  | 1.95                     | 0.65              |
| 4:3:512:G:N1      | 4:3:515:A:OP2     | 2.28                     | 0.65              |
| 4:3:1220:A:P      | 50:q:78:HIS:HE2   | 2.19                     | 0.65              |
| 22:L:33:ILE:HG12  | 22:L:63:TYR:HE2   | 1.62                     | 0.65              |
| 44:k:112:ILE:HG23 | 44:k:128:VAL:HA   | 1.79                     | 0.65              |
| 48:o:34:ALA:HB1   | 48:o:45:ILE:HD11  | 1.78                     | 0.65              |
| 4:3:1518:C:N4     | 4:3:2220:A:OP1    | 2.30                     | 0.65              |
| 6:5:983:G:H21     | 6:5:1012:A:H8     | 1.45                     | 0.65              |
| 11:A:90:ASP:HA    | 11:A:93:LYS:HE2   | 1.78                     | 0.65              |
| 18:H:12:ARG:NH2   | 18:H:109:ASP:OD2  | 2.30                     | 0.65              |
| 27:Q:67:TYR:CE2   | 30:T:2:PRO:HB3    | 2.31                     | 0.65              |
| 31:X:36:LYS:HA    | 31:X:45:LYS:HE2   | 1.78                     | 0.65              |
| 4:3:2667:G:N2     | 4:3:2670:A:OP2    | 2.20                     | 0.65              |
| 6:5:164:C:H2'     | 6:5:165:A:H8      | 1.62                     | 0.65              |
| 6:5:1214:A:H2'    | 6:5:1272:C:H41    | 1.61                     | 0.65              |
| 11:A:181:PRO:HG2  | 11:A:206:THR:HG21 | 1.79                     | 0.65              |
| 29:S:20:ASN:O     | 29:S:24:GLN:NE2   | 2.29                     | 0.65              |
| 58:y:52:ARG:HH22  | 58:y:55:LYS:HA    | 1.60                     | 0.65              |
| 4:3:362:U:O3'     | 53:t:73:LYS:NZ    | 2.30                     | 0.64              |
| 6:5:661:G:OP1     | 27:Q:84:ARG:NH1   | 2.30                     | 0.64              |
| 11:A:41:MET:O     | 11:A:45:ILE:HG13  | 1.97                     | 0.64              |
| 11:A:203:ASN:HB2  | 11:A:219:ASN:HD22 | 1.61                     | 0.64              |
| 15:E:159:VAL:HA   | 17:G:60:LEU:HG    | 1.78                     | 0.64              |
| 24:N:79:VAL:O     | 24:N:85:ARG:NH1   | 2.30                     | 0.64              |
| 32:Y:62:A:H2'     | 32:Y:63:A:C8      | 2.32                     | 0.64              |
| 46:m:102:LYS:C    | 58:y:41:ARG:HH11  | 2.05                     | 0.64              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:5:1342:C:OP1    | 18:H:119:GLY:N    | 2.27                     | 0.64              |
| 18:H:6:TYR:HB2    | 18:H:21:LEU:HB2   | 1.79                     | 0.64              |
| 27:Q:36:ARG:HB3   | 27:Q:38:LYS:HG3   | 1.78                     | 0.64              |
| 46:m:50:THR:HA    | 46:m:53:LYS:HE3   | 1.77                     | 0.64              |
| 2:1:49:ALA:HA     | 2:1:52:PHE:HD2    | 1.63                     | 0.64              |
| 4:3:672:G:OP2     | 44:k:130:LYS:NZ   | 2.30                     | 0.64              |
| 14:D:143:ARG:NH2  | 14:D:145:GLY:O    | 2.30                     | 0.64              |
| 4:3:1343:C:O2'    | 4:3:1420:A:N3     | 2.29                     | 0.64              |
| 6:5:350:G:O2'     | 6:5:385:A:OP1     | 2.10                     | 0.64              |
| 6:5:999:C:OP1     | 6:5:1023:G:N2     | 2.27                     | 0.64              |
| 22:L:50:GLU:HA    | 22:L:53:PHE:HB2   | 1.78                     | 0.64              |
| 34:a:218:ARG:O    | 34:a:222:ARG:NH1  | 2.29                     | 0.64              |
| 52:s:9:LYS:NZ     | 56:w:31:PHE:O     | 2.30                     | 0.64              |
| 6:5:1215:U:P      | 16:F:115:MET:HE1  | 2.37                     | 0.64              |
| 38:e:90:LEU:HD11  | 38:e:136:ILE:HD11 | 1.79                     | 0.64              |
| 43:j:8:LEU:CD2    | 43:j:82:ASN:HB2   | 2.28                     | 0.64              |
| 6:5:1110:C:H2'    | 6:5:1111:G:H8     | 1.62                     | 0.64              |
| 47:n:67:LYS:HZ2   | 47:n:101:ARG:N    | 1.96                     | 0.64              |
| 4:3:633:G:H5''    | 36:c:30:LYS:HD2   | 1.79                     | 0.64              |
| 38:e:112:TYR:HB2  | 38:e:116:ILE:HD11 | 1.80                     | 0.64              |
| 4:3:695:G:H5''    | 36:c:101:LEU:HD22 | 1.79                     | 0.64              |
| 6:5:577:G:H5'     | 6:5:725:A:H1'     | 1.80                     | 0.64              |
| 6:5:683:G:H1      | 6:5:700:G:HO2'    | 1.44                     | 0.64              |
| 6:5:1332:U:OP1    | 23:M:35:SER:OG    | 2.15                     | 0.64              |
| 34:a:39:VAL:O     | 34:a:66:TYR:N     | 2.31                     | 0.64              |
| 36:c:31:GLN:NE2   | 44:k:7:LYS:O      | 2.31                     | 0.64              |
| 37:d:39:GLY:HA2   | 37:d:86:GLY:HA2   | 1.79                     | 0.64              |
| 42:i:18:TRP:HB3   | 42:i:140:PRO:HB3  | 1.78                     | 0.64              |
| 58:y:41:ARG:HE    | 58:y:42:VAL:N     | 1.81                     | 0.64              |
| 4:3:2114:C:H2'    | 4:3:2115:A:H8     | 1.63                     | 0.64              |
| 11:A:28:THR:O     | 11:A:61:GLN:NE2   | 2.31                     | 0.64              |
| 12:B:137:MET:HE2  | 12:B:171:TYR:CE2  | 2.31                     | 0.64              |
| 13:C:179:VAL:HG12 | 13:C:180:ARG:H    | 1.62                     | 0.64              |
| 35:b:33:PRO:HD3   | 35:b:189:MET:SD   | 2.37                     | 0.64              |
| 40:g:110:CYS:HA   | 40:g:123:LEU:HD11 | 1.80                     | 0.64              |
| 6:5:826:G:H1      | 6:5:851:U:H3      | 1.43                     | 0.64              |
| 15:E:16:GLU:OE1   | 15:E:16:GLU:N     | 2.28                     | 0.64              |
| 21:K:42:LEU:HD13  | 21:K:94:LEU:HD21  | 1.80                     | 0.64              |
| 36:c:187:SER:H    | 36:c:190:ASP:CG   | 2.06                     | 0.64              |
| 6:5:293:G:N2      | 6:5:296:A:OP2     | 2.25                     | 0.63              |
| 37:d:30:ARG:O     | 37:d:159:SER:N    | 2.30                     | 0.63              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 42:i:7:LEU:HG    | 49:p:60:TRP:HE1   | 1.63                     | 0.63              |
| 54:u:34:ARG:O    | 54:u:53:ARG:NH1   | 2.29                     | 0.63              |
| 57:x:57:GLY:O    | 57:x:58:ARG:HG2   | 1.98                     | 0.63              |
| 4:3:86:A:N6      | 4:3:101:C:O4'     | 2.31                     | 0.63              |
| 4:3:591:G:H5''   | 42:i:115:ASN:HD21 | 1.63                     | 0.63              |
| 4:3:947:A:H62    | 45:l:12:PRO:HA    | 1.62                     | 0.63              |
| 4:3:1094:G:N2    | 41:h:123:MET:SD   | 2.66                     | 0.63              |
| 16:F:68:VAL:HG13 | 16:F:99:ALA:HB1   | 1.80                     | 0.63              |
| 19:I:15:LYS:HB3  | 19:I:105:ARG:HB3  | 1.79                     | 0.63              |
| 39:f:84:HIS:H    | 39:f:148:VAL:HG13 | 1.62                     | 0.63              |
| 54:u:86:PHE:N    | 54:u:90:GLN:HE22  | 1.97                     | 0.63              |
| 4:3:184:A:O2'    | 4:3:186:A:N7      | 2.26                     | 0.63              |
| 6:5:1438:U:H2'   | 6:5:1439:G:H8     | 1.63                     | 0.63              |
| 38:e:47:GLU:OE1  | 38:e:49:LYS:HG3   | 1.98                     | 0.63              |
| 4:3:2120:G:H3'   | 4:3:2121:A:H8     | 1.64                     | 0.63              |
| 4:3:2266:C:O2'   | 4:3:2435:C:OP2    | 2.16                     | 0.63              |
| 30:T:18:PHE:HA   | 30:T:21:VAL:HG22  | 1.80                     | 0.63              |
| 26:P:8:VAL:HB    | 26:P:62:GLN:NE2   | 2.14                     | 0.63              |
| 30:T:15:LEU:HD12 | 30:T:16:LYS:HD2   | 1.81                     | 0.63              |
| 50:q:27:ALA:HB1  | 50:q:31:LYS:HE3   | 1.80                     | 0.63              |
| 2:1:14:THR:OG1   | 2:1:18:GLN:HG3    | 1.99                     | 0.63              |
| 11:A:59:GLU:OE2  | 11:A:63:GLN:NE2   | 2.31                     | 0.63              |
| 15:E:99:SER:H    | 27:Q:50:ARG:NH2   | 1.97                     | 0.63              |
| 15:E:129:ASP:O   | 15:E:133:THR:HB   | 1.98                     | 0.63              |
| 21:K:86:ASN:HD21 | 21:K:118:VAL:H    | 1.44                     | 0.63              |
| 22:L:2:ALA:O     | 37:d:143:TYR:OH   | 2.12                     | 0.63              |
| 26:P:22:ALA:H    | 26:P:46:GLN:HE22  | 1.46                     | 0.63              |
| 56:w:20:ILE:O    | 56:w:23:LYS:HG2   | 1.99                     | 0.63              |
| 4:3:2799:U:OP1   | 4:3:2896:G:N1     | 2.21                     | 0.63              |
| 6:5:827:C:H5'    | 11:A:37:TRP:HE1   | 1.63                     | 0.63              |
| 11:A:179:ASP:OD1 | 11:A:180:ASP:N    | 2.31                     | 0.63              |
| 50:q:4:ILE:HG13  | 50:q:40:MET:HB3   | 1.80                     | 0.63              |
| 4:3:619:A:N1     | 4:3:844:G:O2'     | 2.27                     | 0.63              |
| 4:3:2794:U:H1'   | 35:b:69:PHE:CE1   | 2.32                     | 0.63              |
| 11:A:87:THR:HG23 | 11:A:183:TYR:CE2  | 2.33                     | 0.63              |
| 14:D:120:LYS:HA  | 14:D:123:HIS:CD2  | 2.34                     | 0.63              |
| 15:E:47:TYR:OH   | 15:E:84:ARG:NH2   | 2.29                     | 0.63              |
| 16:F:52:ARG:HG3  | 16:F:53:THR:HG23  | 1.79                     | 0.63              |
| 17:G:45:LEU:HD12 | 17:G:48:LEU:HD23  | 1.80                     | 0.63              |
| 36:c:131:ASN:O   | 36:c:135:LYS:HG2  | 1.98                     | 0.63              |
| 54:u:46:ARG:HG2  | 54:u:49:GLN:OE1   | 1.99                     | 0.63              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:3:1045:A:N3     | 4:3:1188:C:O2'    | 2.28                     | 0.63              |
| 6:5:1425:A:H2'    | 6:5:1427:U:H3     | 1.64                     | 0.63              |
| 21:K:29:ASN:ND2   | 21:K:31:LEU:HG    | 2.14                     | 0.63              |
| 27:Q:81:MET:N     | 27:Q:81:MET:SD    | 2.72                     | 0.63              |
| 46:m:57:PHE:HB2   | 46:m:60:ARG:HH21  | 1.63                     | 0.63              |
| 50:q:60:GLU:HG3   | 50:q:91:LYS:HZ1   | 1.64                     | 0.63              |
| 4:3:54:A:OP2      | 4:3:118:G:N1      | 2.31                     | 0.62              |
| 6:5:398:G:OP1     | 13:C:73:ARG:NH1   | 2.32                     | 0.62              |
| 31:X:37:ASN:H     | 31:X:45:LYS:HD3   | 1.64                     | 0.62              |
| 54:u:85:LYS:HB3   | 54:u:90:GLN:NE2   | 2.14                     | 0.62              |
| 4:3:15:A:O2'      | 4:3:17:G:N7       | 2.31                     | 0.62              |
| 4:3:2278:G:H4'    | 54:u:34:ARG:NH2   | 2.14                     | 0.62              |
| 4:3:2805:A:H4'    | 4:3:2807:G:H5''   | 1.81                     | 0.62              |
| 21:K:69:ARG:NH1   | 21:K:72:ASN:O     | 2.32                     | 0.62              |
| 25:O:43:LEU:HD23  | 25:O:47:LYS:HA    | 1.81                     | 0.62              |
| 39:f:4:ILE:HG21   | 39:f:47:ARG:CG    | 2.24                     | 0.62              |
| 46:m:103:LEU:HA   | 58:y:41:ARG:HD3   | 1.82                     | 0.62              |
| 49:p:86:ASN:OD1   | 50:q:47:ALA:HB1   | 1.99                     | 0.62              |
| 4:3:1129:U:N3     | 4:3:1132:C:OP2    | 2.25                     | 0.62              |
| 4:3:1619:A:H2'    | 4:3:1620:A:C8     | 2.34                     | 0.62              |
| 4:3:2082:U:OP1    | 34:a:251:ARG:NH2  | 2.32                     | 0.62              |
| 4:3:2159:U:HO2'   | 4:3:2160:U:H6     | 1.47                     | 0.62              |
| 6:5:1062:C:H2'    | 6:5:1063:G:H8     | 1.64                     | 0.62              |
| 4:3:2352:U:H2'    | 59:z:34:LEU:HD11  | 1.81                     | 0.62              |
| 4:3:2038:A:N3     | 4:3:2463:G:O2'    | 2.29                     | 0.62              |
| 6:5:1215:U:C6     | 16:F:115:MET:HE3  | 2.34                     | 0.62              |
| 11:A:51:HIS:CE1   | 11:A:55:HIS:CE1   | 2.88                     | 0.62              |
| 25:O:23:ASP:HB3   | 25:O:26:VAL:HG23  | 1.82                     | 0.62              |
| 39:f:68:LEU:HD13  | 39:f:108:LEU:HD21 | 1.82                     | 0.62              |
| 43:j:58:LEU:HD22  | 43:j:94:ARG:NH1   | 2.12                     | 0.62              |
| 46:m:43:LYS:NZ    | 46:m:47:LYS:HD2   | 2.14                     | 0.62              |
| 48:o:31:VAL:HG22  | 48:o:90:LEU:HD13  | 1.80                     | 0.62              |
| 57:x:58:ARG:HG3   | 57:x:59:ALA:H     | 1.64                     | 0.62              |
| 12:B:127:ILE:HD11 | 12:B:133:LEU:HD13 | 1.81                     | 0.62              |
| 37:d:120:LYS:O    | 37:d:120:LYS:HD3  | 1.99                     | 0.62              |
| 42:i:104:VAL:HG21 | 42:i:127:VAL:HG21 | 1.81                     | 0.62              |
| 43:j:71:ARG:HH22  | 43:j:104:ARG:HH11 | 1.46                     | 0.62              |
| 46:m:43:LYS:HZ3   | 46:m:47:LYS:HD2   | 1.65                     | 0.62              |
| 56:w:39:ASP:OD1   | 56:w:40:LYS:N     | 2.33                     | 0.62              |
| 4:3:2120:G:H3'    | 4:3:2121:A:C8     | 2.35                     | 0.62              |
| 6:5:373:A:H2'     | 6:5:374:G:H8      | 1.63                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:9:59:LEU:HD23  | 10:9:169:ILE:HD11 | 1.80                     | 0.62              |
| 28:R:30:PRO:HA    | 28:R:48:THR:HG23  | 1.82                     | 0.62              |
| 39:f:15:ARG:HD2   | 39:f:16:PHE:H     | 1.64                     | 0.62              |
| 2:1:5:SER:OG      | 4:3:257:C:N4      | 2.33                     | 0.62              |
| 6:5:595:G:H4'     | 26:P:29:ARG:CZ    | 2.30                     | 0.62              |
| 25:O:54:VAL:O     | 25:O:57:GLU:HG3   | 2.00                     | 0.62              |
| 37:d:56:GLU:O     | 37:d:60:ILE:HG12  | 2.00                     | 0.62              |
| 39:f:5:LEU:HA     | 39:f:36:ALA:HA    | 1.82                     | 0.62              |
| 39:f:84:HIS:HB3   | 39:f:125:GLU:OE1  | 2.00                     | 0.62              |
| 45:l:47:ILE:HD11  | 45:l:68:ILE:HD11  | 1.82                     | 0.62              |
| 50:q:54:ARG:HB2   | 50:q:98:VAL:HB    | 1.82                     | 0.62              |
| 4:3:1091:G:H4'    | 4:3:1121:A:H8     | 1.65                     | 0.62              |
| 16:F:112:GLU:HG3  | 16:F:113:LYS:H    | 1.63                     | 0.62              |
| 32:Y:90:G:C2      | 32:Y:91:A:H1'     | 2.35                     | 0.62              |
| 35:b:110:VAL:HG11 | 35:b:197:ILE:HD12 | 1.80                     | 0.62              |
| 26:P:8:VAL:HG12   | 26:P:64:VAL:HG12  | 1.81                     | 0.62              |
| 32:Y:83:A:H2'     | 32:Y:84:A:C8      | 2.35                     | 0.62              |
| 53:t:46:LYS:HE3   | 53:t:63:VAL:HB    | 1.81                     | 0.62              |
| 4:3:573:A:O2'     | 42:i:11:GLN:NE2   | 2.28                     | 0.61              |
| 4:3:993:A:O4'     | 45:l:76:LYS:NZ    | 2.33                     | 0.61              |
| 6:5:416:U:O2'     | 6:5:421:G:N2      | 2.33                     | 0.61              |
| 6:5:952:U:H1'     | 28:R:78:ARG:CZ    | 2.30                     | 0.61              |
| 17:G:29:LYS:HD2   | 17:G:80:ARG:HE    | 1.65                     | 0.61              |
| 25:O:6:LEU:HD13   | 25:O:17:TYR:CD2   | 2.35                     | 0.61              |
| 27:Q:41:CYS:HA    | 27:Q:78:ASN:HA    | 1.82                     | 0.61              |
| 29:S:60:ILE:HD11  | 29:S:64:ARG:HD3   | 1.82                     | 0.61              |
| 3:2:20:HIS:CE1    | 3:2:24:ARG:HH21   | 2.19                     | 0.61              |
| 4:3:600:U:H5''    | 44:k:37:LYS:HE3   | 1.82                     | 0.61              |
| 4:3:638:A:H62     | 4:3:660:U:H3      | 1.48                     | 0.61              |
| 4:3:1703:A:O4'    | 43:j:5:MET:HE2    | 1.99                     | 0.61              |
| 4:3:2121:A:H3'    | 4:3:2122:G:H8     | 1.65                     | 0.61              |
| 4:3:2364:A:H4'    | 54:u:34:ARG:HG2   | 1.81                     | 0.61              |
| 6:5:659:U:H4'     | 6:5:833:G:H5''    | 1.82                     | 0.61              |
| 41:h:32:MET:O     | 41:h:36:THR:HG23  | 2.00                     | 0.61              |
| 58:y:42:VAL:HG21  | 58:y:53:VAL:HG21  | 1.82                     | 0.61              |
| 4:3:1702:A:H5''   | 43:j:5:MET:HE3    | 1.81                     | 0.61              |
| 6:5:1197:G:OP2    | 6:5:1296:C:N4     | 2.33                     | 0.61              |
| 6:5:1332:U:H3     | 6:5:1338:A:N6     | 1.96                     | 0.61              |
| 25:O:51:ASP:OD1   | 25:O:52:GLU:N     | 2.32                     | 0.61              |
| 53:t:71:LEU:HD23  | 53:t:74:LEU:HD12  | 1.82                     | 0.61              |
| 24:N:79:VAL:HG22  | 24:N:85:ARG:HD2   | 1.81                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 37:d:63:GLN:HE21  | 37:d:95:ARG:HD2   | 1.64                     | 0.61              |
| 6:5:550:U:H2'     | 6:5:551:A:H8      | 1.65                     | 0.61              |
| 15:E:38:GLU:OE2   | 15:E:59:ARG:NE    | 2.34                     | 0.61              |
| 22:L:9:ILE:HD12   | 22:L:18:ALA:HB1   | 1.82                     | 0.61              |
| 34:a:128:ILE:HG22 | 34:a:129:ASP:H    | 1.64                     | 0.61              |
| 43:j:70:GLN:HA    | 43:j:76:HIS:HA    | 1.82                     | 0.61              |
| 51:r:114:ARG:HD3  | 51:r:117:LEU:HD21 | 1.81                     | 0.61              |
| 4:3:436:G:O6      | 55:v:56:ARG:NH2   | 2.33                     | 0.61              |
| 6:5:971:A:H5'     | 23:M:31:ARG:NH2   | 2.16                     | 0.61              |
| 32:Y:60:G:H3'     | 32:Y:61:A:C5'     | 2.30                     | 0.61              |
| 41:h:58:TYR:HD1   | 41:h:60:ASP:H     | 1.48                     | 0.61              |
| 47:n:65:GLY:HA2   | 47:n:101:ARG:HH11 | 1.64                     | 0.61              |
| 4:3:562:C:N4      | 4:3:2785:G:O2'    | 2.24                     | 0.61              |
| 4:3:2645:U:O2'    | 35:b:46:LYS:NZ    | 2.18                     | 0.61              |
| 6:5:837:G:H5'     | 15:E:144:SER:CB   | 2.31                     | 0.61              |
| 35:b:213:LYS:HE3  | 35:b:216:VAL:HG21 | 1.82                     | 0.61              |
| 40:g:91:GLU:HA    | 40:g:94:LYS:HG2   | 1.82                     | 0.61              |
| 43:j:75:THR:HG23  | 48:o:77:LYS:HE2   | 1.81                     | 0.61              |
| 4:3:196:G:N2      | 4:3:196:G:OP2     | 2.33                     | 0.61              |
| 31:X:29:LYS:O     | 31:X:32:GLN:HG2   | 2.00                     | 0.61              |
| 32:Y:79:U:H4'     | 32:Y:80:U:O5'     | 2.00                     | 0.61              |
| 58:y:22:LEU:HD23  | 58:y:22:LEU:H     | 1.65                     | 0.61              |
| 4:3:916:U:H3      | 4:3:935:U:H3      | 1.47                     | 0.61              |
| 4:3:1961:A:O2'    | 4:3:1963:U:O4     | 2.14                     | 0.61              |
| 4:3:2268:C:H42    | 54:u:28:ARG:CZ    | 2.13                     | 0.61              |
| 4:3:2475:C:O2     | 45:l:124:LYS:NZ   | 2.28                     | 0.61              |
| 9:8:29:U:H3       | 9:8:41:A:H61      | 1.49                     | 0.61              |
| 11:A:87:THR:HG23  | 11:A:183:TYR:HE2  | 1.65                     | 0.61              |
| 12:B:92:ILE:O     | 12:B:95:ILE:HG22  | 2.01                     | 0.61              |
| 15:E:114:LYS:HZ3  | 15:E:114:LYS:HB2  | 1.66                     | 0.61              |
| 28:R:22:MET:HG2   | 28:R:31:ILE:HD11  | 1.82                     | 0.61              |
| 28:R:36:ARG:HB3   | 28:R:72:GLY:CA    | 2.30                     | 0.61              |
| 5:4:40:U:H4'      | 37:d:64:LYS:HG3   | 1.82                     | 0.61              |
| 2:1:10:ARG:NE     | 44:k:62:LEU:O     | 2.28                     | 0.60              |
| 6:5:710:G:H2'     | 6:5:711:G:C8      | 2.36                     | 0.60              |
| 6:5:823:C:H1'     | 17:G:24:ASN:HD22  | 1.66                     | 0.60              |
| 15:E:207:GLN:HE22 | 32:Y:91:A:H8      | 1.46                     | 0.60              |
| 19:I:46:LEU:H     | 19:I:46:LEU:HD23  | 1.66                     | 0.60              |
| 19:I:56:THR:HG22  | 19:I:68:ARG:HG2   | 1.82                     | 0.60              |
| 22:L:3:ARG:O      | 22:L:57:ARG:NH2   | 2.34                     | 0.60              |
| 49:p:81:LEU:HD23  | 49:p:84:LYS:HZ2   | 1.66                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 53:t:14:THR:HG22  | 53:t:73:LYS:HG3   | 1.81                     | 0.60              |
| 4:3:1096:U:H3     | 41:h:13:ASN:HD21  | 1.48                     | 0.60              |
| 22:L:118:ASN:O    | 28:R:87:ARG:NH2   | 2.34                     | 0.60              |
| 34:a:98:LEU:HG    | 34:a:106:LYS:NZ   | 2.16                     | 0.60              |
| 35:b:101:LEU:HD23 | 35:b:102:PHE:CE1  | 2.36                     | 0.60              |
| 41:h:14:LEU:HD13  | 41:h:19:ALA:HB1   | 1.83                     | 0.60              |
| 6:5:145:G:O2'     | 6:5:147:A:N6      | 2.32                     | 0.60              |
| 6:5:145:G:N2      | 6:5:148:A:OP2     | 2.30                     | 0.60              |
| 12:B:160:LEU:HD12 | 12:B:167:ARG:HB2  | 1.84                     | 0.60              |
| 19:I:27:THR:HG21  | 19:I:102:VAL:HG21 | 1.83                     | 0.60              |
| 6:5:822:A:O4'     | 17:G:11:HIS:HB2   | 2.01                     | 0.60              |
| 6:5:1177:U:H1'    | 23:M:42:LEU:HD11  | 1.84                     | 0.60              |
| 6:5:1320:A:H2'    | 16:F:9:ARG:HH22   | 1.66                     | 0.60              |
| 8:7:26:A:H61      | 8:7:44:G:H1       | 1.47                     | 0.60              |
| 11:A:75:VAL:HG22  | 15:E:181:PHE:HB2  | 1.82                     | 0.60              |
| 34:a:34:GLU:O     | 34:a:38:LEU:HG    | 2.02                     | 0.60              |
| 34:a:98:LEU:HG    | 34:a:106:LYS:HZ1  | 1.65                     | 0.60              |
| 44:k:52:GLU:HB3   | 44:k:55:GLN:HE21  | 1.66                     | 0.60              |
| 4:3:1803:U:O2     | 4:3:1830:G:N2     | 2.30                     | 0.60              |
| 4:3:2116:U:H5''   | 4:3:2156:G:H21    | 1.66                     | 0.60              |
| 4:3:2177:G:H4'    | 10:9:131:THR:HG21 | 1.82                     | 0.60              |
| 15:E:132:VAL:C    | 15:E:134:SER:H    | 2.08                     | 0.60              |
| 36:c:30:LYS:HG2   | 36:c:33:PRO:HD2   | 1.84                     | 0.60              |
| 43:j:75:THR:HG23  | 48:o:77:LYS:NZ    | 2.16                     | 0.60              |
| 45:l:58:LEU:HD11  | 45:l:62:GLY:HA3   | 1.83                     | 0.60              |
| 45:l:134:ARG:HE   | 45:l:135:GLU:N    | 2.00                     | 0.60              |
| 57:x:94:LEU:O     | 57:x:98:ASN:ND2   | 2.35                     | 0.60              |
| 4:3:13:C:H3'      | 4:3:14:U:H5'      | 1.84                     | 0.60              |
| 6:5:136:U:H3      | 6:5:157:A:H62     | 1.48                     | 0.60              |
| 11:A:84:PHE:CE2   | 11:A:105:VAL:HG21 | 2.37                     | 0.60              |
| 12:B:45:PHE:HD1   | 12:B:49:ARG:HH12  | 1.49                     | 0.60              |
| 35:b:163:LYS:HB3  | 35:b:165:MET:HE1  | 1.83                     | 0.60              |
| 58:y:33:CYS:SG    | 58:y:35:LYS:HG2   | 2.41                     | 0.60              |
| 59:z:17:ILE:HD11  | 59:z:50:VAL:HG11  | 1.83                     | 0.60              |
| 4:3:2143:G:H1     | 4:3:2162:U:H3     | 1.47                     | 0.60              |
| 4:3:2183:U:H4'    | 10:9:8:MET:HE1    | 1.84                     | 0.60              |
| 6:5:242:A:N1      | 6:5:274:A:O2'     | 2.35                     | 0.60              |
| 36:c:43:ALA:HA    | 36:c:99:TYR:CE2   | 2.36                     | 0.60              |
| 39:f:33:LYS:O     | 39:f:34:LYS:C     | 2.44                     | 0.60              |
| 43:j:71:ARG:HH22  | 43:j:104:ARG:NH1  | 1.99                     | 0.60              |
| 4:3:1095:U:H1'    | 4:3:1096:U:H3'    | 1.83                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:3:2847:C:H2'    | 4:3:2848:A:H8     | 1.67                     | 0.60              |
| 6:5:195:U:O2'     | 29:S:52:ASP:OD2   | 2.18                     | 0.60              |
| 6:5:1283:G:OP1    | 22:L:87:ARG:NH2   | 2.31                     | 0.60              |
| 6:5:1448:A:H2'    | 6:5:1449:G:C8     | 2.37                     | 0.60              |
| 12:B:153:LYS:HZ1  | 12:B:178:LEU:HD11 | 1.66                     | 0.60              |
| 16:F:26:ILE:HG13  | 16:F:42:LEU:HD13  | 1.83                     | 0.60              |
| 37:d:148:ARG:HE   | 37:d:149:ILE:N    | 1.98                     | 0.60              |
| 4:3:2779:C:H5''   | 35:b:211:LYS:CD   | 2.29                     | 0.60              |
| 6:5:1153:G:N2     | 6:5:1156:G:OP2    | 2.35                     | 0.60              |
| 12:B:16:LYS:HA    | 12:B:216:ASN:ND2  | 2.16                     | 0.60              |
| 15:E:47:TYR:CE2   | 15:E:49:ILE:HB    | 2.36                     | 0.60              |
| 18:H:86:VAL:O     | 18:H:90:LEU:HD23  | 2.01                     | 0.60              |
| 35:b:47:TYR:HB2   | 35:b:85:ARG:HH21  | 1.67                     | 0.60              |
| 37:d:17:GLN:HA    | 37:d:22:PHE:HB2   | 1.82                     | 0.60              |
| 4:3:1123:A:N7     | 41:h:130:GLN:NE2  | 2.49                     | 0.60              |
| 4:3:1296:G:O2'    | 4:3:2019:G:O6     | 2.18                     | 0.60              |
| 11:A:38:ASN:OD1   | 11:A:40:LYS:HE2   | 2.02                     | 0.60              |
| 23:M:21:TYR:HE2   | 23:M:23:ARG:HE    | 1.49                     | 0.60              |
| 27:Q:67:TYR:HA    | 27:Q:103:LYS:HG2  | 1.84                     | 0.60              |
| 45:l:134:ARG:HE   | 45:l:135:GLU:H    | 1.49                     | 0.60              |
| 47:n:31:MET:CE    | 47:n:94:GLY:HA2   | 2.32                     | 0.60              |
| 4:3:78:C:H5'      | 56:w:49:ARG:CZ    | 2.31                     | 0.59              |
| 4:3:1029:A:OP1    | 49:p:49:ARG:NH1   | 2.35                     | 0.59              |
| 4:3:1386:G:O2'    | 4:3:1401:A:N6     | 2.35                     | 0.59              |
| 6:5:1320:A:N6     | 6:5:1349:A:H5''   | 2.16                     | 0.59              |
| 11:A:30:VAL:HG22  | 11:A:55:HIS:NE2   | 2.17                     | 0.59              |
| 12:B:155:LEU:HD23 | 12:B:204:TRP:HZ3  | 1.65                     | 0.59              |
| 16:F:65:VAL:HA    | 16:F:68:VAL:HG12  | 1.84                     | 0.59              |
| 18:H:90:LEU:HD13  | 18:H:97:LYS:HB2   | 1.84                     | 0.59              |
| 19:I:24:LEU:HD21  | 19:I:78:ARG:HG2   | 1.82                     | 0.59              |
| 19:I:57:ILE:HB    | 23:M:45:ARG:CZ    | 2.32                     | 0.59              |
| 23:M:26:ARG:NH2   | 23:M:46:GLU:OE2   | 2.34                     | 0.59              |
| 27:Q:88:LYS:O     | 27:Q:92:ARG:HD3   | 2.02                     | 0.59              |
| 54:u:38:LYS:HD2   | 54:u:53:ARG:NH2   | 2.17                     | 0.59              |
| 4:3:1777:G:H1     | 4:3:1989:U:H3     | 1.47                     | 0.59              |
| 6:5:1321:G:O2'    | 6:5:1348:G:O6     | 2.19                     | 0.59              |
| 16:F:76:VAL:HA    | 16:F:83:ASN:HD22  | 1.68                     | 0.59              |
| 28:R:29:ARG:HB3   | 28:R:30:PRO:HD2   | 1.84                     | 0.59              |
| 48:o:12:LEU:O     | 48:o:15:GLN:HG3   | 2.02                     | 0.59              |
| 4:3:2477:A:H2'    | 4:3:2478:G:O4'    | 2.03                     | 0.59              |
| 21:K:98:GLY:H     | 21:K:107:ARG:HH12 | 1.50                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 43:j:8:LEU:HD22   | 43:j:82:ASN:HB2   | 1.83                     | 0.59              |
| 48:o:53:LEU:HD11  | 48:o:67:ARG:HD2   | 1.85                     | 0.59              |
| 53:t:80:LYS:HD2   | 53:t:109:ASN:HB3  | 1.83                     | 0.59              |
| 1:0:6:GLN:NE2     | 4:3:721:G:O3'     | 2.29                     | 0.59              |
| 4:3:1353:G:OP1    | 4:3:1681:G:O2'    | 2.13                     | 0.59              |
| 6:5:1022:G:H21    | 6:5:1026:A:H62    | 1.50                     | 0.59              |
| 7:6:60:A:OP2      | 7:6:61:C:N4       | 2.25                     | 0.59              |
| 24:N:9:ILE:HG13   | 24:N:28:LEU:HD21  | 1.85                     | 0.59              |
| 25:O:5:ARG:HA     | 25:O:69:VAL:HG21  | 1.84                     | 0.59              |
| 42:i:144:ASN:OD1  | 42:i:145:TRP:HD1  | 1.86                     | 0.59              |
| 43:j:89:GLU:CD    | 43:j:89:GLU:H     | 2.10                     | 0.59              |
| 56:w:18:LEU:HD13  | 56:w:21:LYS:HD2   | 1.83                     | 0.59              |
| 59:z:10:GLY:HA2   | 59:z:17:ILE:HA    | 1.85                     | 0.59              |
| 4:3:679:A:N1      | 4:3:2377:A:O2'    | 2.35                     | 0.59              |
| 6:5:735:C:OP2     | 15:E:92:ARG:NH2   | 2.35                     | 0.59              |
| 10:9:137:ASN:N    | 10:9:142:THR:OG1  | 2.33                     | 0.59              |
| 11:A:255:GLN:OE1  | 11:A:255:GLN:N    | 2.36                     | 0.59              |
| 16:F:1:MET:O      | 16:F:3:LYS:NZ     | 2.29                     | 0.59              |
| 17:G:31:MET:HE3   | 17:G:73:ASN:HB3   | 1.84                     | 0.59              |
| 47:n:93:THR:HB    | 47:n:102:ILE:HD13 | 1.84                     | 0.59              |
| 4:3:1909:C:O2'    | 34:a:251:ARG:O    | 2.19                     | 0.59              |
| 4:3:2106:G:N2     | 4:3:2199:C:O2     | 2.36                     | 0.59              |
| 36:c:165:ASN:HB3  | 36:c:168:LEU:HD23 | 1.84                     | 0.59              |
| 39:f:82:LYS:HA    | 39:f:149:LYS:HE3  | 1.85                     | 0.59              |
| 44:k:98:LEU:HD11  | 44:k:103:VAL:HB   | 1.85                     | 0.59              |
| 56:w:71:LYS:HE2   | 56:w:72:TYR:HD1   | 1.67                     | 0.59              |
| 4:3:1092:A:N6     | 4:3:1122:G:OP1    | 2.35                     | 0.59              |
| 14:D:150:LEU:HD23 | 14:D:183:LEU:HD11 | 1.84                     | 0.59              |
| 16:F:128:ASN:O    | 16:F:130:THR:HG23 | 2.02                     | 0.59              |
| 44:k:126:PHE:HB2  | 44:k:146:VAL:HG22 | 1.85                     | 0.59              |
| 52:s:7:LEU:HD11   | 52:s:29:PHE:CD2   | 2.35                     | 0.59              |
| 4:3:832:C:P       | 36:c:63:LYS:HE3   | 2.43                     | 0.59              |
| 4:3:1602:G:OP2    | 34:a:67:ARG:NH2   | 2.36                     | 0.59              |
| 5:4:2:U:O2        | 5:4:107:G:N2      | 2.36                     | 0.59              |
| 6:5:394:U:H2'     | 6:5:395:G:H8      | 1.68                     | 0.59              |
| 14:D:212:ARG:NE   | 17:G:51:GLU:O     | 2.36                     | 0.59              |
| 18:H:101:LYS:C    | 18:H:103:LYS:H    | 2.10                     | 0.59              |
| 21:K:49:ARG:HH21  | 21:K:77:LEU:HD21  | 1.68                     | 0.59              |
| 34:a:189:THR:HB   | 34:a:279:ILE:HB   | 1.85                     | 0.59              |
| 38:e:19:ASN:OD1   | 38:e:26:ALA:HB3   | 2.03                     | 0.59              |
| 4:3:1798:A:C2     | 4:3:1836:A:H4'    | 2.38                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:5:1138:U:H3     | 6:5:1149:G:H1     | 1.49                     | 0.59              |
| 20:J:72:MET:HE2   | 20:J:75:VAL:HG12  | 1.83                     | 0.59              |
| 38:e:92:LEU:HA    | 38:e:165:VAL:HA   | 1.85                     | 0.59              |
| 43:j:40:VAL:HG22  | 43:j:59:ARG:HG2   | 1.85                     | 0.59              |
| 43:j:93:PRO:HG2   | 43:j:113:LYS:HB3  | 1.85                     | 0.59              |
| 44:k:10:PRO:O     | 44:k:11:LYS:HG3   | 2.03                     | 0.59              |
| 45:l:83:MET:N     | 45:l:83:MET:SD    | 2.75                     | 0.59              |
| 50:q:34:GLN:HE22  | 50:q:56:VAL:HG22  | 1.68                     | 0.59              |
| 53:t:76:LEU:HD22  | 53:t:89:ILE:HG21  | 1.85                     | 0.59              |
| 4:3:549:A:N3      | 4:3:614:C:O2'     | 2.35                     | 0.58              |
| 4:3:814:U:OP1     | 34:a:53:ILE:HD12  | 2.03                     | 0.58              |
| 6:5:640:C:H5'     | 17:G:40:LEU:HD11  | 1.85                     | 0.58              |
| 11:A:174:ASN:HD22 | 15:E:181:PHE:HE1  | 1.50                     | 0.58              |
| 12:B:153:LYS:HG3  | 12:B:170:MET:HE1  | 1.85                     | 0.58              |
| 26:P:22:ALA:HB2   | 26:P:49:ASN:ND2   | 2.16                     | 0.58              |
| 30:T:20:ARG:NH2   | 32:Y:60:G:O5'     | 2.36                     | 0.58              |
| 42:i:17:GLN:HE22  | 42:i:141:THR:HG23 | 1.67                     | 0.58              |
| 49:p:65:ASN:O     | 49:p:69:ARG:HG2   | 2.03                     | 0.58              |
| 50:q:27:ALA:O     | 50:q:62:HIS:NE2   | 2.36                     | 0.58              |
| 9:8:39:U:O3'      | 22:L:120:LYS:NZ   | 2.32                     | 0.58              |
| 14:D:212:ARG:CZ   | 14:D:214:LYS:HD3  | 2.32                     | 0.58              |
| 17:G:48:LEU:HD12  | 17:G:51:GLU:OE2   | 2.02                     | 0.58              |
| 20:J:75:VAL:HG23  | 20:J:100:ILE:HA   | 1.85                     | 0.58              |
| 4:3:2122:G:H2'    | 4:3:2124:A:N7     | 2.18                     | 0.58              |
| 6:5:373:A:H2'     | 6:5:374:G:C8      | 2.38                     | 0.58              |
| 11:A:84:PHE:HE2   | 11:A:105:VAL:HG21 | 1.68                     | 0.58              |
| 12:B:83:LYS:HD2   | 12:B:86:GLN:NE2   | 2.18                     | 0.58              |
| 22:L:50:GLU:OE1   | 22:L:50:GLU:N     | 2.34                     | 0.58              |
| 36:c:60:GLY:HA3   | 36:c:80:ARG:HG3   | 1.85                     | 0.58              |
| 39:f:65:SER:O     | 39:f:134:THR:HG21 | 2.03                     | 0.58              |
| 46:m:59:ASN:OD1   | 46:m:62:GLN:NE2   | 2.35                     | 0.58              |
| 4:3:201:A:N6      | 4:3:2438:A:O2'    | 2.37                     | 0.58              |
| 12:B:109:ILE:HD12 | 12:B:222:ILE:HG23 | 1.84                     | 0.58              |
| 18:H:44:LYS:HG3   | 18:H:46:VAL:H     | 1.68                     | 0.58              |
| 34:a:65:LYS:O     | 34:a:67:ARG:NH1   | 2.36                     | 0.58              |
| 39:f:15:ARG:CD    | 39:f:16:PHE:H     | 2.16                     | 0.58              |
| 46:m:93:THR:HB    | 46:m:97:TYR:CE1   | 2.39                     | 0.58              |
| 4:3:954:A:H5''    | 4:3:2276:A:H61    | 1.67                     | 0.58              |
| 15:E:179:LYS:HB3  | 15:E:180:ARG:HH11 | 1.67                     | 0.58              |
| 16:F:110:ARG:NH1  | 16:F:125:ASP:OD2  | 2.36                     | 0.58              |
| 16:F:111:HIS:ND1  | 16:F:111:HIS:O    | 2.36                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 20:J:103:ILE:HG23 | 30:T:18:PHE:CZ    | 2.39                     | 0.58              |
| 58:y:53:VAL:HG23  | 58:y:54:LYS:H     | 1.68                     | 0.58              |
| 4:3:1722:U:O2'    | 4:3:1734:A:N7     | 2.25                     | 0.58              |
| 4:3:2009:U:OP1    | 46:m:14:ARG:NH1   | 2.33                     | 0.58              |
| 4:3:2152:C:H5''   | 4:3:2153:U:C5     | 2.38                     | 0.58              |
| 50:q:21:PHE:CD2   | 50:q:91:LYS:HB2   | 2.39                     | 0.58              |
| 56:w:18:LEU:HA    | 56:w:21:LYS:HG2   | 1.85                     | 0.58              |
| 4:3:622:U:H4'     | 36:c:94:LYS:HE3   | 1.84                     | 0.58              |
| 6:5:257:U:OP1     | 29:S:64:ARG:NH1   | 2.36                     | 0.58              |
| 6:5:733:A:P       | 27:Q:92:ARG:HH21  | 2.27                     | 0.58              |
| 6:5:1123:G:O2'    | 6:5:1124:U:O5'    | 2.22                     | 0.58              |
| 17:G:90:ILE:HD11  | 17:G:140:TYR:HD2  | 1.69                     | 0.58              |
| 18:H:45:LEU:O     | 18:H:49:ASP:N     | 2.36                     | 0.58              |
| 18:H:49:ASP:HA    | 18:H:52:GLN:NE2   | 2.17                     | 0.58              |
| 19:I:46:LEU:HD21  | 19:I:79:LEU:HD22  | 1.85                     | 0.58              |
| 4:3:1093:U:H3     | 4:3:1115:G:H1     | 1.52                     | 0.58              |
| 4:3:1906:G:H21    | 4:3:1909:C:H41    | 1.51                     | 0.58              |
| 4:3:2100:G:N7     | 4:3:2233:A:H2'    | 2.19                     | 0.58              |
| 6:5:426:U:H5'     | 13:C:8:PHE:CG     | 2.39                     | 0.58              |
| 16:F:25:ILE:HB    | 16:F:100:LEU:HD22 | 1.85                     | 0.58              |
| 27:Q:36:ARG:HB2   | 27:Q:38:LYS:NZ    | 2.19                     | 0.58              |
| 29:S:67:ARG:HB3   | 29:S:71:ARG:HH12  | 1.68                     | 0.58              |
| 35:b:15:GLN:OE1   | 35:b:23:ARG:NH1   | 2.35                     | 0.58              |
| 38:e:89:LYS:NZ    | 38:e:133:GLU:OE2  | 2.36                     | 0.58              |
| 41:h:58:TYR:HE1   | 41:h:60:ASP:HB3   | 1.65                     | 0.58              |
| 41:h:73:SER:HB2   | 41:h:131:MET:HE2  | 1.86                     | 0.58              |
| 4:3:410:G:H4'     | 4:3:411:U:O5'     | 2.03                     | 0.58              |
| 4:3:1033:A:OP2    | 49:p:57:ARG:NH1   | 2.37                     | 0.58              |
| 6:5:523:U:OP1     | 21:K:99:ARG:NH2   | 2.37                     | 0.58              |
| 20:J:6:LYS:NZ     | 20:J:8:ASN:HD22   | 2.01                     | 0.58              |
| 43:j:75:THR:HG23  | 48:o:77:LYS:CE    | 2.33                     | 0.58              |
| 45:l:109:ILE:CG1  | 45:l:110:PRO:HD2  | 2.34                     | 0.58              |
| 50:q:31:LYS:NZ    | 50:q:33:ILE:HD13  | 2.19                     | 0.58              |
| 4:3:1355:C:OP1    | 51:r:11:ARG:NH1   | 2.37                     | 0.58              |
| 6:5:661:G:HO2'    | 6:5:722:G:HO2'    | 1.48                     | 0.58              |
| 7:6:9:A:O2'       | 7:6:10:G:N7       | 2.35                     | 0.58              |
| 15:E:147:GLU:OE2  | 15:E:148:LYS:HD2  | 2.03                     | 0.58              |
| 40:g:27:PHE:O     | 40:g:81:ALA:N     | 2.37                     | 0.58              |
| 43:j:66:LYS:O     | 43:j:78:LYS:NZ    | 2.37                     | 0.58              |
| 51:r:136:LYS:O    | 51:r:139:ARG:HG2  | 2.03                     | 0.58              |
| 4:3:1023:C:O2'    | 4:3:1036:A:N3     | 2.33                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:3:2794:U:H5'    | 35:b:72:LYS:NZ    | 2.19                     | 0.57              |
| 6:5:22:G:H2'      | 6:5:23:G:C8       | 2.39                     | 0.57              |
| 6:5:508:A:HO2'    | 6:5:540:U:HO2'    | 1.47                     | 0.57              |
| 36:c:120:LEU:HA   | 36:c:125:THR:HG21 | 1.86                     | 0.57              |
| 37:d:118:SER:C    | 37:d:120:LYS:H    | 2.12                     | 0.57              |
| 38:e:28:LYS:HD2   | 38:e:33:GLN:HB2   | 1.86                     | 0.57              |
| 57:x:32:LYS:O     | 57:x:34:ILE:HD12  | 2.04                     | 0.57              |
| 4:3:2164:G:O2'    | 4:3:2165:A:H8     | 1.87                     | 0.57              |
| 6:5:515:G:N2      | 6:5:528:G:OP1     | 2.34                     | 0.57              |
| 6:5:535:A:OP1     | 21:K:123:ARG:NH2  | 2.37                     | 0.57              |
| 6:5:1269:U:O2'    | 22:L:14:ARG:NH1   | 2.37                     | 0.57              |
| 6:5:1406:U:O4     | 6:5:1407:A:N6     | 2.37                     | 0.57              |
| 11:A:95:LEU:HD21  | 11:A:226:CYS:HA   | 1.86                     | 0.57              |
| 15:E:98:ALA:HA    | 15:E:101:ASN:HD22 | 1.69                     | 0.57              |
| 17:G:61:GLU:HG2   | 17:G:65:LYS:HE2   | 1.86                     | 0.57              |
| 30:T:42:LEU:HD12  | 30:T:45:LYS:HZ1   | 1.68                     | 0.57              |
| 4:3:287:G:H1      | 39:f:42:LYS:HE2   | 1.69                     | 0.57              |
| 4:3:700:U:H2'     | 4:3:701:A:H8      | 1.70                     | 0.57              |
| 4:3:1091:G:H4'    | 4:3:1121:A:C8     | 2.38                     | 0.57              |
| 4:3:2493:G:O3'    | 45:l:126:PRO:HB3  | 2.05                     | 0.57              |
| 4:3:2813:A:H2'    | 4:3:2814:A:C8     | 2.38                     | 0.57              |
| 6:5:1497:U:H2'    | 6:5:1498:G:H8     | 1.69                     | 0.57              |
| 12:B:192:ALA:HB3  | 12:B:199:ILE:HB   | 1.86                     | 0.57              |
| 13:C:61:GLN:CB    | 13:C:71:PHE:HE2   | 2.16                     | 0.57              |
| 28:R:19:VAL:HG21  | 28:R:44:PHE:CD1   | 2.38                     | 0.57              |
| 46:m:33:THR:O     | 46:m:114:ALA:N    | 2.37                     | 0.57              |
| 4:3:1270:C:H2'    | 4:3:1271:A:H8     | 1.70                     | 0.57              |
| 6:5:251:G:H4'     | 26:P:20:LYS:HD2   | 1.87                     | 0.57              |
| 6:5:304:U:H2'     | 6:5:305:A:H8      | 1.69                     | 0.57              |
| 6:5:945:U:OP2     | 22:L:101:ARG:HD2  | 2.04                     | 0.57              |
| 7:6:25:C:H42      | 7:6:45:G:H22      | 1.50                     | 0.57              |
| 17:G:107:VAL:HG22 | 17:G:140:TYR:HD1  | 1.70                     | 0.57              |
| 36:c:154:ASP:OD1  | 36:c:154:ASP:N    | 2.37                     | 0.57              |
| 38:e:88:LYS:HB2   | 38:e:136:ILE:HB   | 1.85                     | 0.57              |
| 46:m:63:VAL:HG12  | 46:m:79:MET:HE1   | 1.85                     | 0.57              |
| 53:t:10:VAL:HG11  | 53:t:74:LEU:HB3   | 1.86                     | 0.57              |
| 4:3:1314:A:H4'    | 46:m:107:ARG:HH12 | 1.69                     | 0.57              |
| 4:3:2885:U:O2     | 46:m:99:ARG:NH2   | 2.38                     | 0.57              |
| 11:A:17:LEU:HG    | 11:A:18:VAL:H     | 1.68                     | 0.57              |
| 11:A:152:LEU:HA   | 11:A:155:GLU:CD   | 2.29                     | 0.57              |
| 16:F:107:ALA:O    | 16:F:118:LYS:HE3  | 2.04                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 28:R:9:ALA:H      | 57:x:69:GLY:HA3   | 1.69                     | 0.57              |
| 48:o:49:THR:HG23  | 48:o:91:LYS:NZ    | 2.18                     | 0.57              |
| 4:3:585:U:H2'     | 4:3:586:G:H8      | 1.70                     | 0.57              |
| 6:5:1142:G:O2'    | 6:5:1144:A:N6     | 2.31                     | 0.57              |
| 6:5:1144:A:H2'    | 6:5:1145:A:C8     | 2.39                     | 0.57              |
| 34:a:128:ILE:HG22 | 34:a:129:ASP:N    | 2.20                     | 0.57              |
| 47:n:64:ASN:CG    | 47:n:65:GLY:H     | 2.12                     | 0.57              |
| 4:3:619:A:H62     | 4:3:1281:A:H2     | 1.53                     | 0.57              |
| 4:3:2814:A:H4'    | 35:b:64:LYS:HD2   | 1.85                     | 0.57              |
| 4:3:2820:G:N3     | 4:3:2887:A:O2'    | 2.37                     | 0.57              |
| 6:5:92:G:N7       | 29:S:10:ARG:NH2   | 2.53                     | 0.57              |
| 6:5:670:G:H2'     | 6:5:671:G:C8      | 2.39                     | 0.57              |
| 6:5:714:C:O2'     | 6:5:731:A:O4'     | 2.15                     | 0.57              |
| 6:5:952:U:O2      | 28:R:78:ARG:NH2   | 2.30                     | 0.57              |
| 9:8:18:G:N2       | 9:8:58:A:OP2      | 2.35                     | 0.57              |
| 12:B:17:ASN:H     | 12:B:216:ASN:HD22 | 1.51                     | 0.57              |
| 12:B:40:ILE:HG12  | 12:B:95:ILE:HG21  | 1.87                     | 0.57              |
| 30:T:5:GLU:HG3    | 30:T:7:LYS:H      | 1.70                     | 0.57              |
| 39:f:57:HIS:O     | 39:f:60:ILE:HG12  | 2.05                     | 0.57              |
| 48:o:49:THR:HG23  | 48:o:91:LYS:HZ1   | 1.69                     | 0.57              |
| 4:3:140:G:N2      | 4:3:143:A:OP2     | 2.22                     | 0.57              |
| 4:3:246:G:O2'     | 4:3:258:G:O6      | 2.22                     | 0.57              |
| 4:3:1106:G:N2     | 4:3:1124:G:O2'    | 2.37                     | 0.57              |
| 4:3:2308:U:H2'    | 4:3:2309:A:H8     | 1.68                     | 0.57              |
| 4:3:2383:G:N2     | 4:3:2386:A:OP2    | 2.31                     | 0.57              |
| 6:5:930:A:H62     | 16:F:2:ARG:NH2    | 2.02                     | 0.57              |
| 6:5:972:A:N6      | 6:5:1199:U:O5'    | 2.37                     | 0.57              |
| 13:C:68:ASP:OD1   | 13:C:69:LYS:N     | 2.37                     | 0.57              |
| 15:E:94:TYR:HB3   | 27:Q:85:HIS:CD2   | 2.40                     | 0.57              |
| 16:F:76:VAL:HG22  | 16:F:83:ASN:ND2   | 2.20                     | 0.57              |
| 21:K:69:ARG:HH12  | 21:K:73:GLY:HA2   | 1.70                     | 0.57              |
| 39:f:65:SER:HA    | 39:f:134:THR:HB   | 1.87                     | 0.57              |
| 4:3:80:U:H5'      | 56:w:8:ARG:HH22   | 1.70                     | 0.57              |
| 4:3:788:G:H2'     | 4:3:789:A:H8      | 1.70                     | 0.57              |
| 4:3:1796:A:O3'    | 34:a:226:PRO:HB3  | 2.05                     | 0.57              |
| 6:5:711:G:N2      | 20:J:114:CYS:SG   | 2.78                     | 0.57              |
| 6:5:716:C:O2      | 27:Q:70:ILE:HG12  | 2.05                     | 0.57              |
| 6:5:733:A:H2'     | 6:5:734:A:C8      | 2.40                     | 0.57              |
| 6:5:1330:A:H2'    | 6:5:1331:A:C8     | 2.39                     | 0.57              |
| 7:6:46:G:H4'      | 7:6:47:U:OP1      | 2.05                     | 0.57              |
| 17:G:26:ARG:HD3   | 17:G:84:ILE:HG23  | 1.87                     | 0.57              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 43:j:71:ARG:N     | 43:j:75:THR:O    | 2.23                     | 0.57              |
| 4:3:141:A:H2      | 4:3:1437:A:H1'   | 1.68                     | 0.57              |
| 4:3:799:A:H5''    | 34:a:217:GLY:HA3 | 1.85                     | 0.57              |
| 4:3:2106:G:H2'    | 4:3:2107:A:H8    | 1.69                     | 0.57              |
| 4:3:2137:A:H5''   | 4:3:2139:C:C5    | 2.39                     | 0.57              |
| 6:5:55:C:H2'      | 6:5:348:C:H41    | 1.70                     | 0.57              |
| 7:6:73:A:H5''     | 7:6:74:C:C5      | 2.38                     | 0.57              |
| 10:9:113:ILE:HD11 | 10:9:150:ALA:HB3 | 1.87                     | 0.57              |
| 12:B:35:ILE:HG21  | 23:M:25:GLN:HB2  | 1.86                     | 0.57              |
| 14:D:117:LYS:O    | 14:D:120:LYS:HG2 | 2.05                     | 0.57              |
| 20:J:103:ILE:HG23 | 30:T:18:PHE:CE2  | 2.40                     | 0.57              |
| 34:a:41:LEU:HG    | 34:a:66:TYR:HB2  | 1.85                     | 0.57              |
| 57:x:37:ASP:OD1   | 57:x:38:ILE:N    | 2.38                     | 0.57              |
| 4:3:1521:A:N3     | 4:3:1611:C:O2'   | 2.35                     | 0.56              |
| 6:5:1113:U:O4     | 6:5:1114:A:N6    | 2.38                     | 0.56              |
| 13:C:66:ILE:HB    | 13:C:71:PHE:CZ   | 2.40                     | 0.56              |
| 20:J:79:VAL:N     | 20:J:104:ASN:O   | 2.37                     | 0.56              |
| 34:a:178:LYS:HG2  | 34:a:179:TYR:H   | 1.68                     | 0.56              |
| 40:g:37:ALA:O     | 40:g:40:ILE:HG22 | 2.05                     | 0.56              |
| 51:r:124:LEU:HD23 | 51:r:127:LYS:HD3 | 1.86                     | 0.56              |
| 6:5:576:A:O2'     | 6:5:725:A:N3     | 2.30                     | 0.56              |
| 6:5:927:C:OP2     | 16:F:3:LYS:NZ    | 2.37                     | 0.56              |
| 6:5:1215:U:H4'    | 16:F:37:LEU:HD21 | 1.87                     | 0.56              |
| 11:A:26:MET:SD    | 11:A:227:LEU:HG  | 2.45                     | 0.56              |
| 15:E:1:MET:CE     | 15:E:91:GLU:HB3  | 2.32                     | 0.56              |
| 19:I:63:VAL:HG12  | 19:I:64:ASP:N    | 2.19                     | 0.56              |
| 25:O:78:LEU:HA    | 25:O:81:LYS:HZ3  | 1.70                     | 0.56              |
| 39:f:26:ALA:HB1   | 39:f:30:LEU:N    | 2.20                     | 0.56              |
| 43:j:66:LYS:N     | 43:j:82:ASN:OD1  | 2.30                     | 0.56              |
| 45:l:116:LYS:O    | 45:l:120:ARG:HG2 | 2.05                     | 0.56              |
| 47:n:112:ARG:HG3  | 47:n:112:ARG:O   | 2.05                     | 0.56              |
| 56:w:91:LEU:O     | 56:w:95:LYS:HD3  | 2.06                     | 0.56              |
| 4:3:524:G:N2      | 4:3:527:A:OP2    | 2.28                     | 0.56              |
| 4:3:631:A:OP1     | 44:k:11:LYS:NZ   | 2.38                     | 0.56              |
| 4:3:1029:A:OP2    | 49:p:50:ARG:NH2  | 2.38                     | 0.56              |
| 4:3:1393:A:H4'    | 55:v:4:LYS:HZ1   | 1.70                     | 0.56              |
| 4:3:2131:G:H5'    | 4:3:2131:G:H8    | 1.70                     | 0.56              |
| 4:3:2180:U:H3'    | 4:3:2181:A:H8    | 1.70                     | 0.56              |
| 4:3:2186:C:H2'    | 4:3:2187:C:H4'   | 1.86                     | 0.56              |
| 6:5:469:C:H5''    | 25:O:79:TRP:HE1  | 1.70                     | 0.56              |
| 6:5:1330:A:H2'    | 6:5:1331:A:H8    | 1.70                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:E:33:GLU:HG2   | 15:E:63:SER:HB3   | 1.87                     | 0.56              |
| 19:I:56:THR:HG23  | 19:I:70:GLN:HG3   | 1.88                     | 0.56              |
| 24:N:33:ILE:HG13  | 24:N:60:ARG:CZ    | 2.35                     | 0.56              |
| 24:N:41:LEU:O     | 24:N:44:LYS:NZ    | 2.35                     | 0.56              |
| 25:O:17:TYR:O     | 25:O:39:LEU:N     | 2.36                     | 0.56              |
| 27:Q:64:LEU:HD21  | 27:Q:68:ALA:HA    | 1.87                     | 0.56              |
| 30:T:19:LYS:NZ    | 32:Y:61:A:OP2     | 2.35                     | 0.56              |
| 37:d:132:ILE:HB   | 37:d:152:PHE:HB2  | 1.86                     | 0.56              |
| 38:e:27:VAL:HB    | 38:e:34:ILE:HG22  | 1.88                     | 0.56              |
| 44:k:95:ARG:NH2   | 44:k:110:LEU:O    | 2.38                     | 0.56              |
| 46:m:102:LYS:O    | 58:y:41:ARG:NH1   | 2.38                     | 0.56              |
| 49:p:111:LYS:NZ   | 50:q:45:ILE:HG22  | 2.20                     | 0.56              |
| 52:s:43:ALA:O     | 52:s:47:VAL:HG22  | 2.05                     | 0.56              |
| 6:5:832:G:H2'     | 6:5:833:G:H8      | 1.70                     | 0.56              |
| 6:5:1205:C:N4     | 22:L:104:THR:OG1  | 2.39                     | 0.56              |
| 6:5:1321:G:C8     | 18:H:111:ARG:HB3  | 2.41                     | 0.56              |
| 11:A:247:ALA:O    | 11:A:249:LYS:HG2  | 2.05                     | 0.56              |
| 13:C:27:LYS:HD2   | 13:C:27:LYS:C     | 2.31                     | 0.56              |
| 13:C:93:LEU:HA    | 13:C:96:ARG:HH12  | 1.70                     | 0.56              |
| 15:E:20:GLN:CD    | 15:E:81:GLN:HG3   | 2.30                     | 0.56              |
| 18:H:30:ILE:HG23  | 18:H:37:PRO:HG3   | 1.86                     | 0.56              |
| 26:P:59:ASP:O     | 26:P:61:VAL:HG23  | 2.05                     | 0.56              |
| 28:R:21:ASP:O     | 28:R:24:LYS:HG2   | 2.06                     | 0.56              |
| 34:a:213:ILE:HG21 | 34:a:219:ASN:OD1  | 2.06                     | 0.56              |
| 4:3:1125:U:H2'    | 4:3:1126:G:C8     | 2.41                     | 0.56              |
| 4:3:1369:U:OP2    | 4:3:1422:U:O2'    | 2.18                     | 0.56              |
| 8:7:36:C:H2'      | 8:7:37:A:C8       | 2.40                     | 0.56              |
| 13:C:50:TYR:CD1   | 13:C:199:TRP:HH2  | 2.24                     | 0.56              |
| 14:D:151:LEU:HD23 | 14:D:180:THR:HG22 | 1.87                     | 0.56              |
| 21:K:98:GLY:H     | 21:K:107:ARG:NH1  | 2.04                     | 0.56              |
| 22:L:73:ILE:O     | 22:L:77:ILE:HG12  | 2.06                     | 0.56              |
| 36:c:188:VAL:O    | 36:c:192:MET:HG3  | 2.05                     | 0.56              |
| 44:k:69:ARG:NH1   | 44:k:73:LEU:O     | 2.38                     | 0.56              |
| 54:u:39:LYS:HB2   | 54:u:51:ILE:HD12  | 1.86                     | 0.56              |
| 4:3:1557:G:O6     | 4:3:1571:G:O2'    | 2.22                     | 0.56              |
| 4:3:1665:G:N1     | 4:3:1668:G:OP2    | 2.32                     | 0.56              |
| 6:5:971:A:OP2     | 23:M:31:ARG:NE    | 2.38                     | 0.56              |
| 12:B:89:THR:HG23  | 12:B:102:LEU:HD23 | 1.87                     | 0.56              |
| 29:S:19:LEU:O     | 29:S:22:LYS:HG3   | 2.06                     | 0.56              |
| 34:a:29:ASN:O     | 34:a:29:ASN:ND2   | 2.37                     | 0.56              |
| 34:a:151:GLU:HG2  | 34:a:157:GLY:C    | 2.30                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 39:f:33:LYS:O     | 39:f:35:LEU:N     | 2.39                     | 0.56              |
| 39:f:64:LEU:HA    | 39:f:67:LYS:HE2   | 1.87                     | 0.56              |
| 39:f:69:LYS:O     | 39:f:73:GLU:HG2   | 2.06                     | 0.56              |
| 44:k:95:ARG:O     | 44:k:99:ILE:HG12  | 2.06                     | 0.56              |
| 52:s:9:LYS:HZ2    | 56:w:31:PHE:HA    | 1.71                     | 0.56              |
| 4:3:615:G:H2'     | 4:3:616:G:H8      | 1.70                     | 0.56              |
| 4:3:2155:G:H2'    | 4:3:2156:G:C8     | 2.41                     | 0.56              |
| 12:B:44:PHE:CE2   | 12:B:56:VAL:HG21  | 2.40                     | 0.56              |
| 17:G:49:VAL:HG11  | 17:G:57:PHE:HE1   | 1.70                     | 0.56              |
| 22:L:87:ARG:C     | 22:L:87:ARG:HD3   | 2.31                     | 0.56              |
| 38:e:23:ASP:HA    | 38:e:38:LEU:HB2   | 1.87                     | 0.56              |
| 39:f:40:THR:N     | 39:f:47:ARG:HB2   | 2.12                     | 0.56              |
| 39:f:52:LYS:O     | 39:f:56:GLU:HG2   | 2.05                     | 0.56              |
| 39:f:71:VAL:CG1   | 39:f:108:LEU:HB2  | 2.36                     | 0.56              |
| 45:l:37:THR:O     | 45:l:38:LYS:HD3   | 2.05                     | 0.56              |
| 46:m:111:THR:HG23 | 46:m:113:MET:CE   | 2.36                     | 0.56              |
| 48:o:14:GLU:HB2   | 48:o:60:ILE:HB    | 1.88                     | 0.56              |
| 4:3:957:G:H21     | 4:3:2277:A:H8     | 1.53                     | 0.56              |
| 4:3:1617:U:H5''   | 4:3:1619:A:C4     | 2.41                     | 0.56              |
| 4:3:2402:C:H5''   | 44:k:64:LYS:HE2   | 1.88                     | 0.56              |
| 4:3:2798:A:O3'    | 4:3:2896:G:N2     | 2.38                     | 0.56              |
| 5:4:52:G:H21      | 37:d:26:MET:HE1   | 1.70                     | 0.56              |
| 6:5:916:U:O2      | 14:D:79:THR:OG1   | 2.23                     | 0.56              |
| 7:6:18:G:N7       | 7:6:57:G:N2       | 2.54                     | 0.56              |
| 11:A:203:ASN:HB2  | 11:A:219:ASN:ND2  | 2.21                     | 0.56              |
| 13:C:179:VAL:HG12 | 13:C:180:ARG:N    | 2.20                     | 0.56              |
| 42:i:95:MET:HE3   | 42:i:99:GLN:O     | 2.06                     | 0.56              |
| 49:p:43:LYS:HE2   | 50:q:73:HIS:HB3   | 1.86                     | 0.56              |
| 4:3:622:U:H2'     | 4:3:623:A:C8      | 2.41                     | 0.56              |
| 4:3:901:C:H4'     | 4:3:902:U:C5'     | 2.36                     | 0.56              |
| 4:3:1833:G:O2'    | 4:3:1978:U:OP2    | 2.24                     | 0.56              |
| 6:5:1490:G:H2'    | 6:5:1491:A:C8     | 2.41                     | 0.56              |
| 15:E:43:LYS:HD2   | 15:E:44:GLU:O     | 2.06                     | 0.56              |
| 15:E:53:LEU:HD23  | 15:E:53:LEU:H     | 1.69                     | 0.56              |
| 28:R:50:ALA:HB1   | 28:R:57:PHE:HB3   | 1.87                     | 0.56              |
| 31:X:43:PHE:HA    | 52:s:14:GLU:OE2   | 2.06                     | 0.56              |
| 35:b:40:LYS:O     | 35:b:48:SER:HA    | 2.06                     | 0.56              |
| 35:b:175:THR:HG21 | 35:b:208:ARG:HH22 | 1.71                     | 0.56              |
| 37:d:31:LEU:HD11  | 37:d:156:LEU:HD12 | 1.88                     | 0.56              |
| 46:m:111:THR:HG23 | 46:m:113:MET:HE1  | 1.87                     | 0.56              |
| 47:n:109:ALA:HB1  | 47:n:114:LEU:HD12 | 1.88                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 50:q:46:GLY:H     | 50:q:50:LEU:HG    | 1.70                     | 0.56              |
| 56:w:18:LEU:HA    | 56:w:21:LYS:HZ2   | 1.70                     | 0.56              |
| 4:3:2121:A:H3'    | 4:3:2122:G:C8     | 2.41                     | 0.56              |
| 6:5:671:G:H2'     | 6:5:672:A:H8      | 1.71                     | 0.56              |
| 17:G:107:VAL:HG22 | 17:G:140:TYR:CD1  | 2.41                     | 0.56              |
| 18:H:125:ARG:HH11 | 18:H:125:ARG:H    | 1.53                     | 0.56              |
| 39:f:95:LYS:HD2   | 39:f:97:ILE:HD13  | 1.88                     | 0.56              |
| 44:k:99:ILE:HD13  | 44:k:104:ILE:HG23 | 1.88                     | 0.56              |
| 49:p:64:LEU:O     | 49:p:68:LEU:HD23  | 2.06                     | 0.56              |
| 56:w:86:ALA:O     | 56:w:89:GLN:HG2   | 2.05                     | 0.56              |
| 4:3:1239:G:O2'    | 4:3:1267:A:N1     | 2.33                     | 0.55              |
| 6:5:87:G:H2'      | 6:5:88:A:H8       | 1.71                     | 0.55              |
| 6:5:579:G:N1      | 6:5:756:A:OP2     | 2.27                     | 0.55              |
| 6:5:838:A:N6      | 15:E:136:LEU:O    | 2.38                     | 0.55              |
| 13:C:166:PHE:CD1  | 13:C:182:PRO:HG3  | 2.41                     | 0.55              |
| 24:N:82:LEU:HD22  | 24:N:84:LEU:HD23  | 1.87                     | 0.55              |
| 38:e:80:ILE:HG23  | 38:e:84:GLN:NE2   | 2.21                     | 0.55              |
| 6:5:134:G:O2'     | 6:5:1421:A:N3     | 2.31                     | 0.55              |
| 6:5:823:C:H1'     | 17:G:24:ASN:ND2   | 2.20                     | 0.55              |
| 12:B:108:GLU:N    | 12:B:108:GLU:OE1  | 2.39                     | 0.55              |
| 20:J:115:LYS:HG3  | 30:T:35:HIS:HB2   | 1.88                     | 0.55              |
| 53:t:3:ARG:NH1    | 53:t:74:LEU:O     | 2.39                     | 0.55              |
| 4:3:9:G:H2'       | 4:3:10:U:C6       | 2.41                     | 0.55              |
| 4:3:599:U:OP1     | 44:k:30:LYS:NZ    | 2.39                     | 0.55              |
| 6:5:1323:A:P      | 18:H:125:ARG:NH2  | 2.76                     | 0.55              |
| 8:7:19:A:H61      | 8:7:55:C:H42      | 1.54                     | 0.55              |
| 11:A:95:LEU:HD11  | 11:A:226:CYS:SG   | 2.46                     | 0.55              |
| 18:H:49:ASP:CA    | 18:H:52:GLN:HE22  | 2.19                     | 0.55              |
| 28:R:41:PHE:HD1   | 28:R:43:GLU:H     | 1.53                     | 0.55              |
| 29:S:25:LYS:NZ    | 29:S:60:ILE:HB    | 2.21                     | 0.55              |
| 35:b:228:LYS:O    | 35:b:229:ALA:C    | 2.49                     | 0.55              |
| 47:n:32:VAL:HG11  | 47:n:105:LEU:HD11 | 1.87                     | 0.55              |
| 47:n:64:ASN:ND2   | 47:n:65:GLY:H     | 2.04                     | 0.55              |
| 4:3:2181:A:H3'    | 4:3:2182:C:H6     | 1.71                     | 0.55              |
| 6:5:690:G:H5'     | 32:Y:66:U:H6      | 1.72                     | 0.55              |
| 11:A:237:ALA:HB1  | 11:A:242:MET:SD   | 2.46                     | 0.55              |
| 12:B:155:LEU:HD23 | 12:B:204:TRP:CZ3  | 2.41                     | 0.55              |
| 16:F:110:ARG:HG2  | 16:F:112:GLU:HB2  | 1.88                     | 0.55              |
| 29:S:25:LYS:NZ    | 29:S:54:LEU:HD13  | 2.20                     | 0.55              |
| 36:c:192:MET:HE1  | 44:k:3:LEU:N      | 2.22                     | 0.55              |
| 39:f:30:LEU:HD21  | 39:f:36:ALA:HB3   | 1.88                     | 0.55              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:3:427:A:HI1'   | 4:3:447:G:O4'     | 2.06                     | 0.55              |
| 4:3:1081:A:H2    | 40:g:11:VAL:HG11  | 1.72                     | 0.55              |
| 4:3:1103:G:N2    | 4:3:1130:A:O2'    | 2.39                     | 0.55              |
| 4:3:2151:G:O2'   | 4:3:2152:C:H3'    | 2.06                     | 0.55              |
| 6:5:1193:U:H2'   | 6:5:1194:A:C8     | 2.42                     | 0.55              |
| 11:A:220:HIS:ND1 | 11:A:279:SER:HA   | 2.21                     | 0.55              |
| 13:C:57:LYS:HA   | 13:C:60:MET:HE3   | 1.88                     | 0.55              |
| 15:E:50:LYS:O    | 15:E:50:LYS:HG2   | 2.07                     | 0.55              |
| 21:K:79:TYR:O    | 21:K:81:PRO:HD3   | 2.07                     | 0.55              |
| 25:O:49:LYS:HD2  | 25:O:49:LYS:O     | 2.07                     | 0.55              |
| 30:T:34:TYR:CD1  | 30:T:35:HIS:N     | 2.75                     | 0.55              |
| 53:t:93:MET:SD   | 53:t:98:ASN:HA    | 2.47                     | 0.55              |
| 4:3:648:G:O6     | 36:c:181:LYS:NZ   | 2.39                     | 0.55              |
| 4:3:1392:G:H5''  | 55:v:3:LYS:HZ1    | 1.71                     | 0.55              |
| 6:5:1000:A:HO2'  | 6:5:1029:C:HO2'   | 1.53                     | 0.55              |
| 10:9:198:LYS:HZ3 | 10:9:206:TYR:HB2  | 1.70                     | 0.55              |
| 31:X:40:ILE:HD11 | 31:X:56:TYR:HB3   | 1.88                     | 0.55              |
| 35:b:29:ILE:HD13 | 35:b:207:ILE:HD11 | 1.89                     | 0.55              |
| 40:g:43:LYS:HZ3  | 40:g:95:ALA:HB1   | 1.72                     | 0.55              |
| 45:l:39:GLY:N    | 45:l:99:GLN:OE1   | 2.31                     | 0.55              |
| 2:1:2:LYS:HG2    | 4:3:246:G:N7      | 2.21                     | 0.55              |
| 4:3:917:G:H2'    | 4:3:918:G:C8      | 2.42                     | 0.55              |
| 4:3:2628:U:OP2   | 35:b:161:LYS:NZ   | 2.40                     | 0.55              |
| 4:3:2691:C:OP1   | 48:o:56:ARG:NH1   | 2.39                     | 0.55              |
| 6:5:998:G:H5'    | 6:5:999:C:C4      | 2.42                     | 0.55              |
| 15:E:130:VAL:CG1 | 15:E:131:PRO:HD2  | 2.37                     | 0.55              |
| 27:Q:65:SER:OG   | 27:Q:69:LYS:HB3   | 2.07                     | 0.55              |
| 52:s:9:LYS:NZ    | 56:w:31:PHE:HA    | 2.22                     | 0.55              |
| 56:w:10:LYS:HG2  | 56:w:14:GLU:HG3   | 1.88                     | 0.55              |
| 4:3:620:G:H1     | 44:k:34:ARG:HH11  | 1.53                     | 0.55              |
| 4:3:1563:G:N2    | 4:3:1566:A:OP2    | 2.31                     | 0.55              |
| 4:3:2058:G:N2    | 4:3:2059:G:O6     | 2.39                     | 0.55              |
| 5:4:76:A:H62     | 5:4:88:G:H21      | 1.54                     | 0.55              |
| 6:5:231:U:H2'    | 6:5:232:G:H8      | 1.71                     | 0.55              |
| 6:5:752:G:OP1    | 24:N:59:LYS:NZ    | 2.38                     | 0.55              |
| 36:c:30:LYS:HE2  | 36:c:110:ALA:HB1  | 1.87                     | 0.55              |
| 38:e:122:LYS:HD2 | 38:e:123:GLY:N    | 2.22                     | 0.55              |
| 45:l:19:GLY:O    | 45:l:99:GLN:NE2   | 2.40                     | 0.55              |
| 4:3:749:U:H1'    | 4:3:752:C:H5      | 1.72                     | 0.55              |
| 4:3:868:C:H2'    | 4:3:869:U:C6      | 2.42                     | 0.55              |
| 4:3:2152:C:H5''  | 4:3:2153:U:H5     | 1.71                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:3:2292:A:O2'    | 4:3:2296:A:N1     | 2.34                     | 0.55              |
| 4:3:2299:U:H2'    | 4:3:2300:A:C8     | 2.42                     | 0.55              |
| 6:5:871:U:H5''    | 17:G:92:LYS:HE3   | 1.88                     | 0.55              |
| 11:A:51:HIS:HE1   | 11:A:55:HIS:CE1   | 2.25                     | 0.55              |
| 13:C:99:ASN:O     | 13:C:103:ARG:HG2  | 2.07                     | 0.55              |
| 16:F:115:MET:O    | 16:F:119:ILE:HG12 | 2.07                     | 0.55              |
| 20:J:116:PRO:HB2  | 30:T:33:GLU:C     | 2.32                     | 0.55              |
| 24:N:3:ILE:HG13   | 24:N:4:ASP:H      | 1.71                     | 0.55              |
| 30:T:4:ILE:HB     | 30:T:18:PHE:CZ    | 2.42                     | 0.55              |
| 42:i:71:LYS:HA    | 42:i:74:ASN:OD1   | 2.07                     | 0.55              |
| 43:j:71:ARG:NH2   | 43:j:104:ARG:HB3  | 2.22                     | 0.55              |
| 45:l:74:LYS:HZ1   | 45:l:94:VAL:H     | 1.55                     | 0.55              |
| 47:n:75:GLN:HB3   | 47:n:112:ARG:HH21 | 1.71                     | 0.55              |
| 52:s:23:GLU:CD    | 52:s:24:THR:H     | 2.14                     | 0.55              |
| 4:3:1805:U:OP2    | 34:a:282:ARG:NH2  | 2.40                     | 0.55              |
| 4:3:2603:G:N2     | 4:3:2606:A:OP2    | 2.30                     | 0.55              |
| 6:5:1276:U:OP2    | 22:L:21:TYR:OH    | 2.17                     | 0.55              |
| 8:7:36:C:H2'      | 8:7:37:A:H8       | 1.72                     | 0.55              |
| 10:9:166:PHE:HD2  | 10:9:168:ASN:HD21 | 1.55                     | 0.55              |
| 15:E:5:ILE:HD11   | 15:E:62:PHE:CE1   | 2.42                     | 0.55              |
| 15:E:174:TYR:CG   | 15:E:174:TYR:O    | 2.59                     | 0.55              |
| 16:F:48:LEU:O     | 16:F:51:GLN:HG3   | 2.07                     | 0.55              |
| 36:c:17:PRO:O     | 36:c:19:LYS:NZ    | 2.39                     | 0.55              |
| 38:e:150:GLU:O    | 38:e:153:LYS:NZ   | 2.37                     | 0.55              |
| 40:g:41:ARG:NH1   | 40:g:51:ILE:O     | 2.39                     | 0.55              |
| 4:3:552:C:P       | 58:y:10:LYS:HZ3   | 2.28                     | 0.54              |
| 4:3:1871:U:OP1    | 4:3:2418:G:O2'    | 2.25                     | 0.54              |
| 11:A:201:LEU:HD12 | 11:A:217:ALA:HB3  | 1.89                     | 0.54              |
| 15:E:20:GLN:OE1   | 15:E:81:GLN:HG3   | 2.07                     | 0.54              |
| 37:d:4:LEU:HB3    | 37:d:101:GLU:OE2  | 2.06                     | 0.54              |
| 39:f:39:LEU:HG    | 39:f:44:LEU:CA    | 2.35                     | 0.54              |
| 43:j:44:LYS:HE2   | 43:j:44:LYS:HA    | 1.87                     | 0.54              |
| 43:j:53:LYS:HB2   | 43:j:56:GLN:HE21  | 1.72                     | 0.54              |
| 51:r:122:LYS:HA   | 51:r:125:VAL:HG12 | 1.88                     | 0.54              |
| 54:u:82:LYS:HG2   | 54:u:84:GLN:HE21  | 1.71                     | 0.54              |
| 3:2:19:ARG:C      | 3:2:20:HIS:ND1    | 2.66                     | 0.54              |
| 4:3:518:A:H5''    | 53:t:47:LYS:HE2   | 1.88                     | 0.54              |
| 4:3:706:C:H3'     | 44:k:43:LYS:NZ    | 2.22                     | 0.54              |
| 4:3:2100:G:O2'    | 39:f:25:TYR:HA    | 2.07                     | 0.54              |
| 6:5:250:G:H2'     | 6:5:251:G:H8      | 1.72                     | 0.54              |
| 6:5:836:C:H1'     | 15:E:145:ARG:HG2  | 1.90                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 13:C:137:ASN:OD1  | 13:C:138:PRO:HD2  | 2.06                     | 0.54              |
| 26:P:22:ALA:H     | 26:P:46:GLN:NE2   | 2.05                     | 0.54              |
| 45:l:72:MET:O     | 45:l:74:LYS:NZ    | 2.39                     | 0.54              |
| 49:p:32:LYS:O     | 49:p:35:LYS:HG3   | 2.07                     | 0.54              |
| 4:3:87:G:O2'      | 4:3:104:A:N1      | 2.29                     | 0.54              |
| 4:3:742:G:H1      | 4:3:759:U:H3      | 1.56                     | 0.54              |
| 4:3:1111:C:H2'    | 4:3:1112:A:O4'    | 2.06                     | 0.54              |
| 4:3:1262:G:H2'    | 4:3:1263:G:H8     | 1.71                     | 0.54              |
| 4:3:1392:G:N2     | 4:3:1395:A:OP2    | 2.32                     | 0.54              |
| 4:3:2477:A:H5''   | 45:l:56:LYS:NZ    | 2.23                     | 0.54              |
| 5:4:55:A:O4'      | 37:d:27:GLN:NE2   | 2.36                     | 0.54              |
| 11:A:285:THR:HG23 | 11:A:286:ARG:HD2  | 1.88                     | 0.54              |
| 18:H:12:ARG:HH22  | 18:H:111:ARG:HH21 | 1.53                     | 0.54              |
| 19:I:14:ILE:HG22  | 19:I:80:MET:O     | 2.08                     | 0.54              |
| 30:T:27:ARG:HE    | 30:T:30:GLN:NE2   | 2.00                     | 0.54              |
| 35:b:22:GLU:HG3   | 43:j:72:LYS:HD3   | 1.89                     | 0.54              |
| 39:f:2:LYS:HZ3    | 39:f:20:ASP:HB2   | 1.72                     | 0.54              |
| 58:y:46:GLY:O     | 58:y:47:MET:HE2   | 2.07                     | 0.54              |
| 2:1:54:ARG:HH22   | 44:k:52:GLU:HG2   | 1.71                     | 0.54              |
| 4:3:2111:U:H5''   | 4:3:2112:A:C8     | 2.43                     | 0.54              |
| 4:3:2291:U:H5''   | 59:z:5:ARG:HH21   | 1.71                     | 0.54              |
| 6:5:305:A:O2'     | 6:5:605:A:N1      | 2.39                     | 0.54              |
| 6:5:354:U:H2'     | 6:5:355:A:H8      | 1.72                     | 0.54              |
| 6:5:689:U:O2'     | 6:5:691:A:N7      | 2.32                     | 0.54              |
| 6:5:1096:A:H2'    | 6:5:1097:G:H8     | 1.73                     | 0.54              |
| 6:5:1115:G:H1'    | 6:5:1116:U:H5     | 1.73                     | 0.54              |
| 6:5:1433:G:H5''   | 29:S:22:LYS:NZ    | 2.22                     | 0.54              |
| 49:p:20:ALA:HB2   | 49:p:38:VAL:HG23  | 1.90                     | 0.54              |
| 52:s:87:LYS:HE3   | 56:w:89:GLN:HG3   | 1.89                     | 0.54              |
| 54:u:44:MET:N     | 54:u:44:MET:SD    | 2.80                     | 0.54              |
| 56:w:45:ASN:OD1   | 56:w:46:GLN:N     | 2.40                     | 0.54              |
| 4:3:1245:G:H1     | 4:3:1264:U:H3     | 1.55                     | 0.54              |
| 4:3:1696:C:O2'    | 4:3:2695:U:OP1    | 2.25                     | 0.54              |
| 4:3:2098:U:O2     | 55:v:34:GLN:NE2   | 2.40                     | 0.54              |
| 4:3:2854:A:N7     | 4:3:2872:A:O2'    | 2.31                     | 0.54              |
| 6:5:460:A:H2'     | 6:5:461:G:C8      | 2.42                     | 0.54              |
| 6:5:530:A:N6      | 6:5:1181:G:O2'    | 2.40                     | 0.54              |
| 6:5:1351:U:H2'    | 6:5:1352:A:C8     | 2.43                     | 0.54              |
| 12:B:151:GLY:HA3  | 12:B:176:MET:HE3  | 1.89                     | 0.54              |
| 23:M:53:ILE:HD12  | 23:M:56:VAL:HG21  | 1.89                     | 0.54              |
| 39:f:96:GLN:NE2   | 39:f:117:VAL:HG21 | 2.23                     | 0.54              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 53:t:90:LYS:N    | 53:t:103:VAL:O    | 2.34                     | 0.54              |
| 56:w:107:ASP:HA  | 56:w:110:LYS:HG2  | 1.88                     | 0.54              |
| 4:3:1920:A:C8    | 6:5:1469:G:H4'    | 2.41                     | 0.54              |
| 5:4:47:C:H5'     | 47:n:67:LYS:NZ    | 2.22                     | 0.54              |
| 11:A:41:MET:HE3  | 11:A:208:PRO:HD3  | 1.89                     | 0.54              |
| 17:G:54:LEU:HD21 | 17:G:72:PHE:HB2   | 1.89                     | 0.54              |
| 27:Q:83:GLN:HA   | 27:Q:86:VAL:HG22  | 1.90                     | 0.54              |
| 41:h:42:LYS:HG3  | 41:h:67:LEU:HD11  | 1.90                     | 0.54              |
| 52:s:9:LYS:CE    | 56:w:34:ALA:HB3   | 2.38                     | 0.54              |
| 58:y:41:ARG:HH21 | 58:y:42:VAL:CG2   | 2.17                     | 0.54              |
| 4:3:1825:U:OP2   | 34:a:162:ARG:NH2  | 2.41                     | 0.54              |
| 4:3:2299:U:H2'   | 4:3:2300:A:H8     | 1.73                     | 0.54              |
| 6:5:369:A:H61    | 6:5:387:G:H1'     | 1.73                     | 0.54              |
| 6:5:1102:A:N1    | 12:B:180:THR:HG22 | 2.23                     | 0.54              |
| 12:B:170:MET:O   | 12:B:171:TYR:CD1  | 2.61                     | 0.54              |
| 13:C:64:TYR:HD1  | 13:C:110:ARG:NH1  | 2.06                     | 0.54              |
| 16:F:15:PRO:HG3  | 18:H:45:LEU:HD13  | 1.89                     | 0.54              |
| 36:c:32:GLN:NE2  | 44:k:9:VAL:H      | 2.06                     | 0.54              |
| 45:l:64:MET:HE1  | 45:l:66:ILE:HG13  | 1.88                     | 0.54              |
| 46:m:36:LYS:HA   | 46:m:39:LYS:HD3   | 1.90                     | 0.54              |
| 58:y:13:ARG:HD2  | 58:y:17:ARG:NH2   | 2.23                     | 0.54              |
| 4:3:1529:U:H2'   | 4:3:1530:G:H8     | 1.73                     | 0.54              |
| 4:3:2689:C:OP2   | 35:b:115:LYS:NZ   | 2.41                     | 0.54              |
| 6:5:929:C:O2'    | 6:5:1318:C:OP2    | 2.16                     | 0.54              |
| 6:5:1279:G:H21   | 6:5:1306:A:H2     | 1.54                     | 0.54              |
| 13:C:106:PHE:HD1 | 13:C:157:ALA:HB1  | 1.72                     | 0.54              |
| 14:D:96:ASN:ND2  | 14:D:98:LYS:HG2   | 2.23                     | 0.54              |
| 21:K:90:HIS:ND1  | 21:K:90:HIS:O     | 2.40                     | 0.54              |
| 22:L:13:LYS:HE2  | 22:L:21:TYR:CD2   | 2.42                     | 0.54              |
| 25:O:40:ASN:O    | 25:O:47:LYS:HG2   | 2.08                     | 0.54              |
| 28:R:68:GLY:HA2  | 57:x:66:PHE:HZ    | 1.73                     | 0.54              |
| 35:b:50:THR:OG1  | 35:b:87:MET:O     | 2.21                     | 0.54              |
| 37:d:128:TYR:HB3 | 37:d:156:LEU:HB2  | 1.90                     | 0.54              |
| 38:e:15:LYS:NZ   | 38:e:29:GLY:O     | 2.36                     | 0.54              |
| 39:f:71:VAL:HG11 | 39:f:108:LEU:HB2  | 1.90                     | 0.54              |
| 39:f:130:ILE:HB  | 39:f:142:VAL:HB   | 1.89                     | 0.54              |
| 4:3:2181:A:H3'   | 4:3:2182:C:C6     | 2.42                     | 0.54              |
| 6:5:68:C:H2'     | 6:5:69:G:C8       | 2.43                     | 0.54              |
| 6:5:1019:G:O2'   | 6:5:1020:G:OP2    | 2.21                     | 0.54              |
| 15:E:132:VAL:C   | 15:E:134:SER:N    | 2.64                     | 0.54              |
| 18:H:124:ARG:HD3 | 18:H:125:ARG:HH12 | 1.72                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 26:P:29:ARG:HG2   | 26:P:38:SER:HB3   | 1.90                     | 0.54              |
| 42:i:109:LYS:O    | 42:i:109:LYS:HD3  | 2.08                     | 0.54              |
| 45:l:73:SER:O     | 45:l:74:LYS:HD3   | 2.07                     | 0.54              |
| 47:n:68:ASP:OD1   | 47:n:69:ASN:N     | 2.40                     | 0.54              |
| 49:p:104:LYS:HZ3  | 50:q:43:GLU:HA    | 1.72                     | 0.54              |
| 53:t:52:THR:H     | 53:t:55:ALA:HB3   | 1.72                     | 0.54              |
| 57:x:73:LEU:O     | 57:x:76:LYS:HG2   | 2.07                     | 0.54              |
| 4:3:622:U:H2'     | 4:3:623:A:H8      | 1.73                     | 0.54              |
| 4:3:1124:G:N2     | 4:3:1125:U:O4     | 2.41                     | 0.54              |
| 4:3:1393:A:H4'    | 55:v:4:LYS:NZ     | 2.23                     | 0.54              |
| 4:3:2167:G:H2'    | 4:3:2168:C:C6     | 2.43                     | 0.54              |
| 4:3:2235:A:H5''   | 34:a:271:LYS:NZ   | 2.23                     | 0.54              |
| 12:B:158:GLY:HA3  | 12:B:199:ILE:HD13 | 1.88                     | 0.54              |
| 16:F:115:MET:CA   | 16:F:118:LYS:HB2  | 2.31                     | 0.54              |
| 19:I:16:LEU:HD13  | 19:I:80:MET:HE2   | 1.89                     | 0.54              |
| 20:J:62:LYS:HG2   | 20:J:65:LYS:HE3   | 1.90                     | 0.54              |
| 22:L:88:GLY:O     | 22:L:92:ARG:HB2   | 2.08                     | 0.54              |
| 31:X:45:LYS:HZ3   | 31:X:46:GLY:H     | 1.54                     | 0.54              |
| 37:d:31:LEU:HD23  | 37:d:96:MET:HE1   | 1.88                     | 0.54              |
| 43:j:87:ILE:O     | 43:j:94:ARG:NH2   | 2.38                     | 0.54              |
| 48:o:23:PRO:HB2   | 48:o:90:LEU:HD23  | 1.90                     | 0.54              |
| 55:v:10:ARG:HH12  | 55:v:53:ARG:NH2   | 2.02                     | 0.54              |
| 4:3:141:A:C2      | 4:3:1437:A:H1'    | 2.43                     | 0.53              |
| 4:3:672:G:OP1     | 44:k:133:LYS:NZ   | 2.35                     | 0.53              |
| 4:3:2166:U:C2     | 4:3:2167:G:H1'    | 2.42                     | 0.53              |
| 4:3:2813:A:H61    | 4:3:2894:G:H2'    | 1.73                     | 0.53              |
| 11:A:14:LYS:HD2   | 11:A:14:LYS:O     | 2.07                     | 0.53              |
| 11:A:178:VAL:HG13 | 11:A:184:GLU:HG3  | 1.90                     | 0.53              |
| 13:C:97:LEU:HD21  | 13:C:132:PRO:HA   | 1.88                     | 0.53              |
| 35:b:180:ARG:HH22 | 35:b:218:LYS:CE   | 2.15                     | 0.53              |
| 39:f:87:ARG:HB3   | 39:f:88:PRO:HD3   | 1.90                     | 0.53              |
| 57:x:14:PHE:O     | 57:x:22:SER:HA    | 2.08                     | 0.53              |
| 6:5:192:A:H2'     | 6:5:193:G:H8      | 1.73                     | 0.53              |
| 6:5:808:C:O2'     | 6:5:895:A:N1      | 2.40                     | 0.53              |
| 6:5:1126:U:O4     | 6:5:1127:A:N6     | 2.42                     | 0.53              |
| 11:A:201:LEU:O    | 11:A:219:ASN:ND2  | 2.27                     | 0.53              |
| 11:A:222:PRO:HD2  | 11:A:277:ILE:HD11 | 1.89                     | 0.53              |
| 11:A:228:LEU:HD12 | 11:A:229:MET:N    | 2.23                     | 0.53              |
| 14:D:212:ARG:NH2  | 17:G:50:LYS:O     | 2.41                     | 0.53              |
| 20:J:117:PRO:O    | 30:T:34:TYR:HA    | 2.08                     | 0.53              |
| 35:b:150:GLY:HA3  | 35:b:155:SER:HB3  | 1.89                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 39:f:26:ALA:HB1   | 39:f:29:PHE:C     | 2.33                     | 0.53              |
| 46:m:44:ARG:HD3   | 46:m:66:TRP:CD1   | 2.43                     | 0.53              |
| 47:n:71:LYS:HE3   | 47:n:104:ALA:HB1  | 1.90                     | 0.53              |
| 48:o:19:LYS:HG3   | 48:o:82:HIS:ND1   | 2.23                     | 0.53              |
| 56:w:77:LYS:HG2   | 56:w:78:LYS:H     | 1.73                     | 0.53              |
| 4:3:2068:G:N3     | 4:3:2069:A:N6     | 2.56                     | 0.53              |
| 6:5:190:A:H2'     | 6:5:191:A:H8      | 1.73                     | 0.53              |
| 6:5:398:G:OP1     | 13:C:70:GLN:HG3   | 2.08                     | 0.53              |
| 6:5:839:U:H3'     | 6:5:840:C:H6      | 1.73                     | 0.53              |
| 37:d:117:LEU:N    | 37:d:177:LEU:HD12 | 2.20                     | 0.53              |
| 40:g:43:LYS:NZ    | 40:g:95:ALA:HB1   | 2.23                     | 0.53              |
| 48:o:117:ARG:NH1  | 48:o:118:LYS:O    | 2.41                     | 0.53              |
| 51:r:75:VAL:O     | 51:r:103:LEU:HD12 | 2.09                     | 0.53              |
| 4:3:1311:G:N2     | 4:3:1313:G:H3'    | 2.23                     | 0.53              |
| 4:3:1447:A:O2'    | 4:3:1449:G:N7     | 2.33                     | 0.53              |
| 4:3:2819:C:H4'    | 58:y:25:GLN:HE22  | 1.73                     | 0.53              |
| 4:3:2863:G:H2'    | 4:3:2864:A:C8     | 2.43                     | 0.53              |
| 6:5:731:A:HO2'    | 27:Q:95:TYR:HH    | 1.30                     | 0.53              |
| 6:5:733:A:H2'     | 6:5:734:A:H8      | 1.74                     | 0.53              |
| 6:5:1320:A:H2     | 6:5:1350:A:H62    | 1.56                     | 0.53              |
| 11:A:214:ILE:HG13 | 15:E:174:TYR:OH   | 2.08                     | 0.53              |
| 11:A:260:GLN:OE1  | 11:A:261:LYS:HG2  | 2.09                     | 0.53              |
| 18:H:49:ASP:O     | 18:H:52:GLN:NE2   | 2.41                     | 0.53              |
| 27:Q:57:LEU:O     | 27:Q:60:LEU:HG    | 2.08                     | 0.53              |
| 40:g:46:LYS:HG2   | 40:g:48:GLY:H     | 1.73                     | 0.53              |
| 48:o:38:LYS:HG2   | 48:o:43:VAL:HG22  | 1.89                     | 0.53              |
| 4:3:1306:G:H2'    | 4:3:1307:G:H8     | 1.73                     | 0.53              |
| 4:3:2278:G:O2'    | 54:u:34:ARG:NH1   | 2.42                     | 0.53              |
| 4:3:2492:G:O2'    | 45:l:124:LYS:O    | 2.27                     | 0.53              |
| 6:5:172:C:O2'     | 29:S:48:TYR:OH    | 2.20                     | 0.53              |
| 6:5:590:G:H1      | 6:5:644:U:H3      | 1.57                     | 0.53              |
| 6:5:836:C:O3'     | 15:E:144:SER:OG   | 2.16                     | 0.53              |
| 7:6:25:C:H42      | 7:6:45:G:N2       | 2.06                     | 0.53              |
| 12:B:39:LYS:NZ    | 12:B:95:ILE:HG13  | 2.23                     | 0.53              |
| 12:B:113:MET:HG2  | 12:B:114:LEU:N    | 2.23                     | 0.53              |
| 15:E:81:GLN:OE1   | 15:E:81:GLN:N     | 2.39                     | 0.53              |
| 15:E:89:ASN:OD1   | 15:E:91:GLU:HG3   | 2.08                     | 0.53              |
| 15:E:143:LEU:H    | 15:E:143:LEU:HD12 | 1.73                     | 0.53              |
| 15:E:157:TRP:NE1  | 17:G:69:ILE:HG12  | 2.24                     | 0.53              |
| 17:G:61:GLU:OE1   | 17:G:68:ARG:NH1   | 2.41                     | 0.53              |
| 25:O:83:VAL:O     | 25:O:86:LYS:HG2   | 2.07                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 26:P:28:SER:CB    | 26:P:41:ARG:HE    | 2.20                     | 0.53              |
| 34:a:4:LYS:NZ     | 34:a:21:ASP:HA    | 2.24                     | 0.53              |
| 38:e:142:GLU:OE1  | 38:e:142:GLU:N    | 2.39                     | 0.53              |
| 43:j:65:THR:O     | 43:j:79:PHE:HB2   | 2.09                     | 0.53              |
| 43:j:90:ASP:O     | 43:j:91:LYS:HB2   | 2.08                     | 0.53              |
| 44:k:52:GLU:OE1   | 44:k:57:PRO:HA    | 2.08                     | 0.53              |
| 45:l:112:SER:O    | 45:l:116:LYS:HG2  | 2.08                     | 0.53              |
| 53:t:70:PHE:HD2   | 53:t:73:LYS:HZ1   | 1.54                     | 0.53              |
| 4:3:1588:A:H2'    | 4:3:1589:A:C8     | 2.43                     | 0.53              |
| 4:3:1844:C:O2'    | 4:3:1934:A:N3     | 2.39                     | 0.53              |
| 4:3:2313:U:H3     | 37:d:38:MET:HE1   | 1.73                     | 0.53              |
| 4:3:2394:A:O2'    | 54:u:70:ASP:OD1   | 2.24                     | 0.53              |
| 4:3:2427:U:H5''   | 59:z:20:LEU:HD22  | 1.90                     | 0.53              |
| 6:5:181:G:O2'     | 26:P:3:ARG:NH1    | 2.41                     | 0.53              |
| 29:S:44:LEU:HD13  | 29:S:76:LEU:HD22  | 1.89                     | 0.53              |
| 4:3:892:G:H2'     | 4:3:893:A:H8      | 1.72                     | 0.53              |
| 4:3:1805:U:O2'    | 4:3:1809:A:N3     | 2.41                     | 0.53              |
| 4:3:2057:C:O2'    | 35:b:144:GLN:NE2  | 2.41                     | 0.53              |
| 6:5:250:G:H2'     | 6:5:251:G:C8      | 2.44                     | 0.53              |
| 6:5:1316:C:H2'    | 6:5:1317:A:C8     | 2.43                     | 0.53              |
| 19:I:57:ILE:HD12  | 23:M:41:ARG:HB2   | 1.90                     | 0.53              |
| 24:N:33:ILE:O     | 24:N:37:THR:HG23  | 2.08                     | 0.53              |
| 36:c:197:LEU:HD13 | 36:c:199:VAL:HG23 | 1.89                     | 0.53              |
| 37:d:40:VAL:HG22  | 37:d:42:ASP:H     | 1.73                     | 0.53              |
| 40:g:54:ILE:HG21  | 40:g:59:LEU:HD12  | 1.90                     | 0.53              |
| 40:g:63:LEU:HD11  | 40:g:71:ILE:HB    | 1.90                     | 0.53              |
| 44:k:90:LEU:HD11  | 44:k:97:SER:HB3   | 1.90                     | 0.53              |
| 49:p:104:LYS:NZ   | 50:q:43:GLU:HA    | 2.24                     | 0.53              |
| 52:s:60:ARG:HB2   | 52:s:78:GLU:CD    | 2.33                     | 0.53              |
| 1:0:41:GLN:NE2    | 1:0:47:GLU:O      | 2.40                     | 0.53              |
| 4:3:597:C:O2'     | 4:3:1282:G:O6     | 2.27                     | 0.53              |
| 4:3:1456:C:C5     | 4:3:1603:A:H5''   | 2.44                     | 0.53              |
| 4:3:2164:G:HO2'   | 4:3:2165:A:H8     | 1.56                     | 0.53              |
| 12:B:49:ARG:HG3   | 12:B:121:ARG:HE   | 1.73                     | 0.53              |
| 22:L:57:ARG:NH1   | 57:x:37:ASP:OD2   | 2.41                     | 0.53              |
| 22:L:118:ASN:HA   | 28:R:86:ASN:HD21  | 1.73                     | 0.53              |
| 26:P:53:VAL:O     | 26:P:55:ALA:N     | 2.42                     | 0.53              |
| 26:P:58:GLY:HA3   | 26:P:85:LYS:HB3   | 1.91                     | 0.53              |
| 44:k:48:ARG:HG2   | 44:k:49:PRO:HD2   | 1.91                     | 0.53              |
| 45:l:110:PRO:HG2  | 45:l:113:GLN:OE1  | 2.09                     | 0.53              |
| 49:p:81:LEU:HA    | 49:p:84:LYS:HG2   | 1.91                     | 0.53              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:3:98:C:OP1     | 56:w:40:LYS:NZ    | 2.42                     | 0.53              |
| 4:3:728:A:O2'    | 4:3:1381:A:N3     | 2.42                     | 0.53              |
| 4:3:1414:C:H2'   | 4:3:1415:A:H8     | 1.74                     | 0.53              |
| 6:5:195:U:H2'    | 6:5:196:G:H8      | 1.74                     | 0.53              |
| 6:5:661:G:O2'    | 6:5:722:G:O2'     | 2.21                     | 0.53              |
| 6:5:1505:G:O6    | 30:T:43:ARG:NH2   | 2.37                     | 0.53              |
| 6:5:1509:A:H5''  | 6:5:1510:C:H5''   | 1.90                     | 0.53              |
| 11:A:85:VAL:HG21 | 11:A:112:TRP:HE3  | 1.74                     | 0.53              |
| 16:F:152:HIS:HB2 | 20:J:54:TYR:OH    | 2.09                     | 0.53              |
| 21:K:49:ARG:NH2  | 21:K:77:LEU:HD21  | 2.24                     | 0.53              |
| 30:T:20:ARG:O    | 30:T:23:LEU:HG    | 2.08                     | 0.53              |
| 35:b:14:SER:O    | 35:b:26:ILE:N     | 2.25                     | 0.53              |
| 37:d:11:THR:O    | 37:d:15:GLU:HG3   | 2.09                     | 0.53              |
| 39:f:100:GLN:HA  | 39:f:103:THR:HG23 | 1.90                     | 0.53              |
| 40:g:119:ASN:H   | 40:g:122:ASP:HB2  | 1.74                     | 0.53              |
| 55:v:10:ARG:NH1  | 55:v:53:ARG:HH21  | 2.01                     | 0.53              |
| 58:y:47:MET:HE1  | 58:y:52:ARG:HD3   | 1.91                     | 0.53              |
| 4:3:333:A:N3     | 4:3:353:G:O2'     | 2.38                     | 0.53              |
| 4:3:924:C:H3'    | 22:L:92:ARG:HH11  | 1.73                     | 0.53              |
| 4:3:1137:C:H2'   | 4:3:1138:A:C8     | 2.41                     | 0.53              |
| 4:3:2207:A:N1    | 4:3:2234:C:N4     | 2.57                     | 0.53              |
| 8:7:26:A:N1      | 8:7:44:G:N2       | 2.56                     | 0.53              |
| 14:D:177:ASP:N   | 14:D:177:ASP:OD1  | 2.41                     | 0.53              |
| 17:G:18:LEU:HD12 | 17:G:44:ILE:HD11  | 1.91                     | 0.53              |
| 17:G:47:ILE:HD11 | 17:G:115:ILE:HG13 | 1.91                     | 0.53              |
| 25:O:38:HIS:H    | 25:O:49:LYS:HE3   | 1.73                     | 0.53              |
| 35:b:229:ALA:HB2 | 48:o:20:ALA:CB    | 2.36                     | 0.53              |
| 40:g:25:VAL:HA   | 40:g:111:GLY:HA3  | 1.90                     | 0.53              |
| 47:n:47:SER:OG   | 47:n:48:GLN:OE1   | 2.24                     | 0.53              |
| 50:q:65:GLN:O    | 50:q:86:ARG:NH2   | 2.42                     | 0.53              |
| 53:t:77:PHE:O    | 53:t:79:GLN:NE2   | 2.41                     | 0.53              |
| 4:3:196:G:O2'    | 4:3:712:A:N1      | 2.41                     | 0.52              |
| 4:3:275:A:H61    | 4:3:294:G:H1'     | 1.74                     | 0.52              |
| 4:3:615:G:H2'    | 4:3:616:G:C8      | 2.44                     | 0.52              |
| 4:3:880:C:H41    | 4:3:968:U:H2'     | 1.74                     | 0.52              |
| 4:3:892:G:H5''   | 54:u:83:TYR:CZ    | 2.44                     | 0.52              |
| 4:3:1076:U:H3    | 4:3:1149:G:H1     | 1.56                     | 0.52              |
| 4:3:2794:U:H2'   | 4:3:2795:C:C6     | 2.43                     | 0.52              |
| 6:5:133:G:H2'    | 6:5:134:G:C8      | 2.43                     | 0.52              |
| 6:5:1092:A:H61   | 11:A:118:THR:HG21 | 1.74                     | 0.52              |
| 15:E:32:VAL:HG23 | 15:E:62:PHE:CD2   | 2.44                     | 0.52              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 20:J:16:VAL:O    | 20:J:80:LYS:N     | 2.41                     | 0.52              |
| 39:f:39:LEU:HD12 | 39:f:47:ARG:CB    | 2.37                     | 0.52              |
| 42:i:63:ASP:OD1  | 42:i:63:ASP:N     | 2.41                     | 0.52              |
| 4:3:733:C:O2'    | 4:3:769:A:N6      | 2.41                     | 0.52              |
| 6:5:516:C:H4'    | 6:5:517:C:H5''    | 1.90                     | 0.52              |
| 6:5:1261:A:H2'   | 6:5:1262:A:C8     | 2.45                     | 0.52              |
| 13:C:43:ARG:O    | 13:C:43:ARG:HD3   | 2.09                     | 0.52              |
| 15:E:115:TYR:CZ  | 15:E:119:ILE:HD11 | 2.44                     | 0.52              |
| 15:E:170:GLN:HG2 | 17:G:78:GLN:HE22  | 1.74                     | 0.52              |
| 27:Q:73:ARG:NH2  | 27:Q:80:GLN:HA    | 2.24                     | 0.52              |
| 37:d:128:TYR:O   | 37:d:156:LEU:N    | 2.40                     | 0.52              |
| 39:f:68:LEU:HG   | 39:f:114:LYS:HZ2  | 1.74                     | 0.52              |
| 40:g:50:LYS:HD3  | 40:g:52:LYS:HG2   | 1.90                     | 0.52              |
| 4:3:77:G:C2'     | 56:w:49:ARG:HH21  | 2.20                     | 0.52              |
| 4:3:2362:A:P     | 54:u:46:ARG:HH21  | 2.33                     | 0.52              |
| 4:3:2887:A:H5'   | 4:3:2888:U:H5'    | 1.91                     | 0.52              |
| 6:5:732:A:H2'    | 6:5:733:A:H8      | 1.74                     | 0.52              |
| 6:5:1400:A:H2'   | 6:5:1401:A:C8     | 2.45                     | 0.52              |
| 15:E:182:ASN:HB3 | 15:E:185:HIS:CE1  | 2.44                     | 0.52              |
| 30:T:19:LYS:NZ   | 32:Y:60:G:OP1     | 2.39                     | 0.52              |
| 30:T:27:ARG:NE   | 30:T:30:GLN:HE22  | 2.00                     | 0.52              |
| 37:d:12:ILE:HG23 | 37:d:16:LEU:HD23  | 1.91                     | 0.52              |
| 37:d:111:VAL:HB  | 37:d:114:PHE:HB3  | 1.91                     | 0.52              |
| 39:f:56:GLU:O    | 39:f:60:ILE:HG23  | 2.09                     | 0.52              |
| 4:3:316:C:H2'    | 4:3:392:A:H61     | 1.73                     | 0.52              |
| 4:3:894:G:N3     | 4:3:2276:A:H2'    | 2.25                     | 0.52              |
| 4:3:1306:G:H4'   | 46:m:31:ILE:HD12  | 1.91                     | 0.52              |
| 4:3:2254:G:H2'   | 4:3:2255:A:H8     | 1.75                     | 0.52              |
| 6:5:487:A:O2'    | 6:5:488:U:O3'     | 2.28                     | 0.52              |
| 6:5:1022:G:O2'   | 6:5:1023:G:O4'    | 2.28                     | 0.52              |
| 13:C:81:GLN:OE1  | 13:C:88:ASN:ND2   | 2.43                     | 0.52              |
| 19:I:47:PRO:HA   | 19:I:78:ARG:HD2   | 1.90                     | 0.52              |
| 20:J:102:GLU:OE2 | 30:T:3:LYS:HD2    | 2.10                     | 0.52              |
| 21:K:30:LEU:HA   | 21:K:33:LYS:HE2   | 1.92                     | 0.52              |
| 34:a:2:PRO:HD2   | 34:a:24:LYS:HZ1   | 1.75                     | 0.52              |
| 36:c:194:ALA:C   | 36:c:196:ALA:H    | 2.17                     | 0.52              |
| 39:f:95:LYS:HZ3  | 39:f:97:ILE:HB    | 1.75                     | 0.52              |
| 46:m:90:TYR:HB3  | 46:m:97:TYR:CE1   | 2.44                     | 0.52              |
| 53:t:70:PHE:HB2  | 53:t:73:LYS:NZ    | 2.24                     | 0.52              |
| 59:z:25:VAL:HG23 | 59:z:26:LYS:HD3   | 1.91                     | 0.52              |
| 4:3:411:U:H2'    | 4:3:412:A:H8      | 1.74                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:3:1414:C:H2'    | 4:3:1415:A:C8     | 2.45                     | 0.52              |
| 6:5:662:G:H1'     | 6:5:730:G:H5'     | 1.91                     | 0.52              |
| 6:5:922:G:H1      | 6:5:1365:U:H3     | 1.58                     | 0.52              |
| 8:7:34:G:H1       | 32:Y:72:U:H3      | 1.56                     | 0.52              |
| 9:8:40:C:H2'      | 9:8:41:A:C8       | 2.45                     | 0.52              |
| 10:9:67:HIS:ND1   | 10:9:68:SER:O     | 2.41                     | 0.52              |
| 11:A:68:ALA:HB2   | 11:A:215:ILE:HD11 | 1.90                     | 0.52              |
| 12:B:90:LYS:HA    | 12:B:93:LYS:HE2   | 1.91                     | 0.52              |
| 13:C:199:TRP:CE3  | 13:C:202:ARG:NH1  | 2.77                     | 0.52              |
| 18:H:42:PRO:HG2   | 18:H:46:VAL:HG11  | 1.90                     | 0.52              |
| 20:J:22:ASN:OD1   | 20:J:23:THR:N     | 2.39                     | 0.52              |
| 36:c:20:LEU:HD11  | 36:c:24:LEU:HD22  | 1.90                     | 0.52              |
| 44:k:90:LEU:HD22  | 44:k:93:ILE:HG13  | 1.91                     | 0.52              |
| 44:k:97:SER:O     | 44:k:100:GLU:HG2  | 2.09                     | 0.52              |
| 4:3:180:A:H5'     | 4:3:181:G:C8      | 2.44                     | 0.52              |
| 4:3:593:C:O2'     | 49:p:47:ARG:NH1   | 2.42                     | 0.52              |
| 4:3:1098:G:O2'    | 41:h:84:LYS:NZ    | 2.43                     | 0.52              |
| 4:3:1350:A:OP1    | 51:r:9:ARG:NH2    | 2.34                     | 0.52              |
| 4:3:2182:C:O2'    | 10:9:216:MET:HE1  | 2.10                     | 0.52              |
| 4:3:2188:U:H2'    | 4:3:2189:U:O4'    | 2.10                     | 0.52              |
| 5:4:11:A:H2'      | 5:4:12:U:H5''     | 1.90                     | 0.52              |
| 11:A:280:GLN:HG2  | 11:A:282:LEU:HG   | 1.92                     | 0.52              |
| 28:R:11:VAL:HG12  | 28:R:38:SER:HB3   | 1.92                     | 0.52              |
| 44:k:61:ARG:HG2   | 44:k:61:ARG:HH11  | 1.75                     | 0.52              |
| 54:u:59:VAL:HA    | 54:u:93:THR:HG23  | 1.92                     | 0.52              |
| 1:0:38:GLN:HG2    | 4:3:494:G:H5''    | 1.91                     | 0.52              |
| 4:3:629:G:H1      | 4:3:696:U:H3      | 1.55                     | 0.52              |
| 4:3:2028:G:OP1    | 58:y:9:SER:OG     | 2.21                     | 0.52              |
| 6:5:971:A:H5'     | 23:M:31:ARG:CZ    | 2.40                     | 0.52              |
| 14:D:131:ILE:HG22 | 14:D:175:TYR:CE1  | 2.45                     | 0.52              |
| 14:D:154:ALA:HB1  | 14:D:158:THR:HG21 | 1.90                     | 0.52              |
| 15:E:118:ILE:O    | 15:E:121:ARG:HB2  | 2.09                     | 0.52              |
| 27:Q:85:HIS:O     | 27:Q:88:LYS:HG2   | 2.09                     | 0.52              |
| 28:R:69:HIS:HB2   | 28:R:74:PHE:CZ    | 2.45                     | 0.52              |
| 49:p:9:THR:HA     | 49:p:12:ARG:NE    | 2.25                     | 0.52              |
| 52:s:58:LEU:HB2   | 52:s:80:LEU:HB2   | 1.91                     | 0.52              |
| 4:3:299:A:H2'     | 4:3:300:G:H8      | 1.75                     | 0.52              |
| 4:3:2279:G:P      | 54:u:34:ARG:HH12  | 2.31                     | 0.52              |
| 4:3:2548:G:O2'    | 4:3:2748:A:N3     | 2.40                     | 0.52              |
| 4:3:2797:C:H5'    | 4:3:2798:A:O5'    | 2.10                     | 0.52              |
| 6:5:822:A:H5''    | 17:G:9:LYS:CD     | 2.40                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:5:1078:G:H5'    | 6:5:1078:G:H8     | 1.74                     | 0.52              |
| 11:A:77:GLN:NE2   | 11:A:78:ASN:HB2   | 2.25                     | 0.52              |
| 12:B:9:GLY:HA2    | 12:B:12:PHE:HD2   | 1.75                     | 0.52              |
| 13:C:26:SER:OG    | 13:C:27:LYS:N     | 2.43                     | 0.52              |
| 14:D:132:HIS:CE1  | 14:D:137:TYR:HB2  | 2.45                     | 0.52              |
| 16:F:98:LEU:HD23  | 16:F:101:ARG:HH11 | 1.73                     | 0.52              |
| 17:G:115:ILE:HG22 | 17:G:139:ALA:O    | 2.08                     | 0.52              |
| 29:S:38:GLU:O     | 29:S:38:GLU:HG2   | 2.10                     | 0.52              |
| 46:m:19:ARG:NH1   | 46:m:65:LYS:O     | 2.43                     | 0.52              |
| 49:p:89:ILE:HG12  | 50:q:39:LEU:HD13  | 1.91                     | 0.52              |
| 4:3:632:A:H2'     | 4:3:633:G:H8      | 1.75                     | 0.52              |
| 4:3:1831:G:OP1    | 34:a:56:ARG:NE    | 2.43                     | 0.52              |
| 4:3:2736:U:O2'    | 4:3:2737:G:H8     | 1.93                     | 0.52              |
| 6:5:265:U:H2'     | 6:5:266:A:C8      | 2.45                     | 0.52              |
| 6:5:923:G:O2'     | 6:5:1508:C:OP1    | 2.28                     | 0.52              |
| 11:A:70:ASN:O     | 11:A:73:LYS:HG2   | 2.10                     | 0.52              |
| 11:A:209:GLU:OE1  | 11:A:210:LEU:HD23 | 2.09                     | 0.52              |
| 12:B:46:VAL:HG23  | 12:B:47:ASN:N     | 2.24                     | 0.52              |
| 15:E:25:GLN:NE2   | 15:E:35:LEU:HD13  | 2.25                     | 0.52              |
| 19:I:49:PRO:O     | 19:I:77:LYS:NZ    | 2.41                     | 0.52              |
| 24:N:30:THR:HG21  | 24:N:82:LEU:HD21  | 1.92                     | 0.52              |
| 25:O:52:GLU:HG2   | 25:O:78:LEU:HD11  | 1.90                     | 0.52              |
| 25:O:66:THR:HG22  | 25:O:67:ASP:H     | 1.73                     | 0.52              |
| 34:a:98:LEU:HD13  | 34:a:108:TYR:CZ   | 2.45                     | 0.52              |
| 41:h:56:THR:O     | 41:h:58:TYR:CD2   | 2.63                     | 0.52              |
| 44:k:98:LEU:HG    | 44:k:104:ILE:HG22 | 1.91                     | 0.52              |
| 48:o:66:VAL:O     | 48:o:77:LYS:N     | 2.42                     | 0.52              |
| 3:2:7:VAL:HA      | 3:2:34:GLN:NE2    | 2.25                     | 0.52              |
| 4:3:2136:A:H2'    | 4:3:2137:A:C8     | 2.44                     | 0.52              |
| 6:5:941:A:H2'     | 6:5:942:G:C8      | 2.45                     | 0.52              |
| 11:A:107:PHE:HD2  | 11:A:109:THR:HG23 | 1.75                     | 0.52              |
| 13:C:102:TYR:HD2  | 13:C:110:ARG:HH21 | 1.58                     | 0.52              |
| 24:N:82:LEU:CD2   | 24:N:84:LEU:HB3   | 2.38                     | 0.52              |
| 37:d:177:LEU:HB2  | 37:d:180:GLY:O    | 2.10                     | 0.52              |
| 44:k:56:THR:CB    | 44:k:61:ARG:HH12  | 2.22                     | 0.52              |
| 4:3:569:U:H2'     | 4:3:570:C:C6      | 2.45                     | 0.51              |
| 4:3:583:U:O4      | 42:i:3:LYS:HD3    | 2.10                     | 0.51              |
| 4:3:1314:A:H4'    | 46:m:107:ARG:HH22 | 1.73                     | 0.51              |
| 6:5:1302:C:H5''   | 22:L:28:SER:HB3   | 1.92                     | 0.51              |
| 6:5:1332:U:H3     | 6:5:1338:A:H61    | 1.57                     | 0.51              |
| 6:5:1387:U:H2'    | 6:5:1388:A:C8     | 2.45                     | 0.51              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 11:A:46:GLU:OE1  | 11:A:46:GLU:N     | 2.43                     | 0.51              |
| 14:D:152:LYS:HB3 | 14:D:179:TYR:HB2  | 1.92                     | 0.51              |
| 21:K:46:VAL:CG2  | 21:K:69:ARG:HB3   | 2.40                     | 0.51              |
| 38:e:48:LEU:HA   | 38:e:53:LEU:HD13  | 1.92                     | 0.51              |
| 55:v:37:LYS:HB3  | 55:v:45:THR:HG22  | 1.92                     | 0.51              |
| 4:3:481:C:O2'    | 4:3:485:A:N3      | 2.38                     | 0.51              |
| 4:3:604:A:O2'    | 4:3:606:G:OP2     | 2.24                     | 0.51              |
| 4:3:1583:G:O2'   | 4:3:1584:U:OP1    | 2.25                     | 0.51              |
| 6:5:1162:G:H5'   | 18:H:117:LYS:NZ   | 2.24                     | 0.51              |
| 35:b:17:PHE:HB2  | 48:o:17:GLN:NE2   | 2.25                     | 0.51              |
| 4:3:890:U:H2'    | 4:3:891:G:H8      | 1.75                     | 0.51              |
| 4:3:1229:U:H4'   | 49:p:8:GLN:NE2    | 2.25                     | 0.51              |
| 4:3:2144:C:H2'   | 4:3:2145:A:C8     | 2.45                     | 0.51              |
| 4:3:2342:U:N3    | 47:n:10:LEU:HD21  | 2.25                     | 0.51              |
| 6:5:1388:A:H2    | 6:5:1462:G:H22    | 1.59                     | 0.51              |
| 17:G:129:ARG:HG2 | 17:G:129:ARG:HH11 | 1.74                     | 0.51              |
| 20:J:43:MET:SD   | 20:J:59:ALA:HB2   | 2.50                     | 0.51              |
| 22:L:13:LYS:HE2  | 22:L:21:TYR:HD2   | 1.75                     | 0.51              |
| 35:b:34:ASN:ND2  | 35:b:54:PHE:HB3   | 2.26                     | 0.51              |
| 39:f:31:PHE:N    | 39:f:32:PRO:HD2   | 2.26                     | 0.51              |
| 43:j:69:GLN:O    | 43:j:77:LEU:N     | 2.44                     | 0.51              |
| 48:o:63:THR:HB   | 48:o:78:ASN:HD21  | 1.75                     | 0.51              |
| 52:s:48:TYR:HD2  | 52:s:91:ILE:HD13  | 1.75                     | 0.51              |
| 53:t:40:ASN:ND2  | 53:t:67:ALA:HB3   | 2.25                     | 0.51              |
| 56:w:13:GLU:O    | 56:w:16:VAL:HG12  | 2.11                     | 0.51              |
| 1:0:19:LEU:HA    | 1:0:22:MET:HG3    | 1.93                     | 0.51              |
| 2:1:6:ALA:O      | 44:k:59:TYR:CE1   | 2.63                     | 0.51              |
| 4:3:340:U:H2'    | 4:3:341:G:O4'     | 2.10                     | 0.51              |
| 4:3:550:A:H1'    | 4:3:614:C:H1'     | 1.92                     | 0.51              |
| 4:3:816:A:H5''   | 4:3:817:A:N7      | 2.26                     | 0.51              |
| 4:3:963:U:H2'    | 4:3:964:A:H8      | 1.75                     | 0.51              |
| 4:3:1104:A:H5''  | 4:3:1105:A:C5     | 2.45                     | 0.51              |
| 4:3:2183:U:H4'   | 10:9:8:MET:CE     | 2.40                     | 0.51              |
| 4:3:2794:U:H5'   | 35:b:72:LYS:HZ3   | 1.74                     | 0.51              |
| 6:5:192:A:H2'    | 6:5:193:G:C8      | 2.46                     | 0.51              |
| 6:5:499:U:H2'    | 6:5:500:G:H8      | 1.75                     | 0.51              |
| 6:5:1463:A:H2'   | 6:5:1464:G:C8     | 2.46                     | 0.51              |
| 12:B:113:MET:O   | 12:B:115:SER:N    | 2.38                     | 0.51              |
| 16:F:44:GLY:HA3  | 16:F:116:LEU:HD11 | 1.93                     | 0.51              |
| 16:F:52:ARG:HH22 | 16:F:120:ALA:C    | 2.18                     | 0.51              |
| 19:I:83:VAL:HG23 | 19:I:84:ASP:H     | 1.75                     | 0.51              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 22:L:9:ILE:HB     | 22:L:13:LYS:HZ1  | 1.75                     | 0.51              |
| 22:L:19:LEU:HG    | 22:L:25:ILE:HG21 | 1.92                     | 0.51              |
| 34:a:173:GLN:HG3  | 34:a:174:ASP:H   | 1.74                     | 0.51              |
| 39:f:74:GLN:HG3   | 39:f:75:THR:HG23 | 1.92                     | 0.51              |
| 39:f:114:LYS:O    | 39:f:133:ASP:N   | 2.40                     | 0.51              |
| 52:s:86:PRO:HB3   | 56:w:90:HIS:CE1  | 2.45                     | 0.51              |
| 4:3:917:G:H2'     | 4:3:918:G:H8     | 1.75                     | 0.51              |
| 4:3:1117:U:H2'    | 4:3:1118:U:O4'   | 2.11                     | 0.51              |
| 4:3:1166:G:N2     | 4:3:1167:U:O4    | 2.39                     | 0.51              |
| 4:3:1600:A:H1'    | 34:a:62:ASN:HD22 | 1.74                     | 0.51              |
| 4:3:2125:U:OP2    | 4:3:2155:G:H4'   | 2.11                     | 0.51              |
| 6:5:32:U:O2'      | 6:5:49:C:N4      | 2.43                     | 0.51              |
| 6:5:823:C:OP2     | 17:G:9:LYS:NZ    | 2.29                     | 0.51              |
| 6:5:1368:U:O2'    | 6:5:1476:C:O2'   | 2.26                     | 0.51              |
| 12:B:69:VAL:HG23  | 12:B:106:ILE:HA  | 1.92                     | 0.51              |
| 13:C:61:GLN:HB2   | 13:C:71:PHE:HE2  | 1.74                     | 0.51              |
| 15:E:45:LEU:HB3   | 15:E:53:LEU:O    | 2.11                     | 0.51              |
| 15:E:65:ASP:OD1   | 15:E:66:ASN:N    | 2.42                     | 0.51              |
| 15:E:132:VAL:HG13 | 15:E:133:THR:N   | 2.21                     | 0.51              |
| 15:E:211:PHE:HZ   | 32:Y:93:A:C8     | 2.28                     | 0.51              |
| 18:H:34:ARG:HG2   | 18:H:34:ARG:HH11 | 1.76                     | 0.51              |
| 20:J:6:LYS:HZ1    | 20:J:8:ASN:HD22  | 1.56                     | 0.51              |
| 22:L:15:ILE:HG22  | 22:L:45:VAL:HG12 | 1.92                     | 0.51              |
| 27:Q:36:ARG:HB2   | 27:Q:38:LYS:HZ2  | 1.76                     | 0.51              |
| 39:f:23:ASP:OD1   | 39:f:24:GLY:N    | 2.42                     | 0.51              |
| 46:m:103:LEU:HA   | 58:y:41:ARG:CD   | 2.41                     | 0.51              |
| 52:s:12:LEU:HD11  | 56:w:35:HIS:CE1  | 2.45                     | 0.51              |
| 2:1:13:LEU:HD11   | 2:1:17:GLY:HA2   | 1.92                     | 0.51              |
| 4:3:227:A:O2'     | 4:3:456:G:N3     | 2.40                     | 0.51              |
| 4:3:1186:A:O2'    | 49:p:76:SER:O    | 2.28                     | 0.51              |
| 4:3:2133:A:C6     | 4:3:2180:U:H5''  | 2.46                     | 0.51              |
| 4:3:2268:C:H42    | 54:u:28:ARG:NE   | 2.08                     | 0.51              |
| 6:5:499:U:H2'     | 6:5:500:G:C8     | 2.46                     | 0.51              |
| 6:5:1510:C:H41    | 32:Y:60:G:H1     | 1.57                     | 0.51              |
| 22:L:79:HIS:O     | 22:L:82:GLU:HG2  | 2.10                     | 0.51              |
| 44:k:113:LYS:HZ3  | 44:k:130:LYS:HD2 | 1.75                     | 0.51              |
| 45:l:111:GLU:HA   | 45:l:114:MET:HE2 | 1.92                     | 0.51              |
| 2:1:28:HIS:ND1    | 2:1:29:LEU:HG    | 2.25                     | 0.51              |
| 7:6:19:A:C6       | 7:6:57:G:H1'     | 2.46                     | 0.51              |
| 11:A:148:GLU:HA   | 11:A:151:MET:HG3 | 1.91                     | 0.51              |
| 14:D:135:SER:HB3  | 14:D:177:ASP:OD1 | 2.11                     | 0.51              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 17:G:54:LEU:HD11 | 17:G:72:PHE:CD1   | 2.46                     | 0.51              |
| 17:G:95:LEU:O    | 17:G:95:LEU:HD12  | 2.10                     | 0.51              |
| 19:I:56:THR:HG22 | 19:I:68:ARG:CD    | 2.41                     | 0.51              |
| 27:Q:60:LEU:HD13 | 27:Q:90:LEU:HD23  | 1.91                     | 0.51              |
| 39:f:124:HIS:ND1 | 39:f:128:LEU:HD11 | 2.25                     | 0.51              |
| 45:l:40:ASN:OD1  | 45:l:41:TRP:N     | 2.42                     | 0.51              |
| 50:q:71:ILE:HD12 | 50:q:82:LYS:HB3   | 1.93                     | 0.51              |
| 58:y:41:ARG:HG3  | 58:y:42:VAL:N     | 2.26                     | 0.51              |
| 4:3:174:A:H2'    | 4:3:175:A:H8      | 1.75                     | 0.51              |
| 4:3:606:G:N2     | 4:3:2038:A:OP1    | 2.44                     | 0.51              |
| 4:3:1437:A:H2'   | 4:3:1438:G:H8     | 1.76                     | 0.51              |
| 4:3:1437:A:H2'   | 4:3:1438:G:C8     | 2.46                     | 0.51              |
| 4:3:1553:G:N1    | 4:3:1577:A:OP2    | 2.25                     | 0.51              |
| 4:3:1690:C:OP1   | 35:b:142:ARG:HD2  | 2.10                     | 0.51              |
| 4:3:1796:A:H5'   | 34:a:228:VAL:HG22 | 1.93                     | 0.51              |
| 4:3:2194:G:H4'   | 4:3:2195:U:OP1    | 2.08                     | 0.51              |
| 4:3:2311:G:O2'   | 37:d:121:SER:O    | 2.25                     | 0.51              |
| 6:5:473:A:H2'    | 6:5:474:G:C8      | 2.46                     | 0.51              |
| 21:K:45:GLY:O    | 21:K:93:THR:HG22  | 2.10                     | 0.51              |
| 23:M:29:ARG:HE   | 23:M:42:LEU:HD21  | 1.75                     | 0.51              |
| 29:S:25:LYS:HZ2  | 29:S:54:LEU:HD13  | 1.75                     | 0.51              |
| 48:o:68:LYS:HE3  | 48:o:75:ILE:CD1   | 2.41                     | 0.51              |
| 49:p:111:LYS:HZ2 | 50:q:45:ILE:HG22  | 1.75                     | 0.51              |
| 4:3:145:A:O2'    | 52:s:42:LEU:HD11  | 2.11                     | 0.51              |
| 4:3:2117:G:H21   | 4:3:2127:G:H1'    | 1.76                     | 0.51              |
| 6:5:394:U:H2'    | 6:5:395:G:C8      | 2.45                     | 0.51              |
| 6:5:527:G:H22    | 21:K:61:ALA:HB2   | 1.75                     | 0.51              |
| 12:B:49:ARG:HG3  | 12:B:121:ARG:NE   | 2.25                     | 0.51              |
| 12:B:220:ALA:C   | 12:B:222:ILE:H    | 2.18                     | 0.51              |
| 14:D:154:ALA:HB3 | 14:D:177:ASP:HB2  | 1.93                     | 0.51              |
| 21:K:87:LEU:HD12 | 21:K:91:SER:HB2   | 1.93                     | 0.51              |
| 31:X:29:LYS:HG3  | 31:X:30:GLN:N     | 2.20                     | 0.51              |
| 31:X:44:ARG:HH21 | 31:X:47:LYS:HE2   | 1.76                     | 0.51              |
| 45:l:26:TYR:HD2  | 45:l:134:ARG:HH12 | 1.59                     | 0.51              |
| 2:1:2:LYS:HG2    | 4:3:246:G:C8      | 2.45                     | 0.51              |
| 4:3:847:C:H5''   | 4:3:1280:G:O2'    | 2.10                     | 0.51              |
| 4:3:1959:A:P     | 43:j:44:LYS:HZ1   | 2.34                     | 0.51              |
| 4:3:2540:G:O2'   | 4:3:2665:A:N1     | 2.41                     | 0.51              |
| 6:5:447:G:H5''   | 6:5:448:A:H3'     | 1.92                     | 0.51              |
| 6:5:1292:A:N6    | 23:M:18:VAL:HG21  | 2.26                     | 0.51              |
| 12:B:153:LYS:NZ  | 12:B:178:LEU:HD11 | 2.25                     | 0.51              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 15:E:111:LYS:HA  | 15:E:114:LYS:CE   | 2.36                     | 0.51              |
| 35:b:103:GLN:CD  | 35:b:104:VAL:H    | 2.19                     | 0.51              |
| 43:j:71:ARG:HH12 | 43:j:104:ARG:HH11 | 1.57                     | 0.51              |
| 46:m:120:ASP:OD1 | 46:m:120:ASP:N    | 2.43                     | 0.51              |
| 47:n:67:LYS:NZ   | 47:n:101:ARG:HG3  | 2.26                     | 0.51              |
| 48:o:104:MET:HE1 | 48:o:112:ALA:HA   | 1.92                     | 0.51              |
| 4:3:299:A:H2'    | 4:3:300:G:C8      | 2.46                     | 0.50              |
| 4:3:558:C:H5''   | 4:3:575:C:O2'     | 2.11                     | 0.50              |
| 4:3:1279:U:H5'   | 49:p:3:ILE:HB     | 1.94                     | 0.50              |
| 4:3:1281:A:H5'   | 49:p:12:ARG:HH21  | 1.74                     | 0.50              |
| 4:3:1445:U:H2'   | 4:3:1446:G:O4'    | 2.10                     | 0.50              |
| 4:3:1569:A:H2'   | 4:3:1570:A:C2     | 2.46                     | 0.50              |
| 4:3:2032:G:H2'   | 4:3:2033:G:C8     | 2.46                     | 0.50              |
| 4:3:2116:U:H4'   | 4:3:2150:C:H5'    | 1.92                     | 0.50              |
| 4:3:2185:C:H2'   | 4:3:2186:C:C6     | 2.45                     | 0.50              |
| 6:5:9:A:H5'      | 14:D:180:THR:O    | 2.11                     | 0.50              |
| 6:5:378:A:H2'    | 6:5:379:A:C8      | 2.45                     | 0.50              |
| 6:5:1508:C:H42   | 11:A:294:GLU:HA   | 1.76                     | 0.50              |
| 11:A:46:GLU:O    | 11:A:48:GLU:N     | 2.38                     | 0.50              |
| 13:C:47:MET:HG3  | 13:C:52:GLN:HB3   | 1.94                     | 0.50              |
| 15:E:157:TRP:CD1 | 17:G:60:LEU:CB    | 2.88                     | 0.50              |
| 39:f:64:LEU:O    | 39:f:68:LEU:HD23  | 2.11                     | 0.50              |
| 44:k:2:GLU:O     | 44:k:6:LEU:HD23   | 2.11                     | 0.50              |
| 44:k:108:SER:HB2 | 44:k:110:LEU:HD13 | 1.93                     | 0.50              |
| 45:l:12:PRO:HG2  | 45:l:72:MET:SD    | 2.51                     | 0.50              |
| 4:3:1132:C:H3'   | 4:3:1133:A:H8     | 1.76                     | 0.50              |
| 4:3:1603:A:O4'   | 34:a:63:LYS:NZ    | 2.37                     | 0.50              |
| 4:3:1806:G:OP1   | 34:a:268:ARG:NH1  | 2.35                     | 0.50              |
| 6:5:57:U:H2'     | 6:5:58:G:H8       | 1.76                     | 0.50              |
| 6:5:970:A:N1     | 6:5:1341:U:O2'    | 2.40                     | 0.50              |
| 15:E:5:ILE:HD11  | 15:E:62:PHE:HE1   | 1.77                     | 0.50              |
| 18:H:51:GLU:OE1  | 18:H:55:ASP:HB2   | 2.12                     | 0.50              |
| 20:J:40:SER:HA   | 20:J:43:MET:SD    | 2.51                     | 0.50              |
| 35:b:53:SER:HB2  | 35:b:78:THR:OG1   | 2.10                     | 0.50              |
| 45:l:103:MET:HE1 | 45:l:125:LEU:HG   | 1.92                     | 0.50              |
| 55:v:6:GLN:HE22  | 55:v:49:LEU:HB3   | 1.77                     | 0.50              |
| 2:1:10:ARG:HH22  | 4:3:2402:C:H5'    | 1.77                     | 0.50              |
| 2:1:14:THR:HG21  | 2:1:18:GLN:HE21   | 1.77                     | 0.50              |
| 4:3:1544:G:H2'   | 4:3:1545:A:H8     | 1.76                     | 0.50              |
| 4:3:2206:A:H1'   | 4:3:2207:A:H5'    | 1.93                     | 0.50              |
| 6:5:258:A:O3'    | 29:S:63:ASN:ND2   | 2.44                     | 0.50              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 6:5:407:A:H3'    | 13:C:27:LYS:NZ    | 2.26                     | 0.50              |
| 6:5:1505:G:H2'   | 6:5:1506:A:C8     | 2.46                     | 0.50              |
| 12:B:42:ASN:O    | 12:B:46:VAL:HG22  | 2.10                     | 0.50              |
| 26:P:30:PHE:HE2  | 26:P:41:ARG:HB3   | 1.77                     | 0.50              |
| 36:c:142:VAL:O   | 36:c:145:GLN:HG3  | 2.11                     | 0.50              |
| 40:g:27:PHE:HE1  | 40:g:106:MET:HE2  | 1.76                     | 0.50              |
| 48:o:108:SER:HA  | 48:o:112:ALA:HB2  | 1.94                     | 0.50              |
| 2:1:54:ARG:HH21  | 4:3:868:C:H4'     | 1.77                     | 0.50              |
| 3:2:7:VAL:HG12   | 3:2:34:GLN:CD     | 2.36                     | 0.50              |
| 4:3:2154:A:H2'   | 4:3:2155:G:O4'    | 2.11                     | 0.50              |
| 6:5:711:G:H2'    | 6:5:712:A:C8      | 2.46                     | 0.50              |
| 6:5:1110:C:H2'   | 6:5:1111:G:C8     | 2.46                     | 0.50              |
| 12:B:167:ARG:NH2 | 32:Y:78:C:O2      | 2.39                     | 0.50              |
| 15:E:7:LEU:CD2   | 15:E:9:VAL:HG13   | 2.38                     | 0.50              |
| 16:F:78:ARG:O    | 16:F:79:ILE:HG13  | 2.11                     | 0.50              |
| 22:L:19:LEU:HD12 | 22:L:22:ILE:HD12  | 1.92                     | 0.50              |
| 22:L:20:THR:HG22 | 22:L:27:LEU:HA    | 1.92                     | 0.50              |
| 23:M:34:LEU:O    | 23:M:38:GLY:N     | 2.43                     | 0.50              |
| 30:T:30:GLN:HA   | 30:T:33:GLU:OE1   | 2.12                     | 0.50              |
| 37:d:45:ARG:HE   | 37:d:78:LYS:NZ    | 2.09                     | 0.50              |
| 37:d:100:LEU:O   | 37:d:104:ILE:HG22 | 2.11                     | 0.50              |
| 38:e:91:ARG:NH2  | 38:e:167:TYR:O    | 2.44                     | 0.50              |
| 45:l:38:LYS:HZ3  | 45:l:128:THR:HB   | 1.75                     | 0.50              |
| 45:l:43:ASP:OD2  | 45:l:45:ARG:NH1   | 2.44                     | 0.50              |
| 46:m:93:THR:O    | 46:m:97:TYR:OH    | 2.27                     | 0.50              |
| 52:s:10:PRO:HB3  | 52:s:29:PHE:CD1   | 2.47                     | 0.50              |
| 53:t:36:VAL:HG12 | 53:t:69:ILE:HD13  | 1.94                     | 0.50              |
| 56:w:86:ALA:HA   | 56:w:89:GLN:CD    | 2.36                     | 0.50              |
| 1:0:26:SER:HB2   | 4:3:717:U:H5'     | 1.92                     | 0.50              |
| 4:3:552:C:OP1    | 58:y:10:LYS:NZ    | 2.31                     | 0.50              |
| 4:3:1121:A:H5''  | 4:3:1122:G:H5'    | 1.92                     | 0.50              |
| 4:3:1672:C:O2    | 4:3:2706:U:O2'    | 2.29                     | 0.50              |
| 11:A:82:ILE:CD1  | 11:A:175:LEU:HB3  | 2.42                     | 0.50              |
| 14:D:84:ARG:CZ   | 14:D:86:MET:HE2   | 2.41                     | 0.50              |
| 15:E:142:ARG:O   | 15:E:145:ARG:N    | 2.35                     | 0.50              |
| 15:E:182:ASN:O   | 15:E:185:HIS:ND1  | 2.44                     | 0.50              |
| 34:a:27:THR:HG21 | 34:a:85:SER:HA    | 1.93                     | 0.50              |
| 38:e:30:PRO:HD2  | 38:e:83:THR:HA    | 1.93                     | 0.50              |
| 38:e:87:GLU:OE1  | 38:e:137:SER:OG   | 2.26                     | 0.50              |
| 38:e:90:LEU:HB2  | 38:e:134:ILE:HB   | 1.94                     | 0.50              |
| 39:f:38:PRO:O    | 39:f:39:LEU:HD22  | 2.12                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 39:f:81:LEU:O     | 39:f:149:LYS:HG3  | 2.11                     | 0.50              |
| 43:j:28:THR:HG22  | 43:j:29:ARG:HD2   | 1.94                     | 0.50              |
| 48:o:93:ARG:NH2   | 48:o:118:LYS:O    | 2.44                     | 0.50              |
| 4:3:26:G:H1'      | 51:r:77:ASN:HB3   | 1.92                     | 0.50              |
| 4:3:155:A:H2'     | 4:3:156:A:H8      | 1.75                     | 0.50              |
| 4:3:383:U:H2'     | 4:3:384:G:H8      | 1.77                     | 0.50              |
| 4:3:1814:G:N2     | 4:3:1817:A:OP2    | 2.43                     | 0.50              |
| 6:5:295:G:H2'     | 6:5:296:A:C8      | 2.47                     | 0.50              |
| 24:N:3:ILE:HG12   | 24:N:8:ILE:HD11   | 1.92                     | 0.50              |
| 39:f:92:ILE:HB    | 39:f:122:GLY:HA3  | 1.94                     | 0.50              |
| 46:m:106:ARG:HG3  | 46:m:113:MET:HE3  | 1.94                     | 0.50              |
| 4:3:558:C:H1'     | 4:3:587:U:H1'     | 1.94                     | 0.50              |
| 4:3:933:A:O2'     | 9:8:56:C:N3       | 2.45                     | 0.50              |
| 4:3:2189:U:H2'    | 4:3:2190:G:C8     | 2.47                     | 0.50              |
| 4:3:2529:C:O2'    | 4:3:2572:A:N3     | 2.40                     | 0.50              |
| 4:3:2540:G:N2     | 4:3:2671:G:O2'    | 2.44                     | 0.50              |
| 4:3:2584:G:O2'    | 4:3:2587:U:OP2    | 2.23                     | 0.50              |
| 4:3:2683:G:H1'    | 43:j:29:ARG:NH2   | 2.26                     | 0.50              |
| 6:5:35:C:H2'      | 6:5:36:G:H8       | 1.77                     | 0.50              |
| 6:5:259:A:H2'     | 6:5:260:C:C6      | 2.47                     | 0.50              |
| 6:5:690:G:H5'     | 32:Y:66:U:C6      | 2.46                     | 0.50              |
| 12:B:7:SER:O      | 12:B:11:ARG:HD3   | 2.12                     | 0.50              |
| 12:B:217:ARG:NH2  | 19:I:23:LEU:HB2   | 2.26                     | 0.50              |
| 17:G:47:ILE:HD13  | 17:G:122:VAL:HG22 | 1.94                     | 0.50              |
| 19:I:57:ILE:HB    | 23:M:45:ARG:NH2   | 2.27                     | 0.50              |
| 26:P:43:LYS:HD2   | 26:P:45:TYR:CE1   | 2.46                     | 0.50              |
| 37:d:102:LYS:HB2  | 57:x:25:ILE:HG21  | 1.93                     | 0.50              |
| 42:i:3:LYS:HG3    | 42:i:4:THR:N      | 2.23                     | 0.50              |
| 45:l:109:ILE:HG13 | 45:l:110:PRO:HD2  | 1.93                     | 0.50              |
| 48:o:7:GLN:NE2    | 48:o:11:ASP:OD1   | 2.45                     | 0.50              |
| 49:p:97:LEU:HD12  | 49:p:101:GLU:HG3  | 1.94                     | 0.50              |
| 4:3:680:A:H2'     | 4:3:682:A:N7      | 2.27                     | 0.50              |
| 4:3:813:G:H5''    | 34:a:52:LYS:HE3   | 1.93                     | 0.50              |
| 4:3:860:C:H4'     | 4:3:2436:G:C5     | 2.46                     | 0.50              |
| 4:3:869:U:H2'     | 4:3:870:A:H8      | 1.77                     | 0.50              |
| 4:3:1648:A:N1     | 51:r:93:SER:OG    | 2.45                     | 0.50              |
| 6:5:631:C:H2'     | 6:5:632:A:C8      | 2.46                     | 0.50              |
| 6:5:1022:G:O2'    | 6:5:1023:G:O5'    | 2.30                     | 0.50              |
| 6:5:1361:G:H2'    | 6:5:1362:G:H8     | 1.77                     | 0.50              |
| 12:B:37:ASP:O     | 12:B:41:ARG:HG3   | 2.12                     | 0.50              |
| 15:E:28:THR:HG21  | 15:E:72:PHE:HA    | 1.94                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:F:65:VAL:O     | 16:F:68:VAL:HG12  | 2.11                     | 0.50              |
| 18:H:35:ARG:HD3   | 18:H:39:GLU:OE1   | 2.11                     | 0.50              |
| 19:I:27:THR:HG22  | 19:I:30:LYS:HZ1   | 1.77                     | 0.50              |
| 21:K:29:ASN:HD22  | 21:K:32:ASN:ND2   | 2.08                     | 0.50              |
| 25:O:19:ILE:N     | 25:O:37:GLY:O     | 2.45                     | 0.50              |
| 39:f:25:TYR:CE1   | 39:f:29:PHE:HE2   | 2.28                     | 0.50              |
| 39:f:129:HIS:HB3  | 39:f:141:LYS:NZ   | 2.27                     | 0.50              |
| 46:m:51:LEU:HD13  | 46:m:62:GLN:HE21  | 1.76                     | 0.50              |
| 46:m:60:ARG:HG3   | 46:m:61:ARG:N     | 2.27                     | 0.50              |
| 55:v:39:LYS:HZ2   | 55:v:45:THR:HG1   | 1.57                     | 0.50              |
| 58:y:13:ARG:HD2   | 58:y:17:ARG:CZ    | 2.42                     | 0.50              |
| 4:3:1174:G:O2'    | 4:3:1178:A:N1     | 2.41                     | 0.50              |
| 6:5:182:C:H41     | 26:P:3:ARG:HG2    | 1.77                     | 0.50              |
| 6:5:253:G:H1      | 6:5:265:U:H3      | 1.60                     | 0.50              |
| 6:5:259:A:OP1     | 29:S:67:ARG:NH1   | 2.45                     | 0.50              |
| 6:5:1164:U:OP1    | 19:I:59:ARG:NH2   | 2.44                     | 0.50              |
| 6:5:1385:A:H2'    | 6:5:1386:C:C6     | 2.47                     | 0.50              |
| 8:7:10:G:O2'      | 8:7:11:U:OP1      | 2.25                     | 0.50              |
| 22:L:11:ASN:HB2   | 22:L:46:LYS:HB3   | 1.93                     | 0.50              |
| 22:L:86:TRP:O     | 22:L:89:LEU:HG    | 2.12                     | 0.50              |
| 27:Q:72:PRO:HD2   | 27:Q:75:ILE:HD12  | 1.94                     | 0.50              |
| 37:d:148:ARG:HH21 | 37:d:149:ILE:HG12 | 1.75                     | 0.50              |
| 38:e:23:ASP:OD1   | 38:e:23:ASP:N     | 2.45                     | 0.50              |
| 43:j:71:ARG:NH2   | 43:j:104:ARG:HH11 | 2.10                     | 0.50              |
| 4:3:1000:U:O2'    | 4:3:2281:A:N3     | 2.33                     | 0.49              |
| 4:3:1529:U:H2'    | 4:3:1530:G:C8     | 2.46                     | 0.49              |
| 4:3:2078:A:H2'    | 4:3:2079:G:H8     | 1.76                     | 0.49              |
| 4:3:2175:U:H2'    | 4:3:2176:G:C8     | 2.47                     | 0.49              |
| 4:3:2802:C:N4     | 4:3:2803:G:H21    | 2.10                     | 0.49              |
| 11:A:293:ARG:HE   | 30:T:50:GLN:HG2   | 1.77                     | 0.49              |
| 12:B:61:THR:HB    | 12:B:64:THR:HG22  | 1.94                     | 0.49              |
| 14:D:70:ILE:HD13  | 14:D:92:VAL:HG22  | 1.94                     | 0.49              |
| 15:E:121:ARG:O    | 15:E:122:GLU:C    | 2.53                     | 0.49              |
| 24:N:3:ILE:HG13   | 24:N:4:ASP:N      | 2.27                     | 0.49              |
| 35:b:32:GLU:HA    | 35:b:189:MET:SD   | 2.52                     | 0.49              |
| 45:l:37:THR:C     | 45:l:38:LYS:HD3   | 2.37                     | 0.49              |
| 46:m:59:ASN:O     | 46:m:62:GLN:HG2   | 2.11                     | 0.49              |
| 49:p:97:LEU:HD12  | 49:p:101:GLU:CG   | 2.42                     | 0.49              |
| 50:q:60:GLU:HG3   | 50:q:91:LYS:NZ    | 2.27                     | 0.49              |
| 56:w:13:GLU:O     | 56:w:17:LYS:HD2   | 2.12                     | 0.49              |
| 57:x:16:CYS:SG    | 57:x:17:ALA:N     | 2.84                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 58:y:53:VAL:HG23  | 58:y:54:LYS:N     | 2.27                     | 0.49              |
| 4:3:614:C:H2'     | 4:3:615:G:H8      | 1.77                     | 0.49              |
| 4:3:1618:U:H4'    | 4:3:1619:A:OP2    | 2.11                     | 0.49              |
| 6:5:311:A:O2'     | 6:5:326:C:O2'     | 2.26                     | 0.49              |
| 9:8:28:A:H2'      | 9:8:29:U:C6       | 2.47                     | 0.49              |
| 14:D:131:ILE:HG22 | 14:D:175:TYR:HE1  | 1.77                     | 0.49              |
| 22:L:3:ARG:HD2    | 22:L:3:ARG:C      | 2.37                     | 0.49              |
| 24:N:7:GLY:O      | 24:N:10:LYS:HG3   | 2.12                     | 0.49              |
| 24:N:57:VAL:HA    | 24:N:60:ARG:NH2   | 2.27                     | 0.49              |
| 24:N:78:LEU:HD12  | 24:N:79:VAL:N     | 2.28                     | 0.49              |
| 36:c:178:VAL:O    | 36:c:179:GLN:NE2  | 2.44                     | 0.49              |
| 43:j:15:GLY:HA3   | 43:j:47:ILE:HG12  | 1.93                     | 0.49              |
| 43:j:58:LEU:HB3   | 43:j:86:LEU:HD11  | 1.94                     | 0.49              |
| 4:3:580:U:OP1     | 4:3:1249:A:O2'    | 2.20                     | 0.49              |
| 4:3:1248:A:H2'    | 4:3:1249:A:C8     | 2.48                     | 0.49              |
| 4:3:1261:U:H2'    | 4:3:1262:G:C8     | 2.47                     | 0.49              |
| 4:3:2340:U:OP1    | 54:u:92:LYS:NZ    | 2.45                     | 0.49              |
| 6:5:214:U:H2'     | 6:5:215:C:C6      | 2.47                     | 0.49              |
| 6:5:561:A:O2'     | 6:5:564:G:O3'     | 2.30                     | 0.49              |
| 7:6:1:G:O2'       | 7:6:2:G:OP1       | 2.28                     | 0.49              |
| 11:A:148:GLU:O    | 11:A:151:MET:HG3  | 2.13                     | 0.49              |
| 21:K:84:GLY:O     | 21:K:112:ARG:NH2  | 2.45                     | 0.49              |
| 21:K:96:ARG:HG2   | 21:K:111:VAL:CG2  | 2.42                     | 0.49              |
| 34:a:65:LYS:HB2   | 34:a:67:ARG:HH12  | 1.78                     | 0.49              |
| 45:l:41:TRP:CD1   | 45:l:96:VAL:HG22  | 2.47                     | 0.49              |
| 49:p:44:TYR:HD1   | 49:p:47:ARG:HE    | 1.59                     | 0.49              |
| 49:p:45:ALA:O     | 49:p:49:ARG:HG3   | 2.12                     | 0.49              |
| 4:3:355:A:O2'     | 4:3:374:A:N3      | 2.44                     | 0.49              |
| 4:3:625:G:H1      | 4:3:700:U:H3      | 1.60                     | 0.49              |
| 4:3:2031:C:H2'    | 4:3:2032:G:H8     | 1.76                     | 0.49              |
| 4:3:2655:U:H2'    | 4:3:2656:G:H8     | 1.77                     | 0.49              |
| 6:5:949:G:H4'     | 22:L:119:LYS:HD3  | 1.94                     | 0.49              |
| 10:9:116:PRO:HA   | 10:9:119:MET:HE1  | 1.94                     | 0.49              |
| 11:A:293:ARG:HH22 | 30:T:54:ARG:HB2   | 1.75                     | 0.49              |
| 13:C:104:MET:HE1  | 13:C:169:THR:HG23 | 1.94                     | 0.49              |
| 15:E:9:VAL:HG23   | 15:E:56:HIS:HB2   | 1.94                     | 0.49              |
| 38:e:83:THR:HB    | 38:e:84:GLN:OE1   | 2.12                     | 0.49              |
| 39:f:82:LYS:O     | 39:f:83:GLU:C     | 2.54                     | 0.49              |
| 46:m:102:LYS:C    | 58:y:41:ARG:NH1   | 2.69                     | 0.49              |
| 47:n:28:VAL:CG1   | 47:n:89:VAL:HG12  | 2.42                     | 0.49              |
| 48:o:11:ASP:HA    | 48:o:14:GLU:OE2   | 2.11                     | 0.49              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 53:t:78:ASP:OD2  | 53:t:109:ASN:ND2  | 2.45                     | 0.49              |
| 56:w:33:LEU:HB2  | 56:w:38:LEU:HD12  | 1.95                     | 0.49              |
| 4:3:259:A:O2'    | 4:3:422:A:OP1     | 2.28                     | 0.49              |
| 4:3:450:C:H1'    | 4:3:1871:U:H1'    | 1.93                     | 0.49              |
| 4:3:631:A:H2'    | 4:3:632:A:C8      | 2.46                     | 0.49              |
| 4:3:890:U:H2'    | 4:3:891:G:C8      | 2.47                     | 0.49              |
| 4:3:1033:A:H5''  | 49:p:91:ARG:NH1   | 2.27                     | 0.49              |
| 4:3:2365:U:H2'   | 4:3:2367:C:OP2    | 2.13                     | 0.49              |
| 6:5:1283:G:P     | 22:L:87:ARG:HH21  | 2.35                     | 0.49              |
| 10:9:20:LEU:HG   | 10:9:225:PRO:HD2  | 1.93                     | 0.49              |
| 11:A:162:PHE:O   | 11:A:163:PHE:HD1  | 1.95                     | 0.49              |
| 13:C:148:THR:O   | 13:C:151:ILE:HG22 | 2.13                     | 0.49              |
| 16:F:17:PHE:HB3  | 16:F:58:LEU:HD22  | 1.95                     | 0.49              |
| 20:J:9:VAL:HG22  | 20:J:10:SER:H     | 1.77                     | 0.49              |
| 21:K:98:GLY:HA3  | 21:K:109:HIS:ND1  | 2.28                     | 0.49              |
| 23:M:43:CYS:HA   | 23:M:46:GLU:OE1   | 2.12                     | 0.49              |
| 24:N:33:ILE:HG13 | 24:N:60:ARG:NH1   | 2.28                     | 0.49              |
| 39:f:94:THR:O    | 39:f:95:LYS:C     | 2.55                     | 0.49              |
| 39:f:129:HIS:HB3 | 39:f:141:LYS:HZ2  | 1.77                     | 0.49              |
| 42:i:120:ARG:NE  | 42:i:120:ARG:HA   | 2.27                     | 0.49              |
| 45:l:74:LYS:NZ   | 45:l:94:VAL:H     | 2.10                     | 0.49              |
| 49:p:46:TYR:HA   | 49:p:49:ARG:NH1   | 2.28                     | 0.49              |
| 53:t:28:MET:HE2  | 53:t:33:GLN:HB2   | 1.95                     | 0.49              |
| 4:3:29:G:O2'     | 4:3:547:G:N2      | 2.45                     | 0.49              |
| 4:3:118:G:OP2    | 4:3:120:A:O2'     | 2.30                     | 0.49              |
| 4:3:274:A:OP2    | 4:3:294:G:N1      | 2.45                     | 0.49              |
| 4:3:2183:U:H4'   | 10:9:8:MET:SD     | 2.52                     | 0.49              |
| 6:5:519:G:O5'    | 21:K:83:GLU:HG2   | 2.12                     | 0.49              |
| 8:7:46:U:O2'     | 8:7:47:U:OP1      | 2.23                     | 0.49              |
| 9:8:5:C:H2'      | 9:8:6:U:H6        | 1.77                     | 0.49              |
| 13:C:196:VAL:O   | 13:C:199:TRP:HB3  | 2.13                     | 0.49              |
| 15:E:43:LYS:NZ   | 27:Q:98:LEU:HG    | 2.27                     | 0.49              |
| 25:O:67:ASP:O    | 25:O:70:ARG:HG3   | 2.12                     | 0.49              |
| 34:a:56:ARG:HG2  | 34:a:57:HIS:CG    | 2.47                     | 0.49              |
| 38:e:18:LEU:HD12 | 38:e:20:PHE:CZ    | 2.48                     | 0.49              |
| 42:i:104:VAL:CG2 | 42:i:127:VAL:HG21 | 2.43                     | 0.49              |
| 45:l:41:TRP:HB3  | 45:l:94:VAL:HG21  | 1.95                     | 0.49              |
| 46:m:23:SER:OG   | 46:m:68:LEU:N     | 2.45                     | 0.49              |
| 50:q:34:GLN:OE1  | 50:q:54:ARG:HB3   | 2.12                     | 0.49              |
| 53:t:8:ASP:OD1   | 53:t:8:ASP:N      | 2.45                     | 0.49              |
| 4:3:1070:U:H4'   | 38:e:62:LYS:NZ    | 2.28                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:3:2105:G:H2'    | 4:3:2106:G:C8     | 2.48                     | 0.49              |
| 4:3:2177:G:H3'    | 4:3:2178:A:C8     | 2.43                     | 0.49              |
| 6:5:80:U:H2'      | 6:5:81:A:H8       | 1.78                     | 0.49              |
| 6:5:483:U:H2'     | 6:5:484:A:H8      | 1.76                     | 0.49              |
| 6:5:789:A:O2'     | 6:5:791:A:N7      | 2.40                     | 0.49              |
| 10:9:113:ILE:HD13 | 10:9:151:VAL:HG23 | 1.95                     | 0.49              |
| 11:A:75:VAL:HA    | 15:E:181:PHE:CG   | 2.48                     | 0.49              |
| 12:B:170:MET:HE3  | 12:B:172:ILE:N    | 2.27                     | 0.49              |
| 15:E:32:VAL:HG23  | 15:E:62:PHE:HD2   | 1.78                     | 0.49              |
| 15:E:210:ARG:HE   | 15:E:214:LYS:HE3  | 1.76                     | 0.49              |
| 22:L:19:LEU:HD21  | 22:L:33:ILE:HB    | 1.94                     | 0.49              |
| 24:N:29:LEU:O     | 24:N:33:ILE:HG12  | 2.12                     | 0.49              |
| 37:d:60:ILE:HD11  | 37:d:141:ILE:HG13 | 1.95                     | 0.49              |
| 37:d:151:GLY:O    | 37:d:152:PHE:HD1  | 1.96                     | 0.49              |
| 48:o:55:ARG:HH22  | 48:o:62:GLU:CD    | 2.20                     | 0.49              |
| 51:r:19:LEU:O     | 58:y:22:LEU:HD21  | 2.12                     | 0.49              |
| 52:s:9:LYS:HB3    | 52:s:30:VAL:HG22  | 1.94                     | 0.49              |
| 53:t:2:GLN:N      | 53:t:2:GLN:OE1    | 2.45                     | 0.49              |
| 4:3:924:C:O2'     | 4:3:926:U:O2      | 2.30                     | 0.49              |
| 4:3:1032:A:OP2    | 49:p:92:LYS:HE2   | 2.12                     | 0.49              |
| 4:3:1054:U:OP1    | 4:3:1070:U:O2'    | 2.21                     | 0.49              |
| 4:3:2169:G:H21    | 4:3:2173:G:H8     | 1.60                     | 0.49              |
| 4:3:2813:A:H2'    | 4:3:2814:A:H8     | 1.78                     | 0.49              |
| 6:5:369:A:H4'     | 6:5:448:A:H62     | 1.77                     | 0.49              |
| 6:5:452:A:OP1     | 25:O:70:ARG:NH2   | 2.46                     | 0.49              |
| 6:5:1049:G:OP1    | 12:B:202:LYS:NZ   | 2.32                     | 0.49              |
| 13:C:60:MET:HB3   | 13:C:191:ILE:HG12 | 1.95                     | 0.49              |
| 14:D:87:ARG:HG2   | 14:D:109:LEU:HD23 | 1.94                     | 0.49              |
| 15:E:142:ARG:O    | 15:E:144:SER:N    | 2.46                     | 0.49              |
| 15:E:211:PHE:CZ   | 32:Y:93:A:C8      | 3.01                     | 0.49              |
| 16:F:87:PRO:HD2   | 16:F:151:ALA:HA   | 1.95                     | 0.49              |
| 16:F:139:ASP:HA   | 16:F:142:LYS:HG2  | 1.94                     | 0.49              |
| 17:G:16:ALA:HA    | 17:G:19:LEU:HB3   | 1.95                     | 0.49              |
| 29:S:65:ALA:O     | 29:S:68:LEU:HG    | 2.13                     | 0.49              |
| 43:j:64:ARG:HG3   | 43:j:83:ALA:HB3   | 1.94                     | 0.49              |
| 4:3:2886:A:C4'    | 46:m:99:ARG:HE    | 2.26                     | 0.49              |
| 6:5:1323:A:H3'    | 6:5:1324:A:H8     | 1.78                     | 0.49              |
| 12:B:167:ARG:NH2  | 32:Y:78:C:H1'     | 2.27                     | 0.49              |
| 14:D:66:PHE:CD1   | 14:D:96:ASN:HB3   | 2.47                     | 0.49              |
| 21:K:67:LYS:HE2   | 21:K:75:GLU:HB3   | 1.94                     | 0.49              |
| 25:O:23:ASP:OD1   | 25:O:24:SER:N     | 2.46                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 38:e:167:TYR:HB3  | 38:e:170:GLU:OE1  | 2.13                     | 0.49              |
| 42:i:26:LEU:HD21  | 42:i:145:TRP:HA   | 1.93                     | 0.49              |
| 46:m:53:LYS:NZ    | 46:m:97:TYR:OH    | 2.26                     | 0.49              |
| 49:p:104:LYS:O    | 49:p:108:ILE:HD12 | 2.12                     | 0.49              |
| 4:3:1385:U:H2'    | 4:3:1386:G:O4'    | 2.12                     | 0.49              |
| 6:5:822:A:H5''    | 17:G:9:LYS:HD2    | 1.94                     | 0.49              |
| 19:I:8:LYS:O      | 19:I:9:TYR:HD1    | 1.96                     | 0.49              |
| 27:Q:47:GLY:O     | 27:Q:49:LEU:HD23  | 2.12                     | 0.49              |
| 27:Q:67:TYR:OH    | 30:T:4:ILE:HD11   | 2.13                     | 0.49              |
| 34:a:120:LYS:O    | 34:a:121:ILE:HD13 | 2.12                     | 0.49              |
| 38:e:110:LEU:HG   | 38:e:155:ARG:HG3  | 1.95                     | 0.49              |
| 40:g:106:MET:HE1  | 40:g:108:PHE:HB3  | 1.93                     | 0.49              |
| 46:m:57:PHE:HB2   | 46:m:60:ARG:NH2   | 2.27                     | 0.49              |
| 4:3:666:G:N2      | 4:3:669:A:OP2     | 2.31                     | 0.48              |
| 4:3:1691:U:H2'    | 4:3:1692:A:C8     | 2.48                     | 0.48              |
| 17:G:44:ILE:HG22  | 17:G:122:VAL:HG21 | 1.95                     | 0.48              |
| 17:G:100:PRO:HB2  | 17:G:102:GLU:OE2  | 2.13                     | 0.48              |
| 18:H:57:THR:HG21  | 18:H:96:LEU:HG    | 1.95                     | 0.48              |
| 19:I:17:GLU:HB2   | 19:I:77:LYS:HG2   | 1.95                     | 0.48              |
| 34:a:128:ILE:HD12 | 34:a:136:MET:SD   | 2.52                     | 0.48              |
| 34:a:137:PRO:HA   | 34:a:197:ARG:HA   | 1.95                     | 0.48              |
| 35:b:17:PHE:HB2   | 48:o:17:GLN:HE22  | 1.78                     | 0.48              |
| 39:f:77:LEU:HD12  | 39:f:106:MET:HE3  | 1.95                     | 0.48              |
| 46:m:57:PHE:O     | 46:m:60:ARG:HG2   | 2.12                     | 0.48              |
| 50:q:85:HIS:NE2   | 50:q:87:GLN:OE1   | 2.38                     | 0.48              |
| 53:t:14:THR:HA    | 53:t:18:LYS:HE2   | 1.94                     | 0.48              |
| 57:x:10:GLN:OE1   | 57:x:31:GLN:HG2   | 2.13                     | 0.48              |
| 4:3:597:C:C4'     | 49:p:36:GLN:HE22  | 2.26                     | 0.48              |
| 4:3:755:C:H2'     | 4:3:756:A:H8      | 1.76                     | 0.48              |
| 4:3:1103:G:O2'    | 4:3:1104:A:H5'    | 2.13                     | 0.48              |
| 4:3:1493:A:N7     | 4:3:1579:G:H2'    | 2.28                     | 0.48              |
| 4:3:2299:U:O2'    | 4:3:2382:A:N3     | 2.44                     | 0.48              |
| 6:5:399:C:H5'     | 13:C:131:THR:HG23 | 1.95                     | 0.48              |
| 6:5:763:A:N3      | 6:5:1500:G:O2'    | 2.45                     | 0.48              |
| 6:5:1387:U:OP1    | 21:K:49:ARG:NH2   | 2.45                     | 0.48              |
| 11:A:32:MET:HE2   | 11:A:36:TYR:CB    | 2.37                     | 0.48              |
| 12:B:137:MET:HG3  | 12:B:171:TYR:CD2  | 2.48                     | 0.48              |
| 13:C:61:GLN:HB3   | 13:C:71:PHE:CE2   | 2.49                     | 0.48              |
| 21:K:63:ARG:HB3   | 21:K:79:TYR:HE1   | 1.77                     | 0.48              |
| 39:f:5:LEU:HD21   | 39:f:13:GLY:HA3   | 1.95                     | 0.48              |
| 45:l:29:PHE:HB3   | 45:l:65:TRP:CE2   | 2.48                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 55:v:12:PRO:C     | 55:v:13:LEU:HD12  | 2.38                     | 0.48              |
| 56:w:51:LEU:O     | 56:w:55:LEU:HD23  | 2.13                     | 0.48              |
| 4:3:26:G:O2'      | 51:r:78:GLN:O     | 2.23                     | 0.48              |
| 4:3:2100:G:N3     | 4:3:2206:A:N6     | 2.62                     | 0.48              |
| 6:5:991:A:H2'     | 6:5:992:U:C6      | 2.48                     | 0.48              |
| 6:5:1158:A:O2'    | 6:5:1159:A:OP1    | 2.27                     | 0.48              |
| 6:5:1269:U:H2'    | 6:5:1270:C:C6     | 2.47                     | 0.48              |
| 7:6:63:C:H4'      | 10:9:54:LYS:HE2   | 1.95                     | 0.48              |
| 11:A:36:TYR:CD2   | 11:A:281:ARG:HD3  | 2.49                     | 0.48              |
| 15:E:52:GLN:HB3   | 15:E:83:LEU:HD21  | 1.94                     | 0.48              |
| 17:G:90:ILE:HD11  | 17:G:140:TYR:CD2  | 2.47                     | 0.48              |
| 34:a:207:ASP:O    | 34:a:207:ASP:OD1  | 2.31                     | 0.48              |
| 35:b:180:ARG:HH12 | 35:b:218:LYS:NZ   | 2.10                     | 0.48              |
| 41:h:33:GLY:O     | 41:h:37:LYS:NZ    | 2.35                     | 0.48              |
| 1:0:2:LYS:HZ2     | 4:3:1655:U:H5'    | 1.77                     | 0.48              |
| 4:3:246:G:N2      | 4:3:259:A:OP2     | 2.34                     | 0.48              |
| 4:3:1081:A:C2     | 40:g:61:ARG:HD2   | 2.48                     | 0.48              |
| 6:5:1212:C:H3'    | 6:5:1213:A:H5'    | 1.95                     | 0.48              |
| 6:5:1402:U:H2'    | 6:5:1403:A:H8     | 1.79                     | 0.48              |
| 11:A:260:GLN:CD   | 11:A:261:LYS:HG2  | 2.37                     | 0.48              |
| 14:D:219:LEU:H    | 14:D:219:LEU:HD12 | 1.78                     | 0.48              |
| 16:F:63:ARG:NE    | 16:F:127:SER:O    | 2.46                     | 0.48              |
| 19:I:57:ILE:O     | 23:M:45:ARG:NH2   | 2.47                     | 0.48              |
| 34:a:73:ARG:HH21  | 34:a:123:ALA:HB2  | 1.77                     | 0.48              |
| 38:e:107:ASN:HB3  | 38:e:117:LYS:HG2  | 1.95                     | 0.48              |
| 47:n:34:LYS:HG3   | 47:n:39:ILE:HD12  | 1.95                     | 0.48              |
| 47:n:44:TRP:CE3   | 47:n:51:VAL:HG22  | 2.47                     | 0.48              |
| 50:q:21:PHE:HA    | 50:q:91:LYS:HA    | 1.95                     | 0.48              |
| 4:3:196:G:O6      | 4:3:207:C:O2'     | 2.26                     | 0.48              |
| 4:3:334:A:H2'     | 4:3:368:C:H1'     | 1.95                     | 0.48              |
| 4:3:652:U:H2'     | 4:3:653:G:H8      | 1.79                     | 0.48              |
| 4:3:881:A:H2      | 4:3:968:U:H3      | 1.56                     | 0.48              |
| 4:3:1099:C:H3'    | 4:3:1100:U:H6     | 1.79                     | 0.48              |
| 4:3:1566:A:H2'    | 4:3:1567:U:O4'    | 2.14                     | 0.48              |
| 5:4:2:U:H2'       | 5:4:3:U:C6        | 2.49                     | 0.48              |
| 6:5:407:A:OP2     | 13:C:27:LYS:HE2   | 2.13                     | 0.48              |
| 11:A:125:ILE:O    | 11:A:129:LYS:HG3  | 2.14                     | 0.48              |
| 12:B:209:MET:HE2  | 12:B:209:MET:HA   | 1.96                     | 0.48              |
| 14:D:212:ARG:NE   | 14:D:214:LYS:HD3  | 2.29                     | 0.48              |
| 15:E:98:ALA:HB3   | 27:Q:50:ARG:HH21  | 1.77                     | 0.48              |
| 21:K:67:LYS:HD3   | 21:K:77:LEU:HD23  | 1.95                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 34:a:57:HIS:CA    | 34:a:225:ARG:HB3  | 2.39                     | 0.48              |
| 36:c:165:ASN:HB3  | 36:c:168:LEU:CD2  | 2.42                     | 0.48              |
| 39:f:3:VAL:HG23   | 39:f:38:PRO:HA    | 1.96                     | 0.48              |
| 47:n:115:ASN:OD1  | 47:n:115:ASN:O    | 2.32                     | 0.48              |
| 48:o:103:TYR:CD2  | 48:o:106:GLU:OE2  | 2.66                     | 0.48              |
| 50:q:1:MET:SD     | 50:q:2:HIS:ND1    | 2.86                     | 0.48              |
| 4:3:626:A:H2'     | 4:3:627:U:C6      | 2.48                     | 0.48              |
| 4:3:707:C:H5      | 44:k:43:LYS:HD3   | 1.79                     | 0.48              |
| 4:3:1392:G:H5''   | 55:v:3:LYS:NZ     | 2.28                     | 0.48              |
| 4:3:1464:G:H1     | 4:3:1590:U:H3     | 1.60                     | 0.48              |
| 4:3:1691:U:H2'    | 4:3:1692:A:H8     | 1.78                     | 0.48              |
| 4:3:2822:C:O2'    | 4:3:2841:A:H5'    | 2.13                     | 0.48              |
| 61:3:3001:CLM:CL1 | 33:Z:35:ALA:HB2   | 2.50                     | 0.48              |
| 6:5:825:A:H2'     | 6:5:826:G:O4'     | 2.14                     | 0.48              |
| 6:5:868:G:H21     | 17:G:27:LYS:HZ1   | 1.61                     | 0.48              |
| 10:9:73:ILE:HG21  | 10:9:111:LEU:HD12 | 1.94                     | 0.48              |
| 12:B:40:ILE:HD11  | 12:B:96:ILE:HG23  | 1.94                     | 0.48              |
| 12:B:125:ASN:O    | 12:B:128:GLU:HG3  | 2.14                     | 0.48              |
| 15:E:115:TYR:O    | 15:E:119:ILE:HG12 | 2.14                     | 0.48              |
| 16:F:19:ASN:HB2   | 16:F:58:LEU:HD21  | 1.96                     | 0.48              |
| 26:P:60:LYS:NZ    | 26:P:81:ILE:HB    | 2.28                     | 0.48              |
| 27:Q:70:ILE:HG22  | 27:Q:90:LEU:HD13  | 1.95                     | 0.48              |
| 30:T:36:LEU:H     | 30:T:41:ARG:HH21  | 1.61                     | 0.48              |
| 34:a:57:HIS:HB3   | 34:a:225:ARG:O    | 2.14                     | 0.48              |
| 34:a:193:LEU:HB2  | 34:a:196:CYS:SG   | 2.53                     | 0.48              |
| 36:c:162:ASN:HB2  | 36:c:203:VAL:HG22 | 1.95                     | 0.48              |
| 37:d:128:TYR:HD2  | 37:d:156:LEU:HD23 | 1.78                     | 0.48              |
| 50:q:71:ILE:CD1   | 50:q:82:LYS:HB3   | 2.43                     | 0.48              |
| 2:1:10:ARG:HD2    | 44:k:59:TYR:CZ    | 2.48                     | 0.48              |
| 4:3:279:U:H2'     | 4:3:280:A:C8      | 2.48                     | 0.48              |
| 4:3:618:G:N1      | 4:3:1283:A:OP2    | 2.28                     | 0.48              |
| 4:3:845:U:OP2     | 44:k:30:LYS:HE3   | 2.12                     | 0.48              |
| 4:3:1118:U:H5''   | 40:g:41:ARG:CZ    | 2.44                     | 0.48              |
| 4:3:1460:G:H2'    | 4:3:1461:A:C8     | 2.49                     | 0.48              |
| 4:3:1583:G:H2'    | 4:3:1584:U:C6     | 2.49                     | 0.48              |
| 4:3:2119:A:H3'    | 4:3:2120:G:C8     | 2.48                     | 0.48              |
| 4:3:2335:A:H2'    | 4:3:2336:A:C8     | 2.49                     | 0.48              |
| 6:5:1215:U:OP2    | 16:F:114:THR:HG23 | 2.14                     | 0.48              |
| 11:A:249:LYS:HB3  | 11:A:253:GLU:OE2  | 2.14                     | 0.48              |
| 13:C:97:LEU:O     | 13:C:101:VAL:HG23 | 2.14                     | 0.48              |
| 16:F:34:LYS:HD2   | 16:F:37:LEU:HB3   | 1.95                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:L:69:LEU:O     | 22:L:73:ILE:HG13  | 2.13                     | 0.48              |
| 24:N:14:LEU:CD1   | 24:N:15:HIS:HD2   | 2.26                     | 0.48              |
| 27:Q:73:ARG:HH22  | 27:Q:83:GLN:HB3   | 1.79                     | 0.48              |
| 30:T:36:LEU:H     | 30:T:41:ARG:NH2   | 2.11                     | 0.48              |
| 37:d:92:ARG:O     | 37:d:95:ARG:HG2   | 2.14                     | 0.48              |
| 42:i:101:ASP:HB2  | 42:i:127:VAL:HG13 | 1.96                     | 0.48              |
| 57:x:75:ASN:O     | 57:x:75:ASN:ND2   | 2.43                     | 0.48              |
| 2:1:15:LYS:NZ     | 4:3:662:U:OP1     | 2.46                     | 0.48              |
| 4:3:356:A:H5'     | 4:3:374:A:H1'     | 1.95                     | 0.48              |
| 6:5:510:U:H2'     | 6:5:511:A:H8      | 1.79                     | 0.48              |
| 11:A:214:ILE:HD12 | 15:E:174:TYR:CE2  | 2.48                     | 0.48              |
| 13:C:186:GLU:OE1  | 13:C:186:GLU:N    | 2.40                     | 0.48              |
| 15:E:173:PRO:HB3  | 17:G:80:ARG:HG3   | 1.95                     | 0.48              |
| 21:K:53:MET:SD    | 21:K:103:LEU:HD22 | 2.53                     | 0.48              |
| 22:L:68:ASP:OD1   | 22:L:69:LEU:HD12  | 2.14                     | 0.48              |
| 28:R:36:ARG:HH22  | 28:R:77:THR:HG23  | 1.79                     | 0.48              |
| 34:a:240:HIS:CE1  | 34:a:254:PRO:HA   | 2.48                     | 0.48              |
| 37:d:42:ASP:HB3   | 37:d:46:ASP:OD1   | 2.14                     | 0.48              |
| 37:d:45:ARG:HE    | 37:d:78:LYS:HZ3   | 1.61                     | 0.48              |
| 48:o:36:LYS:HE2   | 48:o:85:ASN:C     | 2.38                     | 0.48              |
| 53:t:1:MET:HG3    | 53:t:2:GLN:H      | 1.79                     | 0.48              |
| 2:1:23:HIS:ND1    | 2:1:43:LYS:O      | 2.47                     | 0.48              |
| 4:3:154:U:H2'     | 4:3:155:A:H8      | 1.78                     | 0.48              |
| 4:3:618:G:H3'     | 4:3:1281:A:H61    | 1.78                     | 0.48              |
| 4:3:1032:A:O5'    | 49:p:92:LYS:NZ    | 2.42                     | 0.48              |
| 4:3:2119:A:H3'    | 4:3:2120:G:H8     | 1.77                     | 0.48              |
| 4:3:2644:U:H4'    | 35:b:83:GLU:OE2   | 2.14                     | 0.48              |
| 5:4:6:U:H1'       | 47:n:44:TRP:CH2   | 2.48                     | 0.48              |
| 6:5:853:A:H2'     | 6:5:854:A:C8      | 2.49                     | 0.48              |
| 10:9:52:THR:HG21  | 10:9:164:ASP:O    | 2.13                     | 0.48              |
| 15:E:114:LYS:HB2  | 15:E:114:LYS:NZ   | 2.28                     | 0.48              |
| 21:K:44:ARG:O     | 21:K:70:LEU:HD12  | 2.14                     | 0.48              |
| 35:b:63:ASN:OD1   | 35:b:64:LYS:N     | 2.45                     | 0.48              |
| 37:d:65:PRO:HB2   | 37:d:87:CYS:HB3   | 1.96                     | 0.48              |
| 37:d:70:ALA:HB2   | 37:d:85:ILE:HD11  | 1.95                     | 0.48              |
| 39:f:95:LYS:NZ    | 39:f:97:ILE:HB    | 2.29                     | 0.48              |
| 41:h:39:PHE:HE1   | 41:h:65:PHE:CE2   | 2.32                     | 0.48              |
| 44:k:61:ARG:NH1   | 44:k:61:ARG:HG2   | 2.28                     | 0.48              |
| 46:m:57:PHE:HB2   | 46:m:60:ARG:HE    | 1.79                     | 0.48              |
| 50:q:60:GLU:HB2   | 50:q:91:LYS:HE3   | 1.95                     | 0.48              |
| 51:r:9:ARG:O      | 51:r:9:ARG:HD3    | 2.14                     | 0.48              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:3:339:U:H2'    | 4:3:340:U:C6      | 2.48                     | 0.48              |
| 4:3:574:G:H1     | 4:3:587:U:H3      | 1.60                     | 0.48              |
| 4:3:1554:A:OP2   | 4:3:1576:G:N2     | 2.46                     | 0.48              |
| 4:3:2363:C:O2'   | 54:u:53:ARG:CZ    | 2.62                     | 0.48              |
| 4:3:2376:C:H2'   | 4:3:2377:A:H8     | 1.79                     | 0.48              |
| 5:4:104:C:H2'    | 5:4:105:A:C8      | 2.49                     | 0.48              |
| 6:5:1357:C:H4'   | 16:F:78:ARG:HD3   | 1.96                     | 0.48              |
| 15:E:32:VAL:HG21 | 15:E:35:LEU:HD11  | 1.96                     | 0.48              |
| 15:E:127:ASN:O   | 15:E:128:PRO:C    | 2.56                     | 0.48              |
| 15:E:155:GLU:CD  | 17:G:63:LYS:HZ3   | 2.13                     | 0.48              |
| 16:F:47:ASP:HA   | 16:F:50:GLU:OE1   | 2.14                     | 0.48              |
| 34:a:240:HIS:CE1 | 34:a:249:VAL:HG13 | 2.49                     | 0.48              |
| 39:f:92:ILE:C    | 39:f:94:THR:H     | 2.22                     | 0.48              |
| 41:h:100:LYS:HE3 | 41:h:104:ILE:HD11 | 1.95                     | 0.48              |
| 42:i:96:LEU:HD12 | 42:i:97:LYS:HG3   | 1.96                     | 0.48              |
| 44:k:113:LYS:HZ1 | 44:k:115:ILE:HD11 | 1.78                     | 0.48              |
| 55:v:15:GLY:O    | 55:v:26:ARG:HD3   | 2.13                     | 0.48              |
| 1:0:2:LYS:NZ     | 4:3:1655:U:H5'    | 2.29                     | 0.47              |
| 3:2:15:LYS:HE2   | 3:2:26:ILE:HD11   | 1.95                     | 0.47              |
| 4:3:707:C:C5     | 44:k:43:LYS:HD3   | 2.49                     | 0.47              |
| 4:3:1071:G:H1    | 4:3:1154:U:H3     | 1.62                     | 0.47              |
| 4:3:1093:U:H3    | 4:3:1115:G:H22    | 1.62                     | 0.47              |
| 4:3:1806:G:C4    | 34:a:190:ARG:NH2  | 2.82                     | 0.47              |
| 4:3:2078:A:H2'   | 4:3:2079:G:C8     | 2.49                     | 0.47              |
| 4:3:2088:U:H2'   | 4:3:2089:A:H8     | 1.79                     | 0.47              |
| 4:3:2118:U:H1'   | 4:3:2120:G:OP1    | 2.14                     | 0.47              |
| 4:3:2630:U:O2'   | 4:3:2829:G:N7     | 2.46                     | 0.47              |
| 6:5:214:U:H2'    | 6:5:215:C:H6      | 1.79                     | 0.47              |
| 11:A:75:VAL:HA   | 15:E:181:PHE:CD2  | 2.49                     | 0.47              |
| 11:A:84:PHE:CE1  | 11:A:177:ILE:HD12 | 2.45                     | 0.47              |
| 13:C:3:TYR:CE1   | 13:C:65:GLY:HA2   | 2.49                     | 0.47              |
| 15:E:125:PRO:HB2 | 15:E:127:ASN:O    | 2.13                     | 0.47              |
| 34:a:125:GLU:N   | 34:a:125:GLU:OE1  | 2.47                     | 0.47              |
| 34:a:234:ASN:O   | 34:a:241:GLY:HA3  | 2.13                     | 0.47              |
| 45:l:33:GLY:O    | 45:l:132:LEU:HD23 | 2.14                     | 0.47              |
| 47:n:5:THR:O     | 47:n:9:ARG:HG3    | 2.14                     | 0.47              |
| 4:3:901:C:H4'    | 4:3:902:U:O5'     | 2.15                     | 0.47              |
| 4:3:2132:G:N1    | 4:3:2180:U:OP2    | 2.47                     | 0.47              |
| 6:5:374:G:H2'    | 6:5:375:C:C6      | 2.49                     | 0.47              |
| 12:B:151:GLY:CA  | 12:B:176:MET:HE3  | 2.44                     | 0.47              |
| 15:E:40:LEU:HD12 | 15:E:57:TYR:HB3   | 1.96                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:E:183:ALA:O    | 15:E:186:VAL:HG23 | 2.14                     | 0.47              |
| 20:J:39:SER:O     | 20:J:43:MET:HG3   | 2.14                     | 0.47              |
| 23:M:26:ARG:HD2   | 23:M:27:CYS:N     | 2.29                     | 0.47              |
| 24:N:18:ASP:OD1   | 24:N:21:SER:HB2   | 2.14                     | 0.47              |
| 34:a:29:ASN:C     | 34:a:29:ASN:ND2   | 2.72                     | 0.47              |
| 36:c:157:VAL:HA   | 36:c:196:ALA:O    | 2.14                     | 0.47              |
| 39:f:130:ILE:HB   | 39:f:142:VAL:O    | 2.14                     | 0.47              |
| 41:h:112:LEU:HG   | 41:h:114:ALA:H    | 1.78                     | 0.47              |
| 53:t:24:VAL:HG21  | 53:t:27:ILE:HD11  | 1.95                     | 0.47              |
| 2:1:1:MET:HE1     | 4:3:625:G:N3      | 2.28                     | 0.47              |
| 4:3:502:A:N1      | 4:3:830:A:O2'     | 2.45                     | 0.47              |
| 4:3:756:A:H2'     | 4:3:757:A:H8      | 1.79                     | 0.47              |
| 4:3:1485:A:H4'    | 4:3:1486:U:C4     | 2.49                     | 0.47              |
| 4:3:1575:C:H2'    | 4:3:1576:G:O4'    | 2.14                     | 0.47              |
| 4:3:1688:A:O2'    | 35:b:119:PHE:O    | 2.27                     | 0.47              |
| 4:3:2120:G:O6     | 4:3:2176:G:O2'    | 2.28                     | 0.47              |
| 4:3:2158:C:H2'    | 4:3:2159:U:C6     | 2.48                     | 0.47              |
| 6:5:168:A:N6      | 6:5:219:A:O2'     | 2.47                     | 0.47              |
| 6:5:941:A:H2'     | 6:5:942:G:H8      | 1.78                     | 0.47              |
| 12:B:21:ARG:HH22  | 12:B:57:GLU:CD    | 2.22                     | 0.47              |
| 15:E:130:VAL:HG13 | 15:E:131:PRO:HD2  | 1.95                     | 0.47              |
| 17:G:14:PRO:HB3   | 17:G:41:LYS:NZ    | 2.30                     | 0.47              |
| 21:K:78:THR:HG23  | 21:K:108:TYR:O    | 2.14                     | 0.47              |
| 34:a:2:PRO:HD2    | 34:a:24:LYS:NZ    | 2.29                     | 0.47              |
| 35:b:32:GLU:HG2   | 35:b:33:PRO:HD2   | 1.96                     | 0.47              |
| 36:c:193:LEU:HD23 | 36:c:193:LEU:O    | 2.15                     | 0.47              |
| 37:d:8:TYR:CD1    | 37:d:12:ILE:HG13  | 2.49                     | 0.47              |
| 40:g:24:PHE:N     | 40:g:112:TYR:O    | 2.38                     | 0.47              |
| 41:h:50:MET:O     | 41:h:70:THR:HG22  | 2.15                     | 0.47              |
| 45:l:35:VAL:HG13  | 45:l:132:LEU:CD2  | 2.39                     | 0.47              |
| 46:m:93:THR:HB    | 46:m:97:TYR:HE1   | 1.79                     | 0.47              |
| 48:o:115:LYS:HD3  | 48:o:116:GLU:H    | 1.79                     | 0.47              |
| 4:3:944:U:P       | 45:l:24:ASN:H     | 2.37                     | 0.47              |
| 4:3:1255:G:O2'    | 50:q:82:LYS:HE2   | 2.14                     | 0.47              |
| 4:3:2279:G:H5'    | 54:u:34:ARG:NH1   | 2.30                     | 0.47              |
| 4:3:2299:U:OP1    | 4:3:2388:C:O2'    | 2.32                     | 0.47              |
| 4:3:2334:U:H3     | 4:3:2397:G:H1     | 1.61                     | 0.47              |
| 6:5:36:G:O2'      | 21:K:128:SER:O    | 2.32                     | 0.47              |
| 6:5:169:G:H1      | 6:5:196:G:N2      | 2.12                     | 0.47              |
| 6:5:197:A:H2'     | 6:5:198:A:C8      | 2.50                     | 0.47              |
| 6:5:1212:C:H4'    | 6:5:1274:G:H22    | 1.78                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:5:1472:G:H1'    | 6:5:1493:MA6:H2   | 1.96                     | 0.47              |
| 13:C:69:LYS:HA    | 13:C:72:ARG:HE    | 1.79                     | 0.47              |
| 15:E:1:MET:CG     | 15:E:2:GLN:H      | 2.24                     | 0.47              |
| 18:H:115:ARG:HD2  | 23:M:61:TRP:CD1   | 2.49                     | 0.47              |
| 34:a:233:MET:HG2  | 34:a:238:HIS:HB2  | 1.97                     | 0.47              |
| 35:b:22:GLU:CG    | 43:j:72:LYS:HD3   | 2.43                     | 0.47              |
| 36:c:127:LEU:HD11 | 36:c:201:LYS:HG2  | 1.96                     | 0.47              |
| 42:i:96:LEU:O     | 42:i:100:SER:OG   | 2.32                     | 0.47              |
| 44:k:81:ASN:HA    | 44:k:115:ILE:O    | 2.13                     | 0.47              |
| 54:u:38:LYS:HD2   | 54:u:53:ARG:HH21  | 1.77                     | 0.47              |
| 2:1:31:PRO:HD3    | 59:z:20:LEU:HD21  | 1.96                     | 0.47              |
| 4:3:193:G:O6      | 4:3:209:G:O2'     | 2.29                     | 0.47              |
| 4:3:652:U:H2'     | 4:3:653:G:C8      | 2.50                     | 0.47              |
| 4:3:1036:A:OP2    | 4:3:1189:G:N1     | 2.34                     | 0.47              |
| 4:3:1235:U:H1'    | 44:k:4:ASN:ND2    | 2.29                     | 0.47              |
| 4:3:1958:U:H1'    | 4:3:1961:A:N7     | 2.30                     | 0.47              |
| 4:3:2116:U:H5'    | 4:3:2149:U:O2'    | 2.15                     | 0.47              |
| 6:5:943:C:H2'     | 6:5:944:A:H8      | 1.79                     | 0.47              |
| 9:8:40:C:H4'      | 22:L:119:LYS:HZ1  | 1.80                     | 0.47              |
| 15:E:71:ASP:N     | 15:E:71:ASP:OD1   | 2.46                     | 0.47              |
| 20:J:62:LYS:O     | 20:J:65:LYS:HG2   | 2.13                     | 0.47              |
| 36:c:160:VAL:HG12 | 36:c:203:VAL:HG11 | 1.95                     | 0.47              |
| 4:3:12:A:H2'      | 4:3:13:C:O4'      | 2.14                     | 0.47              |
| 4:3:474:U:H2'     | 4:3:475:A:C8      | 2.49                     | 0.47              |
| 4:3:1143:U:O3'    | 40:g:77:LYS:HD3   | 2.14                     | 0.47              |
| 4:3:2011:G:H3'    | 4:3:2012:A:H8     | 1.79                     | 0.47              |
| 4:3:2254:G:H2'    | 4:3:2255:A:C8     | 2.49                     | 0.47              |
| 5:4:82:U:H2'      | 5:4:83:U:H4'      | 1.95                     | 0.47              |
| 6:5:483:U:H2'     | 6:5:484:A:C8      | 2.50                     | 0.47              |
| 6:5:725:A:H2'     | 6:5:726:A:C8      | 2.49                     | 0.47              |
| 6:5:1384:A:H2'    | 6:5:1385:A:C8     | 2.49                     | 0.47              |
| 11:A:201:LEU:HD13 | 11:A:215:ILE:HB   | 1.97                     | 0.47              |
| 11:A:293:ARG:NH2  | 30:T:50:GLN:HG2   | 2.29                     | 0.47              |
| 13:C:70:GLN:OE1   | 13:C:70:GLN:N     | 2.44                     | 0.47              |
| 15:E:94:TYR:HE2   | 27:Q:84:ARG:HD2   | 1.80                     | 0.47              |
| 25:O:44:LYS:HG3   | 25:O:45:GLU:OE1   | 2.13                     | 0.47              |
| 30:T:23:LEU:O     | 30:T:27:ARG:HG2   | 2.14                     | 0.47              |
| 30:T:45:LYS:O     | 30:T:48:ILE:HG12  | 2.15                     | 0.47              |
| 35:b:14:SER:N     | 35:b:26:ILE:O     | 2.43                     | 0.47              |
| 37:d:85:ILE:HG13  | 37:d:85:ILE:O     | 2.14                     | 0.47              |
| 38:e:136:ILE:HD13 | 38:e:147:PHE:HD2  | 1.78                     | 0.47              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 41:h:9:ILE:N     | 41:h:57:ALA:HB3   | 2.29                     | 0.47              |
| 42:i:40:ARG:HG2  | 42:i:40:ARG:HH11  | 1.80                     | 0.47              |
| 43:j:98:ILE:HD13 | 43:j:114:ILE:HG23 | 1.96                     | 0.47              |
| 46:m:33:THR:OG1  | 46:m:34:THR:N     | 2.47                     | 0.47              |
| 49:p:4:LYS:HD2   | 49:p:4:LYS:C      | 2.39                     | 0.47              |
| 49:p:109:VAL:HA  | 49:p:112:VAL:HG22 | 1.97                     | 0.47              |
| 57:x:59:ALA:O    | 57:x:62:LEU:HG    | 2.14                     | 0.47              |
| 1:0:35:ARG:NH2   | 4:3:56:G:H1'      | 2.29                     | 0.47              |
| 4:3:155:A:H2'    | 4:3:156:A:C8      | 2.49                     | 0.47              |
| 4:3:867:G:H4'    | 44:k:39:GLN:HE21  | 1.80                     | 0.47              |
| 4:3:1440:U:H2'   | 4:3:1441:A:C8     | 2.50                     | 0.47              |
| 4:3:2132:G:H1    | 4:3:2180:U:P      | 2.38                     | 0.47              |
| 4:3:2172:A:O5'   | 4:3:2172:A:H8     | 1.98                     | 0.47              |
| 4:3:2223:C:H2'   | 4:3:2224:A:H8     | 1.79                     | 0.47              |
| 4:3:2587:U:H4'   | 35:b:138:GLY:HA3  | 1.97                     | 0.47              |
| 4:3:2623:U:H1'   | 58:y:4:GLN:HB3    | 1.97                     | 0.47              |
| 5:4:65:G:H2'     | 5:4:66:A:H8       | 1.80                     | 0.47              |
| 6:5:275:A:H5''   | 6:5:276:U:H3'     | 1.96                     | 0.47              |
| 6:5:536:U:H5''   | 21:K:124:ARG:HG2  | 1.97                     | 0.47              |
| 6:5:561:A:H2     | 21:K:12:ARG:NH1   | 2.12                     | 0.47              |
| 6:5:1279:G:HO2'  | 6:5:1280:A:H8     | 1.62                     | 0.47              |
| 6:5:1389:U:H2'   | 6:5:1390:G:H8     | 1.79                     | 0.47              |
| 7:6:33:U:O2'     | 16:F:82:SER:HA    | 2.15                     | 0.47              |
| 11:A:113:LEU:O   | 11:A:116:THR:OG1  | 2.33                     | 0.47              |
| 13:C:7:ILE:HA    | 13:C:62:TYR:OH    | 2.15                     | 0.47              |
| 13:C:60:MET:HA   | 13:C:191:ILE:HG21 | 1.96                     | 0.47              |
| 13:C:199:TRP:HA  | 13:C:202:ARG:HH11 | 1.77                     | 0.47              |
| 14:D:100:LYS:NZ  | 14:D:128:THR:OG1  | 2.48                     | 0.47              |
| 15:E:42:LEU:HA   | 15:E:55:ALA:O     | 2.14                     | 0.47              |
| 15:E:45:LEU:HG   | 15:E:47:TYR:O     | 2.14                     | 0.47              |
| 17:G:125:ASP:OD1 | 17:G:126:LYS:N    | 2.48                     | 0.47              |
| 18:H:51:GLU:CD   | 18:H:55:ASP:HB2   | 2.39                     | 0.47              |
| 19:I:65:LYS:NZ   | 19:I:68:ARG:HH22  | 2.12                     | 0.47              |
| 19:I:85:VAL:HG23 | 19:I:86:ASN:H     | 1.80                     | 0.47              |
| 20:J:115:LYS:HG3 | 30:T:35:HIS:CB    | 2.45                     | 0.47              |
| 22:L:72:GLU:HA   | 22:L:75:LEU:HG    | 1.97                     | 0.47              |
| 27:Q:99:VAL:HG12 | 27:Q:100:PRO:HD2  | 1.97                     | 0.47              |
| 28:R:14:HIS:O    | 28:R:17:LYS:HG2   | 2.14                     | 0.47              |
| 34:a:143:GLU:HA  | 34:a:170:ILE:HB   | 1.96                     | 0.47              |
| 35:b:47:TYR:HD2  | 35:b:85:ARG:NE    | 2.12                     | 0.47              |
| 37:d:151:GLY:O   | 37:d:152:PHE:CD1  | 2.68                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 38:e:42:LEU:HG    | 38:e:44:LEU:CD2   | 2.43                     | 0.47              |
| 40:g:55:LYS:HB2   | 40:g:58:ILE:HG22  | 1.95                     | 0.47              |
| 40:g:100:VAL:HG12 | 40:g:103:LYS:HE3  | 1.95                     | 0.47              |
| 48:o:104:MET:HE2  | 48:o:104:MET:HA   | 1.95                     | 0.47              |
| 51:r:4:PHE:HE2    | 51:r:6:LYS:HE2    | 1.80                     | 0.47              |
| 51:r:119:LYS:O    | 51:r:123:ALA:N    | 2.45                     | 0.47              |
| 55:v:17:ASN:HB2   | 55:v:27:ARG:HD2   | 1.96                     | 0.47              |
| 3:2:11:CYS:SG     | 3:2:32:HIS:CE1    | 3.08                     | 0.47              |
| 4:3:610:G:H2'     | 4:3:611:A:C8      | 2.50                     | 0.47              |
| 4:3:776:U:H2'     | 4:3:777:C:H6      | 1.80                     | 0.47              |
| 6:5:670:G:H4'     | 15:E:84:ARG:NH2   | 2.30                     | 0.47              |
| 10:9:1:MET:HE2    | 10:9:1:MET:N      | 2.30                     | 0.47              |
| 12:B:173:GLU:O    | 12:B:173:GLU:HG2  | 2.15                     | 0.47              |
| 15:E:86:LEU:HD22  | 27:Q:96:LEU:HD21  | 1.97                     | 0.47              |
| 18:H:11:ARG:CZ    | 18:H:83:LEU:HD21  | 2.45                     | 0.47              |
| 23:M:39:VAL:HG13  | 23:M:43:CYS:HB2   | 1.97                     | 0.47              |
| 43:j:24:VAL:HG13  | 43:j:33:ALA:HB2   | 1.97                     | 0.47              |
| 48:o:56:ARG:HG2   | 48:o:57:GLY:N     | 2.30                     | 0.47              |
| 51:r:47:ILE:HG12  | 51:r:103:LEU:HD21 | 1.95                     | 0.47              |
| 53:t:36:VAL:HG13  | 53:t:39:LEU:HB2   | 1.95                     | 0.47              |
| 4:3:223:A:N3      | 4:3:238:U:O2'     | 2.38                     | 0.47              |
| 4:3:334:A:P       | 53:t:105:LYS:HZ1  | 2.38                     | 0.47              |
| 4:3:363:G:P       | 53:t:73:LYS:HZ2   | 2.38                     | 0.47              |
| 4:3:603:G:H2'     | 4:3:2037:A:N7     | 2.30                     | 0.47              |
| 4:3:1598:U:H2'    | 4:3:1599:C:C6     | 2.50                     | 0.47              |
| 4:3:2336:A:H2'    | 4:3:2337:U:C6     | 2.49                     | 0.47              |
| 6:5:1401:A:H2'    | 6:5:1402:U:H6     | 1.78                     | 0.47              |
| 13:C:144:LEU:HG   | 13:C:145:LYS:H    | 1.80                     | 0.47              |
| 15:E:161:GLN:CG   | 17:G:59:VAL:HG12  | 2.44                     | 0.47              |
| 19:I:69:GLU:OE2   | 23:M:45:ARG:CZ    | 2.63                     | 0.47              |
| 21:K:46:VAL:HG22  | 21:K:69:ARG:HB3   | 1.97                     | 0.47              |
| 22:L:65:ILE:HG22  | 22:L:67:GLY:H     | 1.80                     | 0.47              |
| 27:Q:103:LYS:O    | 27:Q:104:ASP:HB2  | 2.15                     | 0.47              |
| 43:j:6:THR:HG22   | 43:j:8:LEU:HG     | 1.96                     | 0.47              |
| 51:r:62:HIS:HB2   | 51:r:64:MET:HE1   | 1.97                     | 0.47              |
| 4:3:768:G:N2      | 4:3:769:A:N7      | 2.63                     | 0.47              |
| 4:3:867:G:N3      | 44:k:53:GLY:HA3   | 2.29                     | 0.47              |
| 4:3:1715:A:O2'    | 4:3:1769:A:H2'    | 2.14                     | 0.47              |
| 4:3:2131:G:H2'    | 4:3:2132:G:O4'    | 2.15                     | 0.47              |
| 4:3:2324:A:H2'    | 4:3:2325:U:C6     | 2.50                     | 0.47              |
| 4:3:2595:A:H61    | 4:3:2616:G:H1'    | 1.80                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:5:540:U:OP1     | 13:C:9:LYS:HE3    | 2.15                     | 0.47              |
| 15:E:43:LYS:HE3   | 15:E:57:TYR:CE2   | 2.49                     | 0.47              |
| 16:F:61:PHE:CE1   | 16:F:65:VAL:HG21  | 2.50                     | 0.47              |
| 26:P:48:HIS:HB3   | 26:P:73:LYS:HD2   | 1.96                     | 0.47              |
| 32:Y:77:U:H3'     | 32:Y:78:C:H6      | 1.80                     | 0.47              |
| 44:k:20:LEU:HB3   | 44:k:32:SER:HB3   | 1.97                     | 0.47              |
| 49:p:97:LEU:HG    | 49:p:105:PHE:HB2  | 1.97                     | 0.47              |
| 2:1:4:LYS:HG3     | 2:1:6:ALA:H       | 1.80                     | 0.46              |
| 4:3:818:A:H2'     | 4:3:819:U:H4'     | 1.97                     | 0.46              |
| 4:3:1135:C:H2'    | 4:3:1136:U:O4'    | 2.15                     | 0.46              |
| 4:3:2197:U:H3'    | 4:3:2198:G:H8     | 1.80                     | 0.46              |
| 4:3:2764:U:H1'    | 4:3:2765:A:H5''   | 1.98                     | 0.46              |
| 6:5:369:A:H2'     | 6:5:370:A:H8      | 1.79                     | 0.46              |
| 6:5:747:C:H2'     | 6:5:748:U:C6      | 2.50                     | 0.46              |
| 6:5:1062:C:H2'    | 6:5:1063:G:C8     | 2.47                     | 0.46              |
| 6:5:1213:A:H5'    | 6:5:1310:C:H41    | 1.80                     | 0.46              |
| 6:5:1323:A:H3'    | 6:5:1324:A:C8     | 2.50                     | 0.46              |
| 11:A:95:LEU:HG    | 11:A:229:MET:CE   | 2.43                     | 0.46              |
| 12:B:34:LEU:HD21  | 23:M:37:PHE:O     | 2.15                     | 0.46              |
| 13:C:144:LEU:HD23 | 13:C:149:ILE:HD11 | 1.97                     | 0.46              |
| 14:D:162:ALA:O    | 14:D:167:ARG:NE   | 2.48                     | 0.46              |
| 16:F:102:TRP:HA   | 16:F:105:MET:HG3  | 1.97                     | 0.46              |
| 16:F:107:ALA:HB2  | 16:F:122:GLU:HG2  | 1.96                     | 0.46              |
| 22:L:16:GLU:OE1   | 22:L:16:GLU:N     | 2.32                     | 0.46              |
| 22:L:87:ARG:HG2   | 22:L:97:VAL:HG13  | 1.96                     | 0.46              |
| 29:S:16:LYS:NZ    | 29:S:20:ASN:OD1   | 2.46                     | 0.46              |
| 35:b:105:GLY:HA2  | 35:b:181:ILE:O    | 2.14                     | 0.46              |
| 46:m:55:ASP:OD1   | 46:m:83:PHE:HD2   | 1.98                     | 0.46              |
| 4:3:51:A:H5''     | 4:3:53:G:O4'      | 2.16                     | 0.46              |
| 4:3:1568:C:H3'    | 4:3:1569:A:C8     | 2.50                     | 0.46              |
| 4:3:1801:U:H2'    | 4:3:1802:C:C6     | 2.50                     | 0.46              |
| 4:3:2057:C:H4'    | 35:b:144:GLN:HE22 | 1.79                     | 0.46              |
| 6:5:989:A:HO2'    | 23:M:12:ARG:HH12  | 1.62                     | 0.46              |
| 6:5:1138:U:H2'    | 6:5:1139:A:H8     | 1.81                     | 0.46              |
| 12:B:29:GLN:HA    | 12:B:32:LYS:HG2   | 1.97                     | 0.46              |
| 12:B:153:LYS:HE3  | 12:B:204:TRP:CE3  | 2.50                     | 0.46              |
| 16:F:113:LYS:O    | 16:F:118:LYS:HG3  | 2.15                     | 0.46              |
| 18:H:65:ILE:HG22  | 18:H:67:VAL:HG23  | 1.97                     | 0.46              |
| 20:J:10:SER:HA    | 20:J:72:MET:HA    | 1.97                     | 0.46              |
| 22:L:29:ARG:O     | 22:L:33:ILE:HG13  | 2.15                     | 0.46              |
| 23:M:19:ARG:HH11  | 23:M:19:ARG:HG3   | 1.81                     | 0.46              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 34:a:73:ARG:NH2  | 34:a:123:ALA:HB2  | 2.30                     | 0.46              |
| 42:i:109:LYS:HE2 | 42:i:122:ILE:HB   | 1.98                     | 0.46              |
| 46:m:22:VAL:HA   | 46:m:25:VAL:HG12  | 1.97                     | 0.46              |
| 48:o:61:SER:O    | 48:o:61:SER:OG    | 2.28                     | 0.46              |
| 49:p:95:SER:O    | 49:p:99:ILE:HG12  | 2.15                     | 0.46              |
| 52:s:47:VAL:HG23 | 52:s:48:TYR:HD1   | 1.80                     | 0.46              |
| 57:x:10:GLN:NE2  | 57:x:11:SER:O     | 2.49                     | 0.46              |
| 4:3:895:G:O2'    | 4:3:953:G:O6      | 2.32                     | 0.46              |
| 4:3:916:U:H2'    | 4:3:917:G:C8      | 2.51                     | 0.46              |
| 4:3:1600:A:H1'   | 34:a:62:ASN:ND2   | 2.29                     | 0.46              |
| 4:3:2120:G:N1    | 4:3:2176:G:O3'    | 2.40                     | 0.46              |
| 4:3:2638:G:H2'   | 4:3:2639:G:H8     | 1.80                     | 0.46              |
| 5:4:3:U:O2'      | 5:4:24:A:N1       | 2.47                     | 0.46              |
| 6:5:682:G:N2     | 6:5:701:A:OP2     | 2.42                     | 0.46              |
| 6:5:989:A:C5     | 6:5:1191:U:H4'    | 2.50                     | 0.46              |
| 7:6:33:U:H6      | 7:6:33:U:H5''     | 1.80                     | 0.46              |
| 8:7:10:G:H2'     | 8:7:11:U:C6       | 2.50                     | 0.46              |
| 11:A:47:PRO:HB3  | 11:A:49:ARG:NH1   | 2.30                     | 0.46              |
| 12:B:138:ARG:O   | 12:B:142:ILE:HG12 | 2.16                     | 0.46              |
| 14:D:96:ASN:CG   | 14:D:98:LYS:HG2   | 2.41                     | 0.46              |
| 15:E:99:SER:H    | 27:Q:50:ARG:HH22  | 1.63                     | 0.46              |
| 20:J:118:LYS:HA  | 30:T:34:TYR:CE1   | 2.50                     | 0.46              |
| 21:K:78:THR:HG21 | 21:K:95:LEU:HD11  | 1.98                     | 0.46              |
| 22:L:4:ILE:HA    | 22:L:57:ARG:HH21  | 1.80                     | 0.46              |
| 37:d:6:ALA:O     | 37:d:10:LYS:HG3   | 2.16                     | 0.46              |
| 37:d:60:ILE:HG22 | 37:d:99:PHE:CE1   | 2.43                     | 0.46              |
| 44:k:82:LEU:HA   | 44:k:85:ILE:HG22  | 1.98                     | 0.46              |
| 47:n:63:LYS:O    | 47:n:63:LYS:HD3   | 2.15                     | 0.46              |
| 50:q:34:GLN:CD   | 50:q:54:ARG:HB3   | 2.40                     | 0.46              |
| 54:u:34:ARG:HG3  | 54:u:53:ARG:NH1   | 2.31                     | 0.46              |
| 2:1:15:LYS:HD3   | 4:3:664:G:H5''    | 1.97                     | 0.46              |
| 3:2:4:ARG:HB2    | 3:2:34:GLN:HE21   | 1.80                     | 0.46              |
| 4:3:50:G:H22     | 4:3:180:A:H5''    | 1.80                     | 0.46              |
| 4:3:783:1MG:C8   | 4:3:785:A:C8      | 3.03                     | 0.46              |
| 4:3:859:G:H2'    | 4:3:860:C:C6      | 2.51                     | 0.46              |
| 4:3:2052:C:H1'   | 58:y:19:HIS:HE2   | 1.80                     | 0.46              |
| 4:3:2136:A:H2'   | 4:3:2137:A:H8     | 1.80                     | 0.46              |
| 4:3:2267:G:H2'   | 4:3:2268:C:C6     | 2.51                     | 0.46              |
| 6:5:147:A:H2'    | 6:5:148:A:C8      | 2.50                     | 0.46              |
| 6:5:404:A:P      | 13:C:111:ARG:HH12 | 2.39                     | 0.46              |
| 6:5:458:G:H2'    | 6:5:459:C:C6      | 2.50                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:5:1074:U:O2'    | 6:5:1093:A:OP2    | 2.28                     | 0.46              |
| 11:A:103:VAL:HG12 | 11:A:105:VAL:HG13 | 1.98                     | 0.46              |
| 13:C:64:TYR:HB2   | 13:C:66:ILE:CD1   | 2.46                     | 0.46              |
| 13:C:123:LEU:HB2  | 13:C:143:ARG:O    | 2.15                     | 0.46              |
| 15:E:132:VAL:HG22 | 15:E:134:SER:H    | 1.80                     | 0.46              |
| 20:J:106:LYS:HB3  | 20:J:106:LYS:HE3  | 1.66                     | 0.46              |
| 21:K:86:ASN:OD1   | 21:K:86:ASN:N     | 2.49                     | 0.46              |
| 25:O:66:THR:HG22  | 25:O:67:ASP:OD1   | 2.15                     | 0.46              |
| 36:c:168:LEU:HD13 | 36:c:180:VAL:HG21 | 1.98                     | 0.46              |
| 37:d:10:LYS:O     | 37:d:14:LYS:HG2   | 2.15                     | 0.46              |
| 54:u:39:LYS:HB2   | 54:u:51:ILE:CD1   | 2.45                     | 0.46              |
| 59:z:11:CYS:SG    | 59:z:12:ASN:N     | 2.89                     | 0.46              |
| 4:3:32:G:P        | 49:p:4:LYS:HZ1    | 2.38                     | 0.46              |
| 4:3:1165:U:O2     | 35:b:158:ARG:NH2  | 2.30                     | 0.46              |
| 4:3:1906:G:H21    | 4:3:1909:C:N4     | 2.12                     | 0.46              |
| 4:3:1959:A:C5     | 43:j:22:ILE:HD12  | 2.50                     | 0.46              |
| 4:3:2155:G:C2     | 4:3:2156:G:C5     | 3.04                     | 0.46              |
| 4:3:2293:C:H5''   | 59:z:27:LYS:HZ1   | 1.79                     | 0.46              |
| 4:3:2841:A:H2'    | 4:3:2842:G:H8     | 1.80                     | 0.46              |
| 6:5:524:C:OP2     | 21:K:101:LYS:HE2  | 2.16                     | 0.46              |
| 6:5:704:U:H2'     | 6:5:705:A:H8      | 1.79                     | 0.46              |
| 12:B:29:GLN:HG3   | 12:B:32:LYS:HD2   | 1.98                     | 0.46              |
| 12:B:88:ILE:O     | 12:B:92:ILE:HG13  | 2.15                     | 0.46              |
| 12:B:170:MET:HE3  | 12:B:171:TYR:C    | 2.41                     | 0.46              |
| 13:C:97:LEU:HD23  | 13:C:97:LEU:H     | 1.80                     | 0.46              |
| 13:C:182:PRO:HA   | 13:C:186:GLU:OE2  | 2.16                     | 0.46              |
| 15:E:6:ILE:HG23   | 27:Q:96:LEU:HD11  | 1.98                     | 0.46              |
| 17:G:36:ILE:HA    | 17:G:69:ILE:HG22  | 1.96                     | 0.46              |
| 17:G:101:PHE:HE1  | 17:G:129:ARG:HA   | 1.81                     | 0.46              |
| 17:G:131:LYS:HB3  | 17:G:133:ILE:HG12 | 1.97                     | 0.46              |
| 21:K:20:LYS:HB3   | 21:K:107:ARG:NH2  | 2.30                     | 0.46              |
| 29:S:16:LYS:HA    | 29:S:19:LEU:HD12  | 1.98                     | 0.46              |
| 45:l:39:GLY:HA2   | 45:l:97:VAL:O     | 2.15                     | 0.46              |
| 51:r:34:ASN:HD21  | 58:y:36:LYS:HG2   | 1.80                     | 0.46              |
| 51:r:74:CYS:HB3   | 51:r:105:VAL:HG23 | 1.97                     | 0.46              |
| 3:2:6:SER:O       | 3:2:34:GLN:NE2    | 2.49                     | 0.46              |
| 4:3:668:A:H2'     | 4:3:669:A:C8      | 2.51                     | 0.46              |
| 4:3:740:A:H4'     | 34:a:9:ARG:CZ     | 2.46                     | 0.46              |
| 4:3:767:C:H2'     | 4:3:768:G:O4'     | 2.16                     | 0.46              |
| 4:3:799:A:H5''    | 34:a:217:GLY:CA   | 2.45                     | 0.46              |
| 4:3:849:C:H2'     | 4:3:850:G:H8      | 1.80                     | 0.46              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:3:1063:A:N6    | 4:3:1160:G:H2'    | 2.31                     | 0.46              |
| 4:3:1381:A:OP2   | 4:3:1405:G:N1     | 2.40                     | 0.46              |
| 4:3:1798:A:O2'   | 34:a:213:ILE:O    | 2.30                     | 0.46              |
| 5:4:12:U:OP2     | 5:4:68:C:O2'      | 2.33                     | 0.46              |
| 6:5:1127:A:H5''  | 19:I:50:THR:HG23  | 1.97                     | 0.46              |
| 15:E:51:LYS:HD3  | 15:E:51:LYS:N     | 2.30                     | 0.46              |
| 22:L:48:LEU:HD11 | 22:L:52:GLU:HG3   | 1.97                     | 0.46              |
| 26:P:52:GLU:HG2  | 26:P:52:GLU:O     | 2.15                     | 0.46              |
| 34:a:27:THR:HG23 | 34:a:86:ILE:H     | 1.81                     | 0.46              |
| 46:m:117:GLN:HG3 | 46:m:118:LEU:N    | 2.30                     | 0.46              |
| 50:q:5:VAL:HG22  | 50:q:12:TYR:HB2   | 1.97                     | 0.46              |
| 52:s:10:PRO:HA   | 52:s:29:PHE:HA    | 1.97                     | 0.46              |
| 53:t:3:ARG:NH2   | 53:t:74:LEU:HB2   | 2.24                     | 0.46              |
| 4:3:1798:A:H2    | 4:3:1836:A:H4'    | 1.79                     | 0.46              |
| 5:4:11:A:N6      | 5:4:67:G:O2'      | 2.48                     | 0.46              |
| 6:5:320:G:OP1    | 29:S:17:ARG:NH2   | 2.49                     | 0.46              |
| 6:5:1436:C:H2'   | 6:5:1437:A:H8     | 1.81                     | 0.46              |
| 12:B:11:ARG:HB3  | 12:B:16:LYS:HD3   | 1.97                     | 0.46              |
| 13:C:64:TYR:OH   | 13:C:94:GLU:OE1   | 2.29                     | 0.46              |
| 15:E:71:ASP:HA   | 15:E:74:ARG:NE    | 2.31                     | 0.46              |
| 18:H:101:LYS:O   | 18:H:103:LYS:N    | 2.47                     | 0.46              |
| 26:P:58:GLY:HA3  | 26:P:85:LYS:HD3   | 1.98                     | 0.46              |
| 27:Q:94:ARG:HB3  | 27:Q:101:PHE:CE1  | 2.50                     | 0.46              |
| 38:e:87:GLU:HA   | 38:e:136:ILE:O    | 2.15                     | 0.46              |
| 42:i:20:ILE:HG12 | 42:i:140:PRO:HB2  | 1.98                     | 0.46              |
| 44:k:34:ARG:HB3  | 44:k:41:ALA:HA    | 1.97                     | 0.46              |
| 49:p:6:GLY:C     | 49:p:8:GLN:H      | 2.23                     | 0.46              |
| 4:3:10:U:H2'     | 4:3:11:U:H4'      | 1.97                     | 0.46              |
| 4:3:2102:U:H2'   | 4:3:2103:C:C6     | 2.51                     | 0.46              |
| 4:3:2224:A:H2'   | 4:3:2225:G:H8     | 1.80                     | 0.46              |
| 6:5:409:G:N2     | 6:5:425:G:H1'     | 2.30                     | 0.46              |
| 6:5:688:G:H1'    | 6:5:693:A:N6      | 2.31                     | 0.46              |
| 6:5:1135:U:O4'   | 6:5:1157:G:N2     | 2.48                     | 0.46              |
| 6:5:1273:A:H2'   | 6:5:1273:A:N3     | 2.30                     | 0.46              |
| 10:9:69:VAL:HG11 | 10:9:159:LYS:NZ   | 2.31                     | 0.46              |
| 15:E:21:VAL:HG21 | 15:E:58:TYR:CD2   | 2.51                     | 0.46              |
| 17:G:29:LYS:CD   | 17:G:80:ARG:HE    | 2.28                     | 0.46              |
| 17:G:61:GLU:HG2  | 17:G:65:LYS:HA    | 1.97                     | 0.46              |
| 18:H:22:THR:OG1  | 18:H:64:ASP:HB3   | 2.16                     | 0.46              |
| 18:H:97:LYS:HA   | 18:H:100:LEU:HD12 | 1.98                     | 0.46              |
| 22:L:89:LEU:HA   | 22:L:92:ARG:HE    | 1.81                     | 0.46              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 35:b:21:ASN:HD21 | 48:o:38:LYS:NZ    | 2.14                     | 0.46              |
| 39:f:4:ILE:HD13  | 39:f:47:ARG:HG3   | 1.98                     | 0.46              |
| 45:l:45:ARG:O    | 45:l:48:GLU:HG3   | 2.16                     | 0.46              |
| 58:y:54:LYS:HB3  | 58:y:54:LYS:HE2   | 1.84                     | 0.46              |
| 4:3:60:G:O2'     | 4:3:75:A:N1       | 2.43                     | 0.46              |
| 4:3:158:U:H2'    | 4:3:159:G:C8      | 2.50                     | 0.46              |
| 4:3:408:G:OP2    | 4:3:459:A:N6      | 2.48                     | 0.46              |
| 4:3:933:A:H2'    | 4:3:933:A:N3      | 2.31                     | 0.46              |
| 4:3:1334:U:H2'   | 4:3:1335:A:H8     | 1.81                     | 0.46              |
| 4:3:2073:C:N4    | 4:3:2074:G:O6     | 2.49                     | 0.46              |
| 4:3:2083:U:OP2   | 4:3:2246:G:N2     | 2.40                     | 0.46              |
| 4:3:2106:G:H2'   | 4:3:2107:A:C8     | 2.50                     | 0.46              |
| 4:3:2531:C:O2'   | 4:3:2772:A:O2'    | 2.28                     | 0.46              |
| 4:3:2838:G:H2'   | 4:3:2883:A:H61    | 1.81                     | 0.46              |
| 4:3:2843:G:OP1   | 46:m:43:LYS:HE2   | 2.16                     | 0.46              |
| 6:5:515:G:H1     | 6:5:531:A:P       | 2.39                     | 0.46              |
| 6:5:716:C:H4'    | 27:Q:69:LYS:HZ1   | 1.81                     | 0.46              |
| 12:B:31:ALA:O    | 12:B:34:LEU:HG    | 2.15                     | 0.46              |
| 12:B:113:MET:HG3 | 12:B:147:ALA:CB   | 2.45                     | 0.46              |
| 14:D:188:PRO:HA  | 14:D:191:MET:HE2  | 1.97                     | 0.46              |
| 16:F:61:PHE:HA   | 16:F:123:ILE:HD11 | 1.96                     | 0.46              |
| 19:I:7:VAL:HG23  | 19:I:8:LYS:N      | 2.31                     | 0.46              |
| 36:c:43:ALA:O    | 36:c:44:SER:OG    | 2.28                     | 0.46              |
| 37:d:102:LYS:NZ  | 37:d:139:PRO:HG2  | 2.30                     | 0.46              |
| 4:3:863:U:O2'    | 4:3:866:G:O6      | 2.33                     | 0.46              |
| 6:5:35:C:H2'     | 6:5:36:G:C8       | 2.51                     | 0.46              |
| 6:5:473:A:H2'    | 6:5:474:G:H8      | 1.80                     | 0.46              |
| 6:5:720:U:O4'    | 30:T:53:ARG:HD2   | 2.16                     | 0.46              |
| 12:B:36:GLU:O    | 12:B:39:LYS:HG2   | 2.15                     | 0.46              |
| 12:B:37:ASP:OD1  | 12:B:38:GLU:N     | 2.49                     | 0.46              |
| 13:C:72:ARG:HG3  | 13:C:204:VAL:HG21 | 1.97                     | 0.46              |
| 17:G:118:THR:OG1 | 17:G:119:SER:N    | 2.48                     | 0.46              |
| 19:I:56:THR:HG22 | 19:I:68:ARG:CG    | 2.45                     | 0.46              |
| 22:L:24:GLY:H    | 22:L:66:GLU:HB2   | 1.81                     | 0.46              |
| 30:T:16:LYS:O    | 30:T:19:LYS:HG2   | 2.15                     | 0.46              |
| 37:d:36:ILE:O    | 37:d:88:LYS:HA    | 2.16                     | 0.46              |
| 39:f:90:GLY:O    | 39:f:125:GLU:HG2  | 2.16                     | 0.46              |
| 45:l:73:SER:HB2  | 45:l:93:TRP:CH2   | 2.51                     | 0.46              |
| 48:o:30:GLU:HG2  | 48:o:91:LYS:HE2   | 1.97                     | 0.46              |
| 55:v:33:LEU:HD22 | 55:v:49:LEU:HG    | 1.98                     | 0.46              |
| 3:2:18:LYS:N     | 3:2:18:LYS:HD2    | 2.31                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:3:621:U:H2'     | 4:3:622:U:C6      | 2.51                     | 0.45              |
| 4:3:622:U:H4'     | 36:c:94:LYS:CE    | 2.45                     | 0.45              |
| 4:3:631:A:H2'     | 4:3:632:A:H8      | 1.81                     | 0.45              |
| 4:3:787:C:OP2     | 4:3:1788:A:N6     | 2.49                     | 0.45              |
| 4:3:852:C:H2'     | 4:3:853:G:O4'     | 2.16                     | 0.45              |
| 4:3:909:U:H2'     | 4:3:910:G:C8      | 2.52                     | 0.45              |
| 4:3:933:A:N6      | 9:8:19:G:O2'      | 2.42                     | 0.45              |
| 4:3:1119:A:C8     | 40:g:53:VAL:HG21  | 2.51                     | 0.45              |
| 4:3:1306:G:H2'    | 4:3:1307:G:C8     | 2.49                     | 0.45              |
| 4:3:1436:C:H2'    | 4:3:1437:A:C8     | 2.51                     | 0.45              |
| 4:3:1509:U:H3     | 4:3:1530:G:H1     | 1.62                     | 0.45              |
| 4:3:1536:C:H2'    | 4:3:1537:A:C8     | 2.51                     | 0.45              |
| 4:3:2081:U:H2'    | 4:3:2082:U:C6     | 2.51                     | 0.45              |
| 6:5:1374:C:O2     | 6:5:1477:A:N6     | 2.49                     | 0.45              |
| 11:A:48:GLU:HA    | 11:A:51:HIS:HB3   | 1.98                     | 0.45              |
| 14:D:131:ILE:HD12 | 14:D:134:GLY:HA2  | 1.97                     | 0.45              |
| 15:E:40:LEU:HB2   | 15:E:57:TYR:HB2   | 1.97                     | 0.45              |
| 15:E:203:ASN:CG   | 15:E:206:ARG:HE   | 2.24                     | 0.45              |
| 16:F:130:THR:O    | 16:F:130:THR:OG1  | 2.32                     | 0.45              |
| 25:O:66:THR:H     | 25:O:69:VAL:HB    | 1.80                     | 0.45              |
| 36:c:136:THR:HG23 | 36:c:143:MET:HG2  | 1.96                     | 0.45              |
| 37:d:25:ILE:H     | 37:d:25:ILE:HD12  | 1.80                     | 0.45              |
| 39:f:55:GLN:HA    | 39:f:58:TYR:HB3   | 1.97                     | 0.45              |
| 45:l:38:LYS:NZ    | 45:l:128:THR:HB   | 2.31                     | 0.45              |
| 49:p:106:ASN:HA   | 49:p:109:VAL:HG22 | 1.98                     | 0.45              |
| 4:3:732:G:H2'     | 4:3:733:C:C6      | 2.50                     | 0.45              |
| 4:3:2106:G:H22    | 4:3:2198:G:H1     | 1.64                     | 0.45              |
| 4:3:2155:G:O2'    | 4:3:2156:G:H5'    | 2.16                     | 0.45              |
| 4:3:2580:A:OP2    | 35:b:151:ARG:N    | 2.49                     | 0.45              |
| 6:5:365:U:H3      | 6:5:388:G:H1      | 1.63                     | 0.45              |
| 6:5:684:A:H4'     | 20:J:42:THR:HG22  | 1.98                     | 0.45              |
| 10:9:54:LYS:HZ1   | 10:9:56:GLU:HB2   | 1.81                     | 0.45              |
| 34:a:251:ARG:HG3  | 34:a:252:ASP:OD1  | 2.16                     | 0.45              |
| 41:h:128:ALA:O    | 41:h:132:GLY:N    | 2.49                     | 0.45              |
| 42:i:20:ILE:N     | 42:i:141:THR:O    | 2.49                     | 0.45              |
| 49:p:3:ILE:H      | 49:p:3:ILE:HD12   | 1.81                     | 0.45              |
| 52:s:9:LYS:CD     | 52:s:10:PRO:HD2   | 2.42                     | 0.45              |
| 55:v:7:LEU:HD21   | 55:v:54:THR:HG21  | 1.99                     | 0.45              |
| 55:v:34:GLN:C     | 55:v:49:LEU:HD12  | 2.40                     | 0.45              |
| 3:2:20:HIS:HE1    | 3:2:24:ARG:HE     | 1.65                     | 0.45              |
| 4:3:989:G:H1      | 4:3:1000:U:H3     | 1.64                     | 0.45              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:3:1002:A:H4'   | 4:3:2279:G:H22    | 1.81                     | 0.45              |
| 4:3:1854:A:H3'   | 4:3:1855:A:H8     | 1.81                     | 0.45              |
| 4:3:1868:A:H5''  | 10:9:204:GLY:HA2  | 1.98                     | 0.45              |
| 4:3:2123:A:H5''  | 4:3:2124:A:C8     | 2.50                     | 0.45              |
| 4:3:2148:U:H2'   | 4:3:2149:U:H6     | 1.81                     | 0.45              |
| 4:3:2781:C:H2'   | 4:3:2782:A:C8     | 2.52                     | 0.45              |
| 6:5:9:A:N1       | 13:C:202:ARG:NE   | 2.62                     | 0.45              |
| 6:5:492:G:O2'    | 6:5:494:A:H1'     | 2.15                     | 0.45              |
| 6:5:1436:C:H2'   | 6:5:1437:A:C8     | 2.50                     | 0.45              |
| 12:B:167:ARG:NH1 | 32:Y:79:U:O4      | 2.50                     | 0.45              |
| 13:C:61:GLN:CB   | 13:C:71:PHE:CE2   | 2.97                     | 0.45              |
| 16:F:59:THR:O    | 16:F:62:GLU:HG3   | 2.16                     | 0.45              |
| 16:F:86:VAL:HB   | 16:F:154:ARG:CZ   | 2.46                     | 0.45              |
| 26:P:50:GLU:HG2  | 26:P:51:GLY:N     | 2.32                     | 0.45              |
| 30:T:12:GLU:HG3  | 30:T:16:LYS:HZ2   | 1.81                     | 0.45              |
| 34:a:251:ARG:HG3 | 34:a:252:ASP:N    | 2.32                     | 0.45              |
| 39:f:48:ASP:O    | 39:f:49:LEU:C     | 2.59                     | 0.45              |
| 39:f:93:ILE:CA   | 39:f:121:PHE:HE1  | 2.28                     | 0.45              |
| 43:j:88:LYS:NZ   | 43:j:93:PRO:O     | 2.50                     | 0.45              |
| 43:j:112:ASN:HA  | 43:j:115:LEU:HD12 | 1.97                     | 0.45              |
| 46:m:25:VAL:HG21 | 46:m:116:LEU:HG   | 1.99                     | 0.45              |
| 46:m:102:LYS:HD3 | 46:m:112:GLU:OE2  | 2.16                     | 0.45              |
| 56:w:22:LEU:HA   | 56:w:25:GLU:OE1   | 2.17                     | 0.45              |
| 58:y:30:CYS:HA   | 58:y:37:LYS:HE3   | 1.98                     | 0.45              |
| 58:y:47:MET:HE1  | 58:y:52:ARG:CD    | 2.46                     | 0.45              |
| 4:3:287:G:N1     | 39:f:42:LYS:HE2   | 2.32                     | 0.45              |
| 4:3:1095:U:H5''  | 41:h:68:LYS:HE2   | 1.98                     | 0.45              |
| 4:3:1176:U:OP1   | 42:i:30:LYS:NZ    | 2.50                     | 0.45              |
| 4:3:1260:U:H2'   | 4:3:1261:U:C6     | 2.51                     | 0.45              |
| 4:3:1809:A:H2'   | 4:3:1810:A:C8     | 2.52                     | 0.45              |
| 4:3:2134:G:H8    | 4:3:2134:G:OP2    | 1.98                     | 0.45              |
| 4:3:2286:A:H8    | 54:u:26:ASN:HD22  | 1.63                     | 0.45              |
| 4:3:2288:G:O6    | 54:u:28:ARG:NH2   | 2.50                     | 0.45              |
| 4:3:2683:G:OP1   | 43:j:31:ARG:HG2   | 2.16                     | 0.45              |
| 5:4:93:U:H2'     | 5:4:94:A:C8       | 2.51                     | 0.45              |
| 11:A:115:GLY:HA2 | 11:A:118:THR:HG22 | 1.98                     | 0.45              |
| 11:A:126:SER:OG  | 11:A:163:PHE:HE2  | 2.00                     | 0.45              |
| 11:A:156:ILE:O   | 11:A:160:GLU:OE1  | 2.34                     | 0.45              |
| 16:F:65:VAL:HG12 | 16:F:69:MET:HE3   | 1.97                     | 0.45              |
| 17:G:95:LEU:HD23 | 21:K:4:ILE:HG13   | 1.99                     | 0.45              |
| 18:H:11:ARG:NH1  | 18:H:87:ARG:HH21  | 2.01                     | 0.45              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 18:H:47:ILE:HA    | 18:H:50:MET:HE3  | 1.98                     | 0.45              |
| 23:M:33:VAL:HA    | 23:M:40:CYS:HA   | 1.99                     | 0.45              |
| 26:P:43:LYS:C     | 26:P:43:LYS:HD3  | 2.41                     | 0.45              |
| 26:P:64:VAL:HG23  | 26:P:76:ARG:HG2  | 1.97                     | 0.45              |
| 28:R:40:ILE:HA    | 28:R:44:PHE:CD2  | 2.51                     | 0.45              |
| 28:R:40:ILE:HA    | 28:R:44:PHE:HD2  | 1.81                     | 0.45              |
| 30:T:50:GLN:HG3   | 30:T:53:ARG:HH21 | 1.81                     | 0.45              |
| 40:g:37:ALA:O     | 40:g:41:ARG:HG2  | 2.17                     | 0.45              |
| 41:h:30:ILE:HG23  | 41:h:35:PHE:HD2  | 1.82                     | 0.45              |
| 42:i:48:THR:HG22  | 42:i:50:ASN:OD1  | 2.17                     | 0.45              |
| 52:s:14:GLU:H     | 52:s:14:GLU:CD   | 2.24                     | 0.45              |
| 54:u:18:LYS:O     | 54:u:19:LYS:HG2  | 2.17                     | 0.45              |
| 4:3:174:A:H2'     | 4:3:175:A:C8     | 2.51                     | 0.45              |
| 4:3:614:C:H2'     | 4:3:615:G:C8     | 2.51                     | 0.45              |
| 4:3:954:A:H5''    | 4:3:2276:A:N6    | 2.30                     | 0.45              |
| 4:3:1436:C:H2'    | 4:3:1437:A:H8    | 1.81                     | 0.45              |
| 4:3:1854:A:H1'    | 6:5:699:A:C4     | 2.52                     | 0.45              |
| 6:5:117:U:H2'     | 6:5:118:C:C6     | 2.52                     | 0.45              |
| 6:5:424:U:OP1     | 13:C:12:ARG:NH2  | 2.49                     | 0.45              |
| 9:8:28:A:H2'      | 9:8:29:U:H6      | 1.81                     | 0.45              |
| 14:D:78:LYS:HG2   | 14:D:85:ASN:HB2  | 1.97                     | 0.45              |
| 14:D:160:ILE:O    | 14:D:167:ARG:NH2 | 2.49                     | 0.45              |
| 15:E:132:VAL:O    | 15:E:134:SER:N   | 2.50                     | 0.45              |
| 16:F:74:LEU:HD11  | 16:F:144:ALA:HA  | 1.98                     | 0.45              |
| 19:I:57:ILE:HD12  | 23:M:41:ARG:CB   | 2.46                     | 0.45              |
| 22:L:55:ALA:O     | 22:L:59:VAL:HG23 | 2.17                     | 0.45              |
| 28:R:22:MET:HE1   | 28:R:29:ARG:H    | 1.81                     | 0.45              |
| 36:c:57:GLU:OE1   | 36:c:57:GLU:N    | 2.50                     | 0.45              |
| 44:k:120:LEU:HD23 | 44:k:120:LEU:H   | 1.81                     | 0.45              |
| 45:l:109:ILE:HG12 | 45:l:110:PRO:HD2 | 1.99                     | 0.45              |
| 4:3:35:U:H2'      | 4:3:482:G:H22    | 1.81                     | 0.45              |
| 4:3:516:A:OP2     | 53:t:44:ARG:HD2  | 2.17                     | 0.45              |
| 4:3:628:A:H2'     | 4:3:629:G:H8     | 1.82                     | 0.45              |
| 4:3:756:A:H2'     | 4:3:757:A:C8     | 2.51                     | 0.45              |
| 4:3:783:1MG:CM1   | 51:r:90:LYS:HE2  | 2.46                     | 0.45              |
| 4:3:1495:A:H2'    | 4:3:1496:A:C8    | 2.52                     | 0.45              |
| 4:3:1623:U:H2'    | 4:3:1624:A:C8    | 2.51                     | 0.45              |
| 4:3:1701:G:O2'    | 4:3:1998:U:O4    | 2.33                     | 0.45              |
| 4:3:2054:C:O2'    | 4:3:2827:A:N1    | 2.44                     | 0.45              |
| 4:3:2294:A:OP1    | 59:z:27:LYS:NZ   | 2.42                     | 0.45              |
| 4:3:2843:G:N2     | 46:m:94:PRO:O    | 2.43                     | 0.45              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 6:5:409:G:H22    | 6:5:425:G:H1'     | 1.82                     | 0.45              |
| 6:5:717:C:H2'    | 6:5:718:A:C8      | 2.51                     | 0.45              |
| 6:5:822:A:C5'    | 17:G:9:LYS:HZ2    | 2.29                     | 0.45              |
| 6:5:1318:C:H4'   | 18:H:124:ARG:NH1  | 2.31                     | 0.45              |
| 7:6:1:G:HO2'     | 7:6:2:G:P         | 2.40                     | 0.45              |
| 25:O:66:THR:HG22 | 25:O:67:ASP:N     | 2.31                     | 0.45              |
| 35:b:4:ARG:HB2   | 35:b:101:LEU:HG   | 1.98                     | 0.45              |
| 42:i:24:ALA:O    | 42:i:64:GLN:HB3   | 2.16                     | 0.45              |
| 47:n:62:LEU:HB3  | 47:n:69:ASN:ND2   | 2.31                     | 0.45              |
| 49:p:73:MET:HE1  | 49:p:78:PHE:HD1   | 1.80                     | 0.45              |
| 54:u:100:HIS:CD2 | 54:u:102:LEU:HG   | 2.52                     | 0.45              |
| 55:v:53:ARG:O    | 55:v:57:THR:HG23  | 2.16                     | 0.45              |
| 56:w:107:ASP:HA  | 56:w:110:LYS:HE3  | 1.99                     | 0.45              |
| 4:3:275:A:N6     | 4:3:294:G:H1'     | 2.31                     | 0.45              |
| 4:3:610:G:H5''   | 4:3:2510:G:C2     | 2.51                     | 0.45              |
| 4:3:1261:U:H2'   | 4:3:1262:G:H8     | 1.81                     | 0.45              |
| 4:3:1879:A:H2'   | 4:3:1880:G:O4'    | 2.17                     | 0.45              |
| 4:3:2032:G:H2'   | 4:3:2033:G:H8     | 1.82                     | 0.45              |
| 4:3:2794:U:H2'   | 4:3:2795:C:H6     | 1.80                     | 0.45              |
| 6:5:18:U:H2'     | 6:5:19:C:C6       | 2.50                     | 0.45              |
| 6:5:882:U:H3'    | 6:5:883:A:H8      | 1.80                     | 0.45              |
| 6:5:1022:G:H2'   | 6:5:1023:G:C8     | 2.51                     | 0.45              |
| 6:5:1302:C:O2'   | 22:L:29:ARG:NH2   | 2.50                     | 0.45              |
| 12:B:48:TYR:HE2  | 12:B:88:ILE:HG22  | 1.82                     | 0.45              |
| 12:B:220:ALA:O   | 12:B:222:ILE:N    | 2.50                     | 0.45              |
| 13:C:97:LEU:HD21 | 13:C:132:PRO:C    | 2.42                     | 0.45              |
| 15:E:140:GLN:HB2 | 15:E:141:PRO:HD2  | 1.98                     | 0.45              |
| 15:E:154:GLU:HG3 | 17:G:5:THR:C      | 2.41                     | 0.45              |
| 15:E:157:TRP:NE1 | 17:G:60:LEU:HB2   | 2.32                     | 0.45              |
| 16:F:74:LEU:HA   | 16:F:74:LEU:HD23  | 1.53                     | 0.45              |
| 21:K:127:ARG:HD2 | 21:K:133:LYS:O    | 2.16                     | 0.45              |
| 22:L:4:ILE:O     | 22:L:4:ILE:HG13   | 2.17                     | 0.45              |
| 32:Y:94:A:H8     | 32:Y:94:A:O5'     | 2.00                     | 0.45              |
| 36:c:30:LYS:NZ   | 36:c:33:PRO:HG2   | 2.32                     | 0.45              |
| 37:d:171:ARG:HA  | 37:d:171:ARG:NE   | 2.31                     | 0.45              |
| 44:k:129:HIS:CE1 | 44:k:149:LEU:HD23 | 2.51                     | 0.45              |
| 48:o:64:PHE:O    | 48:o:78:ASN:HA    | 2.16                     | 0.45              |
| 50:q:54:ARG:HB2  | 50:q:98:VAL:CB    | 2.46                     | 0.45              |
| 56:w:11:SER:OG   | 56:w:14:GLU:HG2   | 2.17                     | 0.45              |
| 58:y:13:ARG:HD2  | 58:y:17:ARG:NE    | 2.31                     | 0.45              |
| 2:1:2:LYS:HE2    | 4:3:246:G:C6      | 2.52                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:3:867:G:H2'     | 4:3:868:C:C6      | 2.51                     | 0.45              |
| 4:3:1092:A:H2'    | 4:3:1093:U:C6     | 2.52                     | 0.45              |
| 4:3:1824:G:C6     | 4:3:1825:U:C4     | 3.04                     | 0.45              |
| 4:3:1828:A:H2'    | 4:3:1829:U:C6     | 2.52                     | 0.45              |
| 4:3:2111:U:N3     | 4:3:2194:G:H1'    | 2.32                     | 0.45              |
| 4:3:2239:U:H5''   | 55:v:29:TRP:HD1   | 1.81                     | 0.45              |
| 5:4:56:A:H3'      | 5:4:57:G:H8       | 1.82                     | 0.45              |
| 6:5:354:U:H2'     | 6:5:355:A:C8      | 2.50                     | 0.45              |
| 6:5:403:A:H2'     | 6:5:404:A:C8      | 2.51                     | 0.45              |
| 6:5:762:G:N1      | 6:5:809:G:O2'     | 2.40                     | 0.45              |
| 6:5:1162:G:H5'    | 18:H:117:LYS:HZ2  | 1.80                     | 0.45              |
| 8:7:50:G:H1       | 8:7:62:C:H42      | 1.65                     | 0.45              |
| 13:C:91:ARG:HG2   | 13:C:181:PHE:CD2  | 2.51                     | 0.45              |
| 19:I:7:VAL:HG23   | 19:I:8:LYS:H      | 1.82                     | 0.45              |
| 19:I:79:LEU:HD23  | 19:I:80:MET:N     | 2.32                     | 0.45              |
| 21:K:43:LYS:HB2   | 21:K:70:LEU:HD11  | 1.99                     | 0.45              |
| 29:S:21:ASN:CG    | 29:S:59:ILE:HD12  | 2.42                     | 0.45              |
| 32:Y:77:U:H3'     | 32:Y:78:C:C6      | 2.52                     | 0.45              |
| 32:Y:79:U:O2      | 32:Y:80:U:N3      | 2.50                     | 0.45              |
| 34:a:154:PRO:HG3  | 34:a:195:GLU:OE2  | 2.16                     | 0.45              |
| 34:a:184:LEU:HD12 | 34:a:190:ARG:NE   | 2.32                     | 0.45              |
| 34:a:218:ARG:CG   | 34:a:222:ARG:HH12 | 2.26                     | 0.45              |
| 35:b:101:LEU:HD23 | 35:b:102:PHE:HE1  | 1.82                     | 0.45              |
| 37:d:132:ILE:N    | 37:d:152:PHE:O    | 2.48                     | 0.45              |
| 38:e:44:LEU:HD12  | 38:e:55:ILE:CG2   | 2.42                     | 0.45              |
| 40:g:88:GLU:OE2   | 40:g:90:VAL:HB    | 2.17                     | 0.45              |
| 42:i:78:TYR:CE1   | 42:i:89:LYS:HB3   | 2.51                     | 0.45              |
| 43:j:7:ARG:O      | 43:j:8:LEU:HD23   | 2.17                     | 0.45              |
| 48:o:104:MET:SD   | 48:o:112:ALA:HB1  | 2.56                     | 0.45              |
| 49:p:39:ILE:HG13  | 49:p:40:GLN:N     | 2.32                     | 0.45              |
| 49:p:86:ASN:OD1   | 49:p:86:ASN:C     | 2.60                     | 0.45              |
| 52:s:45:GLU:OE2   | 52:s:51:LYS:HA    | 2.16                     | 0.45              |
| 4:3:1372:U:O2     | 4:3:1413:A:H5'    | 2.17                     | 0.45              |
| 6:5:654:U:H4'     | 24:N:25:GLN:HG2   | 1.99                     | 0.45              |
| 6:5:894:A:H2'     | 6:5:895:A:C8      | 2.52                     | 0.45              |
| 6:5:1241:G:H21    | 6:5:1243:A:H8     | 1.65                     | 0.45              |
| 11:A:61:GLN:HG2   | 11:A:216:PRO:O    | 2.17                     | 0.45              |
| 11:A:89:ASN:C     | 11:A:93:LYS:HZ3   | 2.25                     | 0.45              |
| 13:C:61:GLN:HB3   | 13:C:71:PHE:HE2   | 1.80                     | 0.45              |
| 24:N:67:LEU:HD23  | 24:N:67:LEU:O     | 2.17                     | 0.45              |
| 25:O:28:ARG:NH1   | 25:O:29:ASP:OD2   | 2.50                     | 0.45              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 28:R:86:ASN:OD1  | 28:R:87:ARG:N     | 2.50                     | 0.45              |
| 31:X:44:ARG:NH2  | 31:X:47:LYS:HE2   | 2.32                     | 0.45              |
| 37:d:136:ILE:H   | 37:d:136:ILE:HD12 | 1.81                     | 0.45              |
| 52:s:10:PRO:HB3  | 52:s:29:PHE:CE1   | 2.52                     | 0.45              |
| 54:u:57:THR:HG23 | 54:u:57:THR:O     | 2.17                     | 0.45              |
| 4:3:226:A:H61    | 4:3:236:G:H1'     | 1.82                     | 0.45              |
| 4:3:279:U:H2'    | 4:3:280:A:H8      | 1.82                     | 0.45              |
| 4:3:479:A:OP1    | 36:c:47:GLN:N     | 2.45                     | 0.45              |
| 4:3:1081:A:C2    | 40:g:11:VAL:HG11  | 2.51                     | 0.45              |
| 4:3:1379:C:H4'   | 4:3:1606:A:H4'    | 1.98                     | 0.45              |
| 4:3:2561:G:C2    | 4:3:2591:G:H1'    | 2.51                     | 0.45              |
| 4:3:2690:U:C6    | 35:b:13:MET:HE1   | 2.51                     | 0.45              |
| 6:5:101:A:H61    | 6:5:309:A:H1'     | 1.82                     | 0.45              |
| 6:5:631:C:H2'    | 6:5:632:A:H8      | 1.81                     | 0.45              |
| 6:5:1201:C:P     | 22:L:90:ARG:HH12  | 2.40                     | 0.45              |
| 6:5:1216:G:H2'   | 6:5:1217:G:H8     | 1.82                     | 0.45              |
| 6:5:1505:G:H2'   | 6:5:1506:A:H8     | 1.82                     | 0.45              |
| 9:8:37:A:H3'     | 9:8:38:A:H8       | 1.81                     | 0.45              |
| 13:C:179:VAL:CG1 | 13:C:180:ARG:H    | 2.30                     | 0.45              |
| 21:K:49:ARG:HG2  | 21:K:67:LYS:CB    | 2.47                     | 0.45              |
| 23:M:46:GLU:HG2  | 23:M:47:LEU:N     | 2.31                     | 0.45              |
| 26:P:35:TYR:HB2  | 26:P:37:LYS:NZ    | 2.32                     | 0.45              |
| 34:a:15:HIS:ND1  | 34:a:214:GLY:O    | 2.49                     | 0.45              |
| 39:f:59:GLU:O    | 39:f:62:LYS:NZ    | 2.49                     | 0.45              |
| 39:f:96:GLN:O    | 39:f:100:GLN:NE2  | 2.50                     | 0.45              |
| 40:g:29:TYR:CZ   | 40:g:53:VAL:HG22  | 2.52                     | 0.45              |
| 42:i:20:ILE:HD13 | 42:i:58:ILE:HB    | 1.99                     | 0.45              |
| 45:l:77:LYS:HE2  | 45:l:77:LYS:HB3   | 1.68                     | 0.45              |
| 46:m:40:ASN:OD1  | 46:m:41:THR:N     | 2.50                     | 0.45              |
| 48:o:9:LEU:HD12  | 48:o:10:ILE:N     | 2.32                     | 0.45              |
| 51:r:97:THR:O    | 51:r:99:ARG:HD3   | 2.17                     | 0.45              |
| 56:w:16:VAL:HA   | 56:w:19:VAL:HG12  | 1.98                     | 0.45              |
| 4:3:1729:G:O2'   | 34:a:9:ARG:HG2    | 2.17                     | 0.44              |
| 4:3:2269:C:N4    | 54:u:28:ARG:HE    | 2.15                     | 0.44              |
| 6:5:425:G:H4'    | 6:5:426:U:O5'     | 2.17                     | 0.44              |
| 6:5:1070:G:H2'   | 6:5:1071:A:C8     | 2.52                     | 0.44              |
| 14:D:166:ILE:H   | 14:D:166:ILE:HD12 | 1.81                     | 0.44              |
| 15:E:105:GLN:O   | 15:E:109:LEU:HG   | 2.17                     | 0.44              |
| 15:E:115:TYR:O   | 15:E:118:ILE:HB   | 2.16                     | 0.44              |
| 15:E:181:PHE:O   | 15:E:183:ALA:N    | 2.50                     | 0.44              |
| 16:F:36:GLY:O    | 16:F:39:GLN:HG3   | 2.18                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 35:b:39:VAL:H     | 35:b:92:MET:HE1   | 1.82                     | 0.44              |
| 37:d:114:PHE:HE2  | 57:x:43:HIS:CD2   | 2.34                     | 0.44              |
| 43:j:54:LYS:HE3   | 43:j:54:LYS:HB3   | 1.81                     | 0.44              |
| 45:l:35:VAL:HG12  | 45:l:102:VAL:HG22 | 1.99                     | 0.44              |
| 48:o:6:LYS:O      | 48:o:10:ILE:HG12  | 2.17                     | 0.44              |
| 49:p:92:LYS:HG3   | 49:p:93:VAL:N     | 2.31                     | 0.44              |
| 4:3:71:C:O2       | 4:3:75:A:O2'      | 2.31                     | 0.44              |
| 4:3:193:G:OP1     | 55:v:26:ARG:HG2   | 2.16                     | 0.44              |
| 4:3:1090:G:H4'    | 40:g:32:MET:O     | 2.18                     | 0.44              |
| 4:3:1572:U:H2'    | 4:3:1573:A:H8     | 1.83                     | 0.44              |
| 4:3:1761:C:H1'    | 48:o:103:TYR:CD2  | 2.52                     | 0.44              |
| 4:3:1778:G:H2'    | 4:3:1779:G:C8     | 2.52                     | 0.44              |
| 4:3:2861:G:N2     | 4:3:2864:A:OP2    | 2.41                     | 0.44              |
| 5:4:76:A:H62      | 5:4:88:G:N2       | 2.15                     | 0.44              |
| 6:5:212:G:H2'     | 6:5:213:U:C6      | 2.52                     | 0.44              |
| 11:A:43:PHE:CE2   | 15:E:173:PRO:HG3  | 2.52                     | 0.44              |
| 11:A:158:ARG:O    | 11:A:161:LYS:HG2  | 2.17                     | 0.44              |
| 11:A:249:LYS:HB3  | 11:A:253:GLU:CD   | 2.41                     | 0.44              |
| 13:C:64:TYR:HD1   | 13:C:110:ARG:HH12 | 1.63                     | 0.44              |
| 14:D:169:ILE:HD12 | 14:D:196:MET:HE3  | 1.98                     | 0.44              |
| 20:J:72:MET:HE2   | 20:J:75:VAL:CG1   | 2.46                     | 0.44              |
| 28:R:40:ILE:HG23  | 28:R:68:GLY:N     | 2.26                     | 0.44              |
| 28:R:67:VAL:O     | 57:x:58:ARG:NH2   | 2.50                     | 0.44              |
| 48:o:6:LYS:O      | 48:o:9:LEU:HG     | 2.17                     | 0.44              |
| 51:r:115:GLN:O    | 51:r:118:ILE:HG22 | 2.17                     | 0.44              |
| 51:r:125:VAL:O    | 51:r:129:VAL:HG23 | 2.17                     | 0.44              |
| 58:y:42:VAL:HG12  | 58:y:43:CYS:O     | 2.16                     | 0.44              |
| 1:0:1:MET:HE1     | 4:3:787:C:P       | 2.58                     | 0.44              |
| 4:3:944:U:OP1     | 45:l:24:ASN:N     | 2.47                     | 0.44              |
| 4:3:2886:A:H5'    | 46:m:99:ARG:HE    | 1.82                     | 0.44              |
| 6:5:506:U:H4'     | 13:C:50:TYR:CD2   | 2.52                     | 0.44              |
| 6:5:525:7MG:O2'   | 6:5:533:A:N1      | 2.40                     | 0.44              |
| 6:5:1038:G:C5'    | 23:M:4:LYS:HE2    | 2.47                     | 0.44              |
| 6:5:1232:C:H42    | 57:x:82:LYS:HG2   | 1.82                     | 0.44              |
| 6:5:1248:U:H2'    | 6:5:1249:G:O4'    | 2.17                     | 0.44              |
| 6:5:1348:G:H4'    | 16:F:30:MET:CE    | 2.47                     | 0.44              |
| 13:C:60:MET:HE2   | 13:C:191:ILE:HD11 | 1.98                     | 0.44              |
| 13:C:155:LYS:O    | 13:C:159:GLU:HG2  | 2.16                     | 0.44              |
| 14:D:211:LEU:HD23 | 17:G:83:SER:HA    | 2.00                     | 0.44              |
| 16:F:128:ASN:O    | 16:F:129:ASN:OD1  | 2.35                     | 0.44              |
| 20:J:7:ILE:O      | 20:J:7:ILE:HG12   | 2.16                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 20:J:29:ASP:HB3   | 20:J:30:PRO:HD2   | 2.00                     | 0.44              |
| 21:K:86:ASN:ND2   | 21:K:118:VAL:H    | 2.14                     | 0.44              |
| 32:Y:65:C:H1'     | 32:Y:66:U:C2      | 2.52                     | 0.44              |
| 35:b:10:LYS:HB2   | 35:b:205:VAL:HG21 | 1.98                     | 0.44              |
| 35:b:11:VAL:CG2   | 48:o:9:LEU:HD11   | 2.44                     | 0.44              |
| 35:b:177:GLN:HE22 | 35:b:212:LYS:HZ3  | 1.66                     | 0.44              |
| 37:d:15:GLU:OE2   | 37:d:16:LEU:HD22  | 2.17                     | 0.44              |
| 38:e:128:VAL:HG13 | 38:e:128:VAL:O    | 2.17                     | 0.44              |
| 41:h:100:LYS:HD2  | 41:h:103:GLU:OE2  | 2.17                     | 0.44              |
| 42:i:119:ARG:HH21 | 42:i:120:ARG:HH12 | 1.66                     | 0.44              |
| 50:q:67:LYS:HD2   | 50:q:86:ARG:HD2   | 1.99                     | 0.44              |
| 51:r:12:ILE:HG12  | 51:r:43:ALA:HB2   | 1.99                     | 0.44              |
| 59:z:12:ASN:HD21  | 59:z:48:LYS:HB2   | 1.83                     | 0.44              |
| 4:3:1350:A:P      | 51:r:9:ARG:HH22   | 2.39                     | 0.44              |
| 4:3:1558:A:H5''   | 4:3:1570:A:H62    | 1.81                     | 0.44              |
| 4:3:1946:U:OP1    | 4:3:2612:G:O2'    | 2.31                     | 0.44              |
| 4:3:2176:G:N2     | 4:3:2178:A:H3'    | 2.32                     | 0.44              |
| 5:4:47:C:H5'      | 47:n:67:LYS:HZ3   | 1.82                     | 0.44              |
| 6:5:18:U:H2'      | 6:5:19:C:H6       | 1.81                     | 0.44              |
| 6:5:433:C:H2'     | 6:5:434:U:C6      | 2.53                     | 0.44              |
| 6:5:732:A:H5''    | 27:Q:92:ARG:NH1   | 2.32                     | 0.44              |
| 6:5:961:G:N2      | 8:7:34:G:H5'      | 2.31                     | 0.44              |
| 6:5:991:A:H2'     | 6:5:992:U:H6      | 1.83                     | 0.44              |
| 6:5:1320:A:H5'    | 16:F:9:ARG:NH2    | 2.33                     | 0.44              |
| 6:5:1324:A:H2'    | 6:5:1325:U:O4'    | 2.17                     | 0.44              |
| 8:7:61:C:H2'      | 8:7:62:C:H6       | 1.83                     | 0.44              |
| 11:A:162:PHE:O    | 11:A:163:PHE:CD1  | 2.70                     | 0.44              |
| 16:F:52:ARG:NH2   | 16:F:120:ALA:O    | 2.49                     | 0.44              |
| 18:H:48:GLN:NE2   | 18:H:51:GLU:OE1   | 2.41                     | 0.44              |
| 25:O:43:LEU:O     | 25:O:44:LYS:HG2   | 2.17                     | 0.44              |
| 27:Q:39:LYS:HD2   | 27:Q:77:GLY:HA2   | 2.00                     | 0.44              |
| 28:R:49:PHE:O     | 28:R:59:ASN:HA    | 2.17                     | 0.44              |
| 35:b:123:ILE:HG23 | 35:b:128:PHE:O    | 2.17                     | 0.44              |
| 36:c:127:LEU:HD21 | 36:c:201:LYS:HG2  | 1.98                     | 0.44              |
| 48:o:36:LYS:HE2   | 48:o:85:ASN:HA    | 1.99                     | 0.44              |
| 51:r:122:LYS:O    | 51:r:125:VAL:HG12 | 2.17                     | 0.44              |
| 51:r:133:GLN:O    | 51:r:137:MET:HG2  | 2.17                     | 0.44              |
| 4:3:1102:A:H2'    | 4:3:1102:A:N3     | 2.31                     | 0.44              |
| 4:3:1128:G:H2'    | 4:3:1129:U:C6     | 2.53                     | 0.44              |
| 4:3:2094:A:H2'    | 4:3:2095:A:H8     | 1.82                     | 0.44              |
| 6:5:818:A:H2'     | 6:5:819:G:H8      | 1.83                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:5:1032:G:H2'    | 6:5:1033:U:O4'    | 2.18                     | 0.44              |
| 6:5:1162:G:H2'    | 6:5:1163:A:C8     | 2.53                     | 0.44              |
| 6:5:1276:U:P      | 22:L:21:TYR:HH    | 2.35                     | 0.44              |
| 10:9:59:LEU:HG    | 10:9:161:TYR:HE2  | 1.83                     | 0.44              |
| 11:A:22:LYS:HD3   | 11:A:22:LYS:HA    | 1.76                     | 0.44              |
| 13:C:46:THR:O     | 13:C:46:THR:HG22  | 2.16                     | 0.44              |
| 13:C:170:ASN:O    | 13:C:173:THR:OG1  | 2.31                     | 0.44              |
| 15:E:24:LYS:HE3   | 15:E:79:ASN:OD1   | 2.17                     | 0.44              |
| 15:E:53:LEU:HD23  | 15:E:53:LEU:N     | 2.32                     | 0.44              |
| 17:G:48:LEU:O     | 17:G:51:GLU:HG3   | 2.17                     | 0.44              |
| 18:H:28:GLY:O     | 18:H:64:ASP:HA    | 2.17                     | 0.44              |
| 19:I:57:ILE:HB    | 23:M:45:ARG:NH1   | 2.33                     | 0.44              |
| 19:I:57:ILE:C     | 19:I:68:ARG:HG3   | 2.42                     | 0.44              |
| 26:P:20:LYS:O     | 26:P:48:HIS:HA    | 2.16                     | 0.44              |
| 39:f:26:ALA:CB    | 39:f:30:LEU:HB2   | 2.46                     | 0.44              |
| 39:f:68:LEU:HA    | 39:f:108:LEU:HD21 | 1.99                     | 0.44              |
| 51:r:69:LEU:HA    | 51:r:108:SER:O    | 2.17                     | 0.44              |
| 51:r:117:LEU:HD12 | 51:r:118:ILE:N    | 2.32                     | 0.44              |
| 1:0:6:GLN:OE1     | 1:0:6:GLN:N       | 2.49                     | 0.44              |
| 2:1:4:LYS:NZ      | 4:3:255:A:OP2     | 2.40                     | 0.44              |
| 4:3:909:U:H2'     | 4:3:910:G:H8      | 1.83                     | 0.44              |
| 4:3:1446:G:N2     | 4:3:1613:A:OP2    | 2.40                     | 0.44              |
| 6:5:1024:U:O2'    | 6:5:1025:U:OP1    | 2.34                     | 0.44              |
| 7:6:35:G:H2'      | 7:6:36:C:C6       | 2.52                     | 0.44              |
| 9:8:29:U:H3       | 9:8:41:A:N6       | 2.12                     | 0.44              |
| 12:B:22:TRP:CE3   | 12:B:33:TRP:HE3   | 2.36                     | 0.44              |
| 13:C:68:ASP:OD1   | 13:C:72:ARG:NH2   | 2.50                     | 0.44              |
| 16:F:34:LYS:HD2   | 16:F:37:LEU:CB    | 2.48                     | 0.44              |
| 17:G:54:LEU:HG    | 17:G:73:ASN:O     | 2.17                     | 0.44              |
| 21:K:30:LEU:HA    | 21:K:33:LYS:CE    | 2.48                     | 0.44              |
| 22:L:26:GLY:O     | 22:L:30:SER:HB3   | 2.18                     | 0.44              |
| 26:P:18:ASN:HB2   | 26:P:21:THR:OG1   | 2.17                     | 0.44              |
| 28:R:11:VAL:HG21  | 28:R:16:LEU:HD12  | 1.98                     | 0.44              |
| 34:a:251:ARG:HG3  | 34:a:252:ASP:H    | 1.82                     | 0.44              |
| 36:c:35:PHE:CD1   | 44:k:6:LEU:HD13   | 2.53                     | 0.44              |
| 36:c:157:VAL:HG12 | 36:c:196:ALA:HB3  | 1.99                     | 0.44              |
| 37:d:34:ILE:HG13  | 37:d:156:LEU:HD13 | 1.99                     | 0.44              |
| 38:e:118:GLU:OE2  | 38:e:150:GLU:HG3  | 2.17                     | 0.44              |
| 39:f:47:ARG:HE    | 39:f:51:LEU:HB2   | 1.81                     | 0.44              |
| 40:g:41:ARG:CZ    | 40:g:51:ILE:HG13  | 2.47                     | 0.44              |
| 42:i:115:ASN:OD1  | 42:i:116:ARG:N    | 2.48                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 43:j:64:ARG:NH2   | 43:j:79:PHE:HD1   | 2.16                     | 0.44              |
| 47:n:13:LYS:HB2   | 47:n:13:LYS:HE3   | 1.66                     | 0.44              |
| 56:w:29:TYR:O     | 56:w:38:LEU:HD11  | 2.18                     | 0.44              |
| 4:3:710:A:N3      | 4:3:2451:C:O2'    | 2.49                     | 0.44              |
| 4:3:874:U:H2'     | 4:3:875:G:H8      | 1.82                     | 0.44              |
| 4:3:1073:A:H2'    | 4:3:1074:A:C8     | 2.53                     | 0.44              |
| 4:3:1242:G:H1'    | 4:3:1267:A:H61    | 1.82                     | 0.44              |
| 6:5:1307:A:H2'    | 6:5:1308:G:O4'    | 2.18                     | 0.44              |
| 6:5:1488:A:H2'    | 6:5:1489:C:C6     | 2.52                     | 0.44              |
| 12:B:86:GLN:HE21  | 12:B:87:LYS:NZ    | 2.16                     | 0.44              |
| 16:F:100:LEU:HA   | 16:F:103:ILE:HG12 | 1.98                     | 0.44              |
| 16:F:115:MET:HE2  | 16:F:115:MET:HB2  | 1.77                     | 0.44              |
| 18:H:26:ASP:O     | 18:H:27:LYS:HB2   | 2.18                     | 0.44              |
| 18:H:90:LEU:HD13  | 18:H:97:LYS:HD2   | 1.98                     | 0.44              |
| 22:L:10:PRO:N     | 22:L:13:LYS:HE3   | 2.33                     | 0.44              |
| 22:L:36:GLN:NE2   | 22:L:59:VAL:HG11  | 2.33                     | 0.44              |
| 24:N:14:LEU:HD11  | 24:N:15:HIS:HD2   | 1.83                     | 0.44              |
| 34:a:160:ILE:HG21 | 34:a:184:LEU:HD13 | 2.00                     | 0.44              |
| 38:e:58:ASN:OD1   | 38:e:59:ASN:ND2   | 2.50                     | 0.44              |
| 40:g:77:LYS:HG3   | 40:g:77:LYS:O     | 2.18                     | 0.44              |
| 41:h:79:ALA:HB1   | 41:h:100:LYS:HG2  | 2.00                     | 0.44              |
| 48:o:33:VAL:CG1   | 48:o:48:PHE:HB3   | 2.47                     | 0.44              |
| 48:o:64:PHE:CZ    | 48:o:79:PHE:HB2   | 2.53                     | 0.44              |
| 48:o:93:ARG:HE    | 48:o:118:LYS:HB3  | 1.83                     | 0.44              |
| 50:q:2:HIS:HB3    | 50:q:15:HIS:CE1   | 2.53                     | 0.44              |
| 52:s:9:LYS:O      | 52:s:30:VAL:N     | 2.43                     | 0.44              |
| 4:3:706:C:H3'     | 44:k:43:LYS:HZ1   | 1.83                     | 0.44              |
| 4:3:739:G:HO2'    | 4:3:761:G:H1      | 1.53                     | 0.44              |
| 4:3:1114:C:H3'    | 4:3:1115:G:H8     | 1.83                     | 0.44              |
| 4:3:1115:G:H21    | 41:h:123:MET:HE1  | 1.83                     | 0.44              |
| 4:3:2235:A:H5''   | 34:a:271:LYS:HZ1  | 1.82                     | 0.44              |
| 4:3:2352:U:OP1    | 59:z:35:ASN:ND2   | 2.42                     | 0.44              |
| 4:3:2403:C:H2'    | 4:3:2404:G:C8     | 2.52                     | 0.44              |
| 4:3:2593:U:C6     | 33:Z:36:ASP:O     | 2.71                     | 0.44              |
| 4:3:2644:U:H2'    | 4:3:2645:U:C6     | 2.53                     | 0.44              |
| 6:5:140:U:H2'     | 6:5:141:A:C8      | 2.53                     | 0.44              |
| 6:5:835:G:H4'     | 15:E:150:GLN:NE2  | 2.33                     | 0.44              |
| 9:8:5:C:H2'       | 9:8:6:U:C6        | 2.53                     | 0.44              |
| 10:9:126:GLY:HA2  | 10:9:135:MET:HE3  | 1.98                     | 0.44              |
| 11:A:46:GLU:CD    | 11:A:55:HIS:HB2   | 2.42                     | 0.44              |
| 15:E:157:TRP:CE2  | 17:G:69:ILE:HG12  | 2.52                     | 0.44              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 15:E:211:PHE:CE1 | 32:Y:93:A:H3'     | 2.52                     | 0.44              |
| 25:O:19:ILE:HG22 | 25:O:36:ILE:HB    | 2.00                     | 0.44              |
| 26:P:9:LEU:O     | 26:P:63:ILE:HG22  | 2.17                     | 0.44              |
| 26:P:59:ASP:OD1  | 26:P:83:ARG:HA    | 2.17                     | 0.44              |
| 29:S:65:ALA:O    | 29:S:69:LYS:HG3   | 2.18                     | 0.44              |
| 40:g:123:LEU:O   | 40:g:126:ILE:HG22 | 2.18                     | 0.44              |
| 45:l:73:SER:HB2  | 45:l:93:TRP:CZ3   | 2.52                     | 0.44              |
| 45:l:74:LYS:HZ1  | 45:l:94:VAL:N     | 2.16                     | 0.44              |
| 48:o:67:ARG:HA   | 48:o:76:GLU:HA    | 2.00                     | 0.44              |
| 50:q:73:HIS:CE1  | 50:q:75:SER:HA    | 2.53                     | 0.44              |
| 54:u:86:PHE:CD1  | 54:u:94:ARG:HB2   | 2.52                     | 0.44              |
| 58:y:42:VAL:CG2  | 58:y:48:TYR:HB2   | 2.31                     | 0.44              |
| 3:2:17:ILE:C     | 3:2:18:LYS:HD2    | 2.43                     | 0.44              |
| 4:3:580:U:C2     | 4:3:1251:G:H1'    | 2.52                     | 0.44              |
| 4:3:1956:G:H2'   | 4:3:1957:G:H8     | 1.83                     | 0.44              |
| 4:3:2130:A:H4'   | 10:9:170:HIS:CD2  | 2.53                     | 0.44              |
| 4:3:2174:G:H8    | 4:3:2174:G:O5'    | 2.01                     | 0.44              |
| 4:3:2269:C:H41   | 54:u:28:ARG:HE    | 1.66                     | 0.44              |
| 4:3:2294:A:H4'   | 4:3:2295:A:O4'    | 2.17                     | 0.44              |
| 4:3:2565:G:H2'   | 4:3:2566:C:C6     | 2.53                     | 0.44              |
| 4:3:2755:G:O6    | 4:3:2763:C:H5''   | 2.17                     | 0.44              |
| 4:3:2811:G:H2'   | 4:3:2812:U:C6     | 2.53                     | 0.44              |
| 6:5:335:C:H2'    | 6:5:336:U:C6      | 2.53                     | 0.44              |
| 19:I:8:LYS:O     | 19:I:9:TYR:CD1    | 2.70                     | 0.44              |
| 19:I:11:GLU:OE2  | 19:I:81:ILE:HD11  | 2.17                     | 0.44              |
| 21:K:67:LYS:HD3  | 21:K:77:LEU:CD2   | 2.48                     | 0.44              |
| 21:K:86:ASN:O    | 21:K:88:GLN:OE1   | 2.36                     | 0.44              |
| 22:L:19:LEU:HD21 | 22:L:33:ILE:HD12  | 2.00                     | 0.44              |
| 34:a:225:ARG:HD2 | 34:a:226:PRO:HD2  | 1.99                     | 0.44              |
| 35:b:222:LEU:H   | 35:b:222:LEU:HD23 | 1.83                     | 0.44              |
| 37:d:102:LYS:HZ3 | 37:d:139:PRO:HG2  | 1.82                     | 0.44              |
| 39:f:5:LEU:HD21  | 39:f:17:ASP:HB2   | 2.00                     | 0.44              |
| 44:k:47:THR:OG1  | 44:k:48:ARG:N     | 2.51                     | 0.44              |
| 46:m:81:HIS:HA   | 46:m:85:LYS:HD3   | 1.99                     | 0.44              |
| 46:m:99:ARG:HA   | 46:m:99:ARG:HD3   | 1.48                     | 0.44              |
| 48:o:15:GLN:HA   | 48:o:18:LEU:HG    | 1.99                     | 0.44              |
| 48:o:31:VAL:HG11 | 48:o:88:ILE:HG23  | 1.99                     | 0.44              |
| 48:o:35:ILE:HD11 | 48:o:46:GLN:OE1   | 2.17                     | 0.44              |
| 50:q:71:ILE:O    | 50:q:71:ILE:HG23  | 2.18                     | 0.44              |
| 51:r:1:MET:HG2   | 51:r:1:MET:O      | 2.18                     | 0.44              |
| 4:3:287:G:N2     | 39:f:42:LYS:HZ1   | 2.16                     | 0.43              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:3:410:G:C8     | 55:v:60:LYS:HD2   | 2.53                     | 0.43              |
| 4:3:1237:G:H2'   | 4:3:1238:A:H8     | 1.83                     | 0.43              |
| 4:3:1422:U:H2'   | 4:3:1423:A:O4'    | 2.18                     | 0.43              |
| 4:3:1688:A:N7    | 4:3:2012:A:H2     | 2.16                     | 0.43              |
| 4:3:2896:G:H3'   | 4:3:2897:G:H5'    | 2.00                     | 0.43              |
| 6:5:231:U:H2'    | 6:5:232:G:C8      | 2.53                     | 0.43              |
| 6:5:640:C:H2'    | 6:5:641:U:C6      | 2.53                     | 0.43              |
| 6:5:1215:U:OP1   | 16:F:115:MET:HE1  | 2.18                     | 0.43              |
| 6:5:1347:U:H2'   | 6:5:1348:G:O4'    | 2.18                     | 0.43              |
| 8:7:61:C:H2'     | 8:7:62:C:C6       | 2.52                     | 0.43              |
| 9:8:41:A:H2'     | 9:8:42:U:O4'      | 2.18                     | 0.43              |
| 11:A:68:ALA:O    | 11:A:72:VAL:HG12  | 2.17                     | 0.43              |
| 11:A:152:LEU:HA  | 11:A:155:GLU:OE1  | 2.18                     | 0.43              |
| 15:E:5:ILE:HA    | 15:E:86:LEU:O     | 2.18                     | 0.43              |
| 17:G:46:GLU:O    | 17:G:49:VAL:HG12  | 2.18                     | 0.43              |
| 19:I:58:ILE:HG12 | 19:I:68:ARG:NE    | 2.25                     | 0.43              |
| 20:J:31:GLY:O    | 20:J:32:GLY:C     | 2.60                     | 0.43              |
| 21:K:55:PRO:HG2  | 21:K:60:SER:HA    | 1.99                     | 0.43              |
| 22:L:33:ILE:HG12 | 22:L:63:TYR:CE2   | 2.48                     | 0.43              |
| 24:N:33:ILE:HG13 | 24:N:60:ARG:NH2   | 2.33                     | 0.43              |
| 27:Q:38:LYS:HE2  | 27:Q:38:LYS:HB2   | 1.80                     | 0.43              |
| 29:S:9:LYS:HE2   | 29:S:13:GLN:NE2   | 2.32                     | 0.43              |
| 35:b:163:LYS:HB3 | 35:b:165:MET:CE   | 2.48                     | 0.43              |
| 39:f:89:TYR:CD1  | 39:f:89:TYR:N     | 2.75                     | 0.43              |
| 40:g:88:GLU:OE1  | 40:g:91:GLU:HG3   | 2.17                     | 0.43              |
| 44:k:113:LYS:NZ  | 44:k:115:ILE:HD11 | 2.33                     | 0.43              |
| 48:o:37:LEU:HD11 | 48:o:44:ARG:HB2   | 2.00                     | 0.43              |
| 51:r:125:VAL:O   | 51:r:128:ARG:HB2  | 2.18                     | 0.43              |
| 53:t:3:ARG:HH12  | 53:t:74:LEU:C     | 2.25                     | 0.43              |
| 53:t:7:GLY:H     | 53:t:24:VAL:HG13  | 1.83                     | 0.43              |
| 4:3:1896:A:N3    | 4:3:2093:U:O2'    | 2.50                     | 0.43              |
| 4:3:2098:U:C3'   | 4:3:2099:U:H5''   | 2.48                     | 0.43              |
| 4:3:2695:U:H2'   | 4:3:2696:G:O4'    | 2.18                     | 0.43              |
| 4:3:2845:U:H2'   | 4:3:2846:A:C8     | 2.53                     | 0.43              |
| 6:5:196:G:O3'    | 29:S:53:ARG:NH1   | 2.51                     | 0.43              |
| 6:5:732:A:H2'    | 6:5:733:A:C8      | 2.52                     | 0.43              |
| 6:5:1026:A:N3    | 6:5:1026:A:H2'    | 2.33                     | 0.43              |
| 6:5:1306:A:N3    | 6:5:1306:A:H5'    | 2.33                     | 0.43              |
| 8:7:28:C:H2'     | 8:7:29:U:C6       | 2.53                     | 0.43              |
| 16:F:106:PHE:HE2 | 16:F:136:LYS:HE2  | 1.83                     | 0.43              |
| 18:H:94:PRO:HA   | 18:H:97:LYS:HG2   | 1.99                     | 0.43              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 18:H:101:LYS:C   | 18:H:103:LYS:N    | 2.75                     | 0.43              |
| 19:I:12:LEU:HD23 | 19:I:85:VAL:HG11  | 2.00                     | 0.43              |
| 19:I:56:THR:HG22 | 19:I:68:ARG:HD3   | 1.99                     | 0.43              |
| 36:c:182:HIS:O   | 36:c:186:VAL:HG13 | 2.18                     | 0.43              |
| 37:d:29:PRO:HG2  | 37:d:169:LEU:HB2  | 2.00                     | 0.43              |
| 39:f:95:LYS:NZ   | 39:f:98:ILE:HG12  | 2.34                     | 0.43              |
| 43:j:93:PRO:HG3  | 43:j:114:ILE:HG13 | 2.00                     | 0.43              |
| 4:3:69:U:H3      | 4:3:76:A:H2       | 1.64                     | 0.43              |
| 4:3:125:G:OP1    | 4:3:1404:C:O2'    | 2.29                     | 0.43              |
| 4:3:925:C:OP2    | 22:L:92:ARG:HG2   | 2.19                     | 0.43              |
| 4:3:1120:A:H2'   | 4:3:1121:A:N9     | 2.32                     | 0.43              |
| 4:3:1950:U:O4'   | 4:3:1952:G:H5'    | 2.18                     | 0.43              |
| 4:3:2123:A:H61   | 4:3:2169:G:H3'    | 1.83                     | 0.43              |
| 4:3:2183:U:H2'   | 4:3:2184:A:H4'    | 2.01                     | 0.43              |
| 4:3:2223:C:H2'   | 4:3:2224:A:C8     | 2.53                     | 0.43              |
| 6:5:1023:G:O2'   | 6:5:1024:U:H5''   | 2.18                     | 0.43              |
| 6:5:1403:A:H2'   | 6:5:1404:U:C6     | 2.54                     | 0.43              |
| 9:8:74:C:OP1     | 9:8:75:C:H5'      | 2.19                     | 0.43              |
| 12:B:92:ILE:O    | 12:B:96:ILE:HG12  | 2.18                     | 0.43              |
| 14:D:132:HIS:ND1 | 14:D:137:TYR:HB2  | 2.34                     | 0.43              |
| 15:E:156:LEU:HB3 | 17:G:63:LYS:NZ    | 2.32                     | 0.43              |
| 20:J:86:LYS:HB2  | 20:J:86:LYS:HE3   | 1.80                     | 0.43              |
| 26:P:8:VAL:O     | 26:P:9:LEU:HD22   | 2.18                     | 0.43              |
| 29:S:25:LYS:HE2  | 29:S:59:ILE:HG22  | 2.00                     | 0.43              |
| 31:X:37:ASN:N    | 31:X:45:LYS:HD3   | 2.31                     | 0.43              |
| 37:d:60:ILE:HD13 | 37:d:140:GLU:HB2  | 1.99                     | 0.43              |
| 38:e:20:PHE:HD2  | 38:e:46:PHE:CD1   | 2.36                     | 0.43              |
| 39:f:67:LYS:O    | 39:f:71:VAL:HG23  | 2.18                     | 0.43              |
| 49:p:20:ALA:HB3  | 49:p:34:ALA:HB1   | 1.99                     | 0.43              |
| 50:q:27:ALA:HB1  | 50:q:31:LYS:CE    | 2.48                     | 0.43              |
| 52:s:8:LEU:HB2   | 52:s:30:VAL:HG23  | 2.01                     | 0.43              |
| 52:s:9:LYS:HD2   | 52:s:9:LYS:HA     | 1.73                     | 0.43              |
| 57:x:77:THR:O    | 57:x:79:LYS:N     | 2.51                     | 0.43              |
| 2:1:13:LEU:HD12  | 2:1:14:THR:N      | 2.27                     | 0.43              |
| 4:3:526:G:H2'    | 4:3:527:A:C8      | 2.53                     | 0.43              |
| 4:3:606:G:O2'    | 4:3:608:A:OP1     | 2.36                     | 0.43              |
| 4:3:1017:A:N1    | 4:3:2034:G:O2'    | 2.43                     | 0.43              |
| 4:3:1393:A:OP1   | 55:v:3:LYS:HE2    | 2.18                     | 0.43              |
| 4:3:2323:U:O2    | 37:d:125:ARG:NH1  | 2.45                     | 0.43              |
| 6:5:207:C:H2'    | 6:5:208:A:O4'     | 2.19                     | 0.43              |
| 6:5:459:C:H2'    | 6:5:460:A:O4'     | 2.18                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:5:476:U:H5'     | 6:5:477:U:OP1     | 2.18                     | 0.43              |
| 6:5:537:A:H2'     | 6:5:538:G:C8      | 2.54                     | 0.43              |
| 6:5:573:G:H4'     | 6:5:574:C:O5'     | 2.17                     | 0.43              |
| 6:5:707:G:H2'     | 6:5:708:A:H8      | 1.84                     | 0.43              |
| 6:5:1323:A:N6     | 6:5:1348:G:O2'    | 2.48                     | 0.43              |
| 9:8:1:G:O6        | 9:8:73:A:N6       | 2.50                     | 0.43              |
| 11:A:24:GLY:HA2   | 11:A:29:HIS:CE1   | 2.53                     | 0.43              |
| 13:C:165:PRO:HG2  | 13:C:180:ARG:HH22 | 1.82                     | 0.43              |
| 15:E:85:GLU:C     | 15:E:86:LEU:HD12  | 2.43                     | 0.43              |
| 16:F:68:VAL:CG1   | 16:F:99:ALA:HB1   | 2.48                     | 0.43              |
| 17:G:125:ASP:OD1  | 17:G:126:LYS:HD2  | 2.18                     | 0.43              |
| 19:I:63:VAL:CG1   | 19:I:64:ASP:H     | 2.29                     | 0.43              |
| 21:K:70:LEU:HD23  | 21:K:72:ASN:HD21  | 1.84                     | 0.43              |
| 24:N:83:ASN:HA    | 24:N:85:ARG:NH1   | 2.34                     | 0.43              |
| 29:S:25:LYS:HZ2   | 29:S:60:ILE:HB    | 1.83                     | 0.43              |
| 34:a:152:LEU:HD12 | 34:a:159:GLN:HG2  | 2.01                     | 0.43              |
| 35:b:13:MET:HG2   | 35:b:26:ILE:O     | 2.18                     | 0.43              |
| 36:c:136:THR:HA   | 36:c:143:MET:HE3  | 2.00                     | 0.43              |
| 36:c:192:MET:HE1  | 44:k:3:LEU:HB3    | 1.99                     | 0.43              |
| 43:j:53:LYS:HE2   | 43:j:56:GLN:NE2   | 2.33                     | 0.43              |
| 45:l:24:ASN:HA    | 45:l:67:ARG:NH2   | 2.33                     | 0.43              |
| 48:o:32:ASN:HB3   | 48:o:89:GLU:OE2   | 2.18                     | 0.43              |
| 48:o:62:GLU:HB3   | 48:o:81:ILE:HD12  | 1.99                     | 0.43              |
| 51:r:36:LEU:HD21  | 51:r:47:ILE:HB    | 2.01                     | 0.43              |
| 4:3:591:G:H5'     | 42:i:117:LEU:HD12 | 2.00                     | 0.43              |
| 4:3:703:A:H2'     | 4:3:705:A:N6      | 2.28                     | 0.43              |
| 4:3:900:G:H2'     | 4:3:901:C:C6      | 2.54                     | 0.43              |
| 4:3:1485:A:H4'    | 4:3:1486:U:C5     | 2.54                     | 0.43              |
| 4:3:1690:C:P      | 35:b:142:ARG:HD2  | 2.58                     | 0.43              |
| 4:3:2107:A:H2'    | 4:3:2108:C:C6     | 2.54                     | 0.43              |
| 4:3:2343:A:H5''   | 4:3:2343:A:H8     | 1.84                     | 0.43              |
| 4:3:2704:U:H2'    | 4:3:2705:G:C8     | 2.53                     | 0.43              |
| 6:5:441:U:H2'     | 6:5:442:G:C8      | 2.52                     | 0.43              |
| 6:5:732:A:H5''    | 27:Q:92:ARG:CZ    | 2.48                     | 0.43              |
| 6:5:1002:A:H2'    | 6:5:1003:A:O4'    | 2.19                     | 0.43              |
| 7:6:74:C:O2'      | 7:6:75:C:P        | 2.77                     | 0.43              |
| 8:7:23:C:H2'      | 8:7:24:A:C8       | 2.54                     | 0.43              |
| 12:B:45:PHE:O     | 12:B:49:ARG:HD2   | 2.18                     | 0.43              |
| 12:B:176:MET:HE1  | 12:B:206:ASN:CB   | 2.48                     | 0.43              |
| 15:E:21:VAL:HG13  | 15:E:60:TRP:CZ2   | 2.53                     | 0.43              |
| 17:G:116:ILE:HG23 | 17:G:136:GLU:O    | 2.18                     | 0.43              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 18:H:86:VAL:HG23 | 18:H:100:LEU:HD13 | 2.01                     | 0.43              |
| 20:J:27:ALA:O    | 20:J:35:LEU:N     | 2.43                     | 0.43              |
| 21:K:20:LYS:HB3  | 21:K:107:ARG:HH21 | 1.83                     | 0.43              |
| 21:K:43:LYS:CB   | 21:K:70:LEU:HD11  | 2.48                     | 0.43              |
| 26:P:43:LYS:HD2  | 26:P:45:TYR:CD1   | 2.54                     | 0.43              |
| 28:R:19:VAL:HG11 | 28:R:44:PHE:HD1   | 1.84                     | 0.43              |
| 29:S:37:LYS:HD3  | 29:S:38:GLU:OE1   | 2.19                     | 0.43              |
| 29:S:41:LEU:CD1  | 29:S:76:LEU:HD21  | 2.47                     | 0.43              |
| 37:d:114:PHE:O   | 37:d:114:PHE:CG   | 2.72                     | 0.43              |
| 48:o:102:SER:HA  | 48:o:105:ARG:HH21 | 1.83                     | 0.43              |
| 56:w:96:ALA:O    | 56:w:99:LEU:HG    | 2.18                     | 0.43              |
| 57:x:62:LEU:HD13 | 57:x:66:PHE:HE2   | 1.84                     | 0.43              |
| 3:2:7:VAL:HA     | 3:2:34:GLN:HE22   | 1.83                     | 0.43              |
| 4:3:433:A:OP1    | 55:v:53:ARG:NH2   | 2.51                     | 0.43              |
| 4:3:831:U:H2'    | 4:3:832:C:C6      | 2.53                     | 0.43              |
| 4:3:832:C:OP1    | 36:c:63:LYS:HE3   | 2.19                     | 0.43              |
| 4:3:983:A:N3     | 4:3:1020:G:H8     | 2.17                     | 0.43              |
| 4:3:2026:A:N7    | 58:y:6:ARG:NH2    | 2.66                     | 0.43              |
| 4:3:2094:A:H2'   | 4:3:2095:A:C8     | 2.54                     | 0.43              |
| 4:3:2119:A:H2'   | 4:3:2120:G:O4'    | 2.19                     | 0.43              |
| 4:3:2269:C:OP1   | 54:u:31:HIS:HB2   | 2.17                     | 0.43              |
| 6:5:408:U:H1'    | 13:C:28:GLY:HA2   | 2.00                     | 0.43              |
| 6:5:709:A:H2'    | 6:5:710:G:C8      | 2.54                     | 0.43              |
| 6:5:787:A:OP1    | 8:7:38:C:O2'      | 2.36                     | 0.43              |
| 6:5:1098:C:H2'   | 6:5:1099:G:O4'    | 2.19                     | 0.43              |
| 6:5:1384:A:H2'   | 6:5:1385:A:H8     | 1.84                     | 0.43              |
| 10:9:15:VAL:HG13 | 10:9:220:LEU:HD23 | 2.01                     | 0.43              |
| 10:9:20:LEU:HD23 | 10:9:224:LEU:HD22 | 2.01                     | 0.43              |
| 11:A:78:ASN:HB3  | 15:E:181:PHE:CE2  | 2.54                     | 0.43              |
| 13:C:16:PHE:CD1  | 13:C:190:GLY:HA2  | 2.53                     | 0.43              |
| 13:C:186:GLU:O   | 13:C:188:PRO:HD3  | 2.17                     | 0.43              |
| 15:E:137:ALA:O   | 15:E:139:THR:N    | 2.46                     | 0.43              |
| 25:O:8:ARG:HB2   | 25:O:28:ARG:NH1   | 2.32                     | 0.43              |
| 36:c:116:TRP:CZ2 | 36:c:207:LEU:HD11 | 2.54                     | 0.43              |
| 36:c:143:MET:O   | 36:c:147:LEU:HG   | 2.18                     | 0.43              |
| 37:d:31:LEU:CD2  | 37:d:96:MET:HE1   | 2.47                     | 0.43              |
| 37:d:91:LEU:C    | 37:d:96:MET:HB3   | 2.44                     | 0.43              |
| 38:e:84:GLN:OE1  | 38:e:84:GLN:N     | 2.52                     | 0.43              |
| 40:g:16:HIS:O    | 40:g:20:THR:HG23  | 2.18                     | 0.43              |
| 48:o:33:VAL:HG11 | 48:o:79:PHE:CE2   | 2.54                     | 0.43              |
| 52:s:19:ASN:C    | 52:s:21:MET:H     | 2.26                     | 0.43              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 52:s:30:VAL:HG12 | 52:s:80:LEU:HD13  | 1.99                     | 0.43              |
| 4:3:19:G:H5''    | 58:y:11:HIS:CE1   | 2.54                     | 0.43              |
| 4:3:530:G:H5''   | 51:r:4:PHE:CZ     | 2.53                     | 0.43              |
| 4:3:634:C:O2'    | 4:3:639:G:H5''    | 2.18                     | 0.43              |
| 4:3:1323:A:H2'   | 4:3:1324:A:C8     | 2.54                     | 0.43              |
| 4:3:1479:A:H4'   | 4:3:1480:A:C4     | 2.54                     | 0.43              |
| 4:3:1821:G:C6    | 4:3:1822:A:C6     | 3.06                     | 0.43              |
| 4:3:2504:C:H5'   | 45:l:83:MET:HE1   | 2.01                     | 0.43              |
| 4:3:2638:G:H2'   | 4:3:2639:G:C8     | 2.54                     | 0.43              |
| 5:4:41:C:H2'     | 5:4:43:A:C8       | 2.54                     | 0.43              |
| 6:5:57:U:H2'     | 6:5:58:G:C8       | 2.53                     | 0.43              |
| 6:5:862:C:H2'    | 6:5:863:A:O4'     | 2.19                     | 0.43              |
| 6:5:1146:A:H2'   | 6:5:1147:U:C6     | 2.52                     | 0.43              |
| 11:A:85:VAL:HG12 | 11:A:176:LEU:HD11 | 2.01                     | 0.43              |
| 13:C:143:ARG:HE  | 13:C:174:PHE:HE1  | 1.66                     | 0.43              |
| 16:F:83:ASN:HD21 | 16:F:85:GLN:NE2   | 2.15                     | 0.43              |
| 18:H:96:LEU:O    | 18:H:99:ILE:HG22  | 2.19                     | 0.43              |
| 19:I:106:PHE:CE1 | 57:x:92:ARG:HB3   | 2.53                     | 0.43              |
| 24:N:3:ILE:CG1   | 24:N:8:ILE:HD11   | 2.49                     | 0.43              |
| 25:O:73:PHE:HD1  | 25:O:78:LEU:HB3   | 1.82                     | 0.43              |
| 26:P:8:VAL:C     | 26:P:9:LEU:HD22   | 2.44                     | 0.43              |
| 27:Q:73:ARG:HH22 | 27:Q:83:GLN:CB    | 2.31                     | 0.43              |
| 30:T:37:ARG:HG3  | 30:T:40:MET:H     | 1.83                     | 0.43              |
| 35:b:30:TYR:CZ   | 35:b:189:MET:HE3  | 2.53                     | 0.43              |
| 35:b:56:THR:HG23 | 35:b:77:PRO:O     | 2.18                     | 0.43              |
| 37:d:55:ASN:O    | 37:d:58:HIS:HB3   | 2.18                     | 0.43              |
| 42:i:31:LEU:HD12 | 42:i:32:ALA:N     | 2.34                     | 0.43              |
| 42:i:106:ASN:OD1 | 42:i:107:ALA:N    | 2.51                     | 0.43              |
| 48:o:55:ARG:NE   | 48:o:81:ILE:HD11  | 2.34                     | 0.43              |
| 4:3:397:G:H2'    | 4:3:398:C:C6      | 2.54                     | 0.43              |
| 4:3:573:A:H2'    | 4:3:574:G:O4'     | 2.19                     | 0.43              |
| 4:3:1091:G:OP1   | 40:g:34:ALA:N     | 2.30                     | 0.43              |
| 4:3:1755:A:H2'   | 4:3:1756:A:C8     | 2.54                     | 0.43              |
| 4:3:2885:U:O2'   | 46:m:99:ARG:NE    | 2.51                     | 0.43              |
| 6:5:359:A:H5''   | 21:K:44:ARG:NH1   | 2.34                     | 0.43              |
| 6:5:380:G:H2'    | 6:5:381:C:O4'     | 2.18                     | 0.43              |
| 6:5:395:G:H2'    | 6:5:396:C:H6      | 1.83                     | 0.43              |
| 6:5:434:U:H2'    | 6:5:435:U:C6      | 2.54                     | 0.43              |
| 6:5:510:U:H2'    | 6:5:511:A:C8      | 2.53                     | 0.43              |
| 6:5:884:G:O2'    | 6:5:900:G:O6      | 2.34                     | 0.43              |
| 6:5:1071:A:H5''  | 14:D:76:ILE:HD12  | 2.01                     | 0.43              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 6:5:1097:G:O3'   | 12:B:175:ASN:HA   | 2.18                     | 0.43              |
| 6:5:1432:A:H2'   | 6:5:1433:G:H8     | 1.83                     | 0.43              |
| 18:H:6:TYR:CZ    | 18:H:92:PHE:HB2   | 2.53                     | 0.43              |
| 18:H:83:LEU:O    | 18:H:86:VAL:HG12  | 2.19                     | 0.43              |
| 18:H:124:ARG:NH1 | 18:H:125:ARG:HG3  | 2.34                     | 0.43              |
| 20:J:18:CYS:H    | 20:J:81:GLY:HA3   | 1.84                     | 0.43              |
| 36:c:30:LYS:HZ2  | 36:c:33:PRO:HG2   | 1.82                     | 0.43              |
| 40:g:29:TYR:HB2  | 40:g:79:LYS:HD3   | 1.99                     | 0.43              |
| 42:i:7:LEU:HD13  | 49:p:96:GLU:HG3   | 2.00                     | 0.43              |
| 48:o:14:GLU:O    | 48:o:18:LEU:HG    | 2.19                     | 0.43              |
| 49:p:4:LYS:HZ2   | 49:p:6:GLY:HA3    | 1.84                     | 0.43              |
| 50:q:36:ASP:OD1  | 50:q:36:ASP:N     | 2.44                     | 0.43              |
| 1:0:32:LYS:NZ    | 4:3:183:A:OP2     | 2.34                     | 0.43              |
| 4:3:353:G:H2'    | 4:3:354:C:C6      | 2.54                     | 0.43              |
| 4:3:1099:C:H3'   | 4:3:1100:U:C6     | 2.54                     | 0.43              |
| 4:3:1522:U:H5''  | 4:3:1523:C:H5     | 1.84                     | 0.43              |
| 4:3:1815:U:O2'   | 4:3:1816:A:O4'    | 2.36                     | 0.43              |
| 4:3:2010:A:H2'   | 4:3:2011:G:O4'    | 2.19                     | 0.43              |
| 4:3:2176:G:H2'   | 4:3:2178:A:OP2    | 2.18                     | 0.43              |
| 4:3:2205:U:O3'   | 4:3:2206:A:H8     | 2.01                     | 0.43              |
| 4:3:2452:G:OP2   | 36:c:69:LYS:HD2   | 2.18                     | 0.43              |
| 4:3:2691:C:H5''  | 48:o:56:ARG:HH22  | 1.83                     | 0.43              |
| 5:4:81:U:H2'     | 5:4:82:U:O4'      | 2.18                     | 0.43              |
| 6:5:111:A:H2'    | 6:5:112:U:O4'     | 2.19                     | 0.43              |
| 6:5:197:A:H1'    | 6:5:218:U:O2'     | 2.19                     | 0.43              |
| 6:5:625:U:H2'    | 6:5:626:G:H8      | 1.83                     | 0.43              |
| 6:5:786:U:O2'    | 6:5:788:G:N7      | 2.37                     | 0.43              |
| 6:5:836:C:O2'    | 15:E:145:ARG:N    | 2.52                     | 0.43              |
| 8:7:35:U:H2'     | 8:7:36:C:C6       | 2.54                     | 0.43              |
| 12:B:34:LEU:HD12 | 12:B:35:ILE:HG23  | 2.00                     | 0.43              |
| 13:C:93:LEU:HA   | 13:C:96:ARG:NH1   | 2.33                     | 0.43              |
| 13:C:102:TYR:HB3 | 13:C:110:ARG:HE   | 1.82                     | 0.43              |
| 14:D:206:ARG:O   | 14:D:210:ILE:HG12 | 2.19                     | 0.43              |
| 21:K:86:ASN:ND2  | 21:K:118:VAL:HG22 | 2.34                     | 0.43              |
| 35:b:13:MET:HA   | 35:b:27:THR:HA    | 2.00                     | 0.43              |
| 39:f:47:ARG:O    | 39:f:48:ASP:C     | 2.62                     | 0.43              |
| 43:j:13:ASN:HD22 | 43:j:96:THR:HG1   | 1.61                     | 0.43              |
| 44:k:61:ARG:HA   | 44:k:61:ARG:NE    | 2.34                     | 0.43              |
| 47:n:8:ARG:HG2   | 47:n:94:GLY:O     | 2.18                     | 0.43              |
| 47:n:65:GLY:HA2  | 47:n:101:ARG:NH1  | 2.32                     | 0.43              |
| 49:p:73:MET:HE1  | 49:p:78:PHE:CD1   | 2.53                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 52:s:25:LYS:HE3  | 52:s:90:ALA:HB2  | 2.00                     | 0.43              |
| 4:3:38:G:N3      | 4:3:486:G:O2'    | 2.52                     | 0.43              |
| 4:3:190:G:H2'    | 4:3:191:G:H8     | 1.84                     | 0.43              |
| 4:3:496:A:H62    | 4:3:505:G:H21    | 1.66                     | 0.43              |
| 4:3:567:U:OP1    | 4:3:594:G:N2     | 2.44                     | 0.43              |
| 4:3:833:C:OP2    | 36:c:63:LYS:NZ   | 2.47                     | 0.43              |
| 4:3:1077:G:H2'   | 4:3:1078:C:C6    | 2.54                     | 0.43              |
| 4:3:1959:A:N3    | 4:3:2568:G:O2'   | 2.42                     | 0.43              |
| 4:3:2025:C:H2'   | 4:3:2026:A:H8    | 1.84                     | 0.43              |
| 4:3:2140:G:H2'   | 4:3:2164:G:H22   | 1.83                     | 0.43              |
| 4:3:2169:G:N2    | 4:3:2173:G:O4'   | 2.52                     | 0.43              |
| 4:3:2183:U:H3'   | 4:3:2184:A:C5'   | 2.45                     | 0.43              |
| 4:3:2502:G:H4'   | 45:l:80:GLU:CD   | 2.44                     | 0.43              |
| 5:4:28:C:OP2     | 47:n:36:LEU:HD11 | 2.19                     | 0.43              |
| 6:5:9:A:C6       | 13:C:202:ARG:NE  | 2.81                     | 0.43              |
| 6:5:421:G:H5''   | 6:5:422:A:OP2    | 2.19                     | 0.43              |
| 6:5:648:C:H2'    | 6:5:649:U:C6     | 2.54                     | 0.43              |
| 6:5:839:U:H3'    | 6:5:840:C:C6     | 2.53                     | 0.43              |
| 6:5:909:A:O2'    | 6:5:911:G:H5''   | 2.18                     | 0.43              |
| 6:5:1019:G:OP2   | 6:5:1019:G:H8    | 2.02                     | 0.43              |
| 12:B:8:ASN:OD1   | 12:B:9:GLY:N     | 2.52                     | 0.43              |
| 14:D:212:ARG:O   | 14:D:212:ARG:HD3 | 2.19                     | 0.43              |
| 16:F:69:MET:HE1  | 16:F:96:ILE:HA   | 2.01                     | 0.43              |
| 16:F:141:HIS:O   | 16:F:145:GLU:OE1 | 2.37                     | 0.43              |
| 20:J:32:GLY:O    | 20:J:33:ASN:C    | 2.61                     | 0.43              |
| 28:R:41:PHE:CD2  | 57:x:66:PHE:HB3  | 2.54                     | 0.43              |
| 34:a:138:LEU:N   | 34:a:196:CYS:O   | 2.47                     | 0.43              |
| 43:j:71:ARG:HH12 | 43:j:104:ARG:NH1 | 2.17                     | 0.43              |
| 46:m:59:ASN:HA   | 46:m:62:GLN:HG2  | 2.00                     | 0.43              |
| 46:m:72:LEU:O    | 46:m:73:PHE:HD1  | 2.02                     | 0.43              |
| 47:n:91:PHE:CZ   | 47:n:106:ALA:HB2 | 2.54                     | 0.43              |
| 48:o:95:LYS:HB2  | 48:o:117:ARG:O   | 2.19                     | 0.43              |
| 55:v:31:VAL:HG23 | 55:v:33:LEU:HG   | 2.01                     | 0.43              |
| 55:v:57:THR:O    | 55:v:61:HIS:ND1  | 2.50                     | 0.43              |
| 4:3:142:A:N3     | 4:3:1436:C:O2'   | 2.35                     | 0.42              |
| 4:3:410:G:O2'    | 4:3:436:G:O6     | 2.26                     | 0.42              |
| 4:3:548:A:H2'    | 4:3:549:A:C8     | 2.54                     | 0.42              |
| 4:3:1118:U:O2'   | 4:3:1120:A:N7    | 2.48                     | 0.42              |
| 4:3:1583:G:HO2'  | 4:3:1584:U:P     | 2.41                     | 0.42              |
| 4:3:1613:A:H2'   | 4:3:1614:G:O4'   | 2.18                     | 0.42              |
| 4:3:2237:U:H2'   | 4:3:2238:G:H8    | 1.83                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:3:2288:G:O6     | 54:u:28:ARG:CZ    | 2.67                     | 0.42              |
| 4:3:2490:A:O2'    | 9:8:63:C:O2'      | 2.23                     | 0.42              |
| 6:5:196:G:HO2'    | 6:5:197:A:P       | 2.41                     | 0.42              |
| 6:5:212:G:O2'     | 6:5:464:A:N6      | 2.31                     | 0.42              |
| 6:5:358:G:N1      | 6:5:361:U:OP2     | 2.51                     | 0.42              |
| 6:5:423:U:H2'     | 6:5:424:U:C6      | 2.54                     | 0.42              |
| 6:5:948:U:O4      | 22:L:103:ARG:NH1  | 2.51                     | 0.42              |
| 6:5:1076:U:H3'    | 6:5:1077:U:C5     | 2.54                     | 0.42              |
| 6:5:1323:A:OP1    | 18:H:125:ARG:CZ   | 2.66                     | 0.42              |
| 10:9:51:ASP:OD1   | 10:9:53:THR:OG1   | 2.35                     | 0.42              |
| 11:A:82:ILE:HD12  | 11:A:175:LEU:HB3  | 1.99                     | 0.42              |
| 11:A:137:GLN:OE1  | 11:A:144:LEU:HD11 | 2.18                     | 0.42              |
| 12:B:114:LEU:HD23 | 12:B:114:LEU:H    | 1.84                     | 0.42              |
| 16:F:52:ARG:NH1   | 16:F:120:ALA:HB1  | 2.34                     | 0.42              |
| 18:H:11:ARG:HD3   | 18:H:11:ARG:N     | 2.34                     | 0.42              |
| 18:H:98:LYS:C     | 18:H:100:LEU:N    | 2.77                     | 0.42              |
| 19:I:18:SER:HB3   | 19:I:102:VAL:HA   | 2.01                     | 0.42              |
| 34:a:209:ASN:N    | 34:a:209:ASN:OD1  | 2.53                     | 0.42              |
| 37:d:63:GLN:HE21  | 37:d:95:ARG:CD    | 2.32                     | 0.42              |
| 37:d:135:GLN:NE2  | 37:d:149:ILE:HA   | 2.33                     | 0.42              |
| 53:t:90:LYS:O     | 53:t:102:ARG:HA   | 2.19                     | 0.42              |
| 54:u:46:ARG:HA    | 54:u:78:ASP:OD1   | 2.18                     | 0.42              |
| 4:3:593:C:H1'     | 49:p:47:ARG:HH12  | 1.84                     | 0.42              |
| 4:3:1889:U:H2'    | 4:3:1890:U:C6     | 2.54                     | 0.42              |
| 4:3:2133:A:N6     | 4:3:2180:U:OP2    | 2.53                     | 0.42              |
| 4:3:2155:G:N1     | 4:3:2156:G:C6     | 2.87                     | 0.42              |
| 4:3:2545:U:H2'    | 4:3:2546:U:C6     | 2.53                     | 0.42              |
| 6:5:680:G:H1      | 6:5:704:U:H3      | 1.67                     | 0.42              |
| 6:5:1226:A:H2'    | 6:5:1227:A:C8     | 2.54                     | 0.42              |
| 15:E:154:GLU:OE2  | 15:E:155:GLU:N    | 2.53                     | 0.42              |
| 17:G:16:ALA:HB2   | 17:G:89:GLN:OE1   | 2.20                     | 0.42              |
| 22:L:27:LEU:HD23  | 22:L:27:LEU:H     | 1.85                     | 0.42              |
| 29:S:56:ARG:HH12  | 29:S:57:LYS:NZ    | 2.17                     | 0.42              |
| 38:e:130:LYS:HG2  | 38:e:133:GLU:HB3  | 2.01                     | 0.42              |
| 44:k:3:LEU:HA     | 44:k:6:LEU:CD2    | 2.50                     | 0.42              |
| 48:o:22:VAL:HG23  | 48:o:81:ILE:HG21  | 2.01                     | 0.42              |
| 48:o:52:VAL:O     | 48:o:101:ILE:HD11 | 2.20                     | 0.42              |
| 49:p:81:LEU:HA    | 49:p:84:LYS:HZ2   | 1.83                     | 0.42              |
| 54:u:60:TYR:OH    | 54:u:92:LYS:NZ    | 2.49                     | 0.42              |
| 4:3:1315:A:P      | 46:m:107:ARG:HH12 | 2.41                     | 0.42              |
| 4:3:1380:U:H1'    | 4:3:1604:A:H2     | 1.85                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:3:1654:G:H2'   | 4:3:1655:U:C6    | 2.53                     | 0.42              |
| 4:3:1758:C:H2'   | 4:3:1759:C:C6    | 2.54                     | 0.42              |
| 4:3:2057:C:H4'   | 35:b:144:GLN:NE2 | 2.34                     | 0.42              |
| 4:3:2068:G:H2'   | 4:3:2509:C:O2'   | 2.19                     | 0.42              |
| 4:3:2399:G:C6    | 4:3:2435:C:H1'   | 2.54                     | 0.42              |
| 4:3:2438:A:H2'   | 4:3:2438:A:N3    | 2.34                     | 0.42              |
| 4:3:2513:G:O6    | 4:3:2584:G:H2'   | 2.20                     | 0.42              |
| 4:3:2797:C:H4'   | 4:3:2895:A:H2    | 1.83                     | 0.42              |
| 4:3:2803:G:O2'   | 4:3:2804:C:O5'   | 2.34                     | 0.42              |
| 4:3:2890:G:H1'   | 58:y:39:PHE:HE1  | 1.84                     | 0.42              |
| 6:5:128:A:O2'    | 6:5:198:A:N1     | 2.49                     | 0.42              |
| 6:5:271:G:C5'    | 26:P:17:LYS:HZ1  | 2.30                     | 0.42              |
| 6:5:945:U:H2'    | 6:5:946:G:H8     | 1.84                     | 0.42              |
| 7:6:71:C:H5'     | 7:6:72:C:OP2     | 2.19                     | 0.42              |
| 8:7:5:C:H2'      | 8:7:6:C:C6       | 2.54                     | 0.42              |
| 12:B:48:TYR:CE2  | 12:B:88:ILE:HG22 | 2.55                     | 0.42              |
| 12:B:115:SER:HB2 | 12:B:221:HIS:CD2 | 2.54                     | 0.42              |
| 14:D:211:LEU:O   | 17:G:75:LYS:NZ   | 2.40                     | 0.42              |
| 17:G:24:ASN:OD1  | 17:G:27:LYS:NZ   | 2.52                     | 0.42              |
| 27:Q:38:LYS:O    | 27:Q:39:LYS:C    | 2.62                     | 0.42              |
| 35:b:56:THR:HA   | 35:b:78:THR:HG22 | 2.01                     | 0.42              |
| 36:c:128:VAL:HB  | 36:c:198:LEU:HG  | 2.00                     | 0.42              |
| 38:e:98:ARG:NH1  | 38:e:109:GLN:OE1 | 2.51                     | 0.42              |
| 39:f:77:LEU:H    | 39:f:77:LEU:HG   | 1.63                     | 0.42              |
| 39:f:90:GLY:HA3  | 39:f:125:GLU:OE2 | 2.19                     | 0.42              |
| 42:i:19:TYR:HD2  | 42:i:38:LEU:HD21 | 1.84                     | 0.42              |
| 42:i:39:ILE:O    | 42:i:54:GLY:HA3  | 2.19                     | 0.42              |
| 45:l:56:LYS:HE3  | 45:l:56:LYS:HB3  | 1.81                     | 0.42              |
| 4:3:154:U:H2'    | 4:3:155:A:C8     | 2.54                     | 0.42              |
| 4:3:567:U:H4'    | 4:3:568:G:C8     | 2.54                     | 0.42              |
| 4:3:901:C:O2     | 4:3:946:A:N6     | 2.53                     | 0.42              |
| 4:3:963:U:H2'    | 4:3:964:A:C8     | 2.54                     | 0.42              |
| 4:3:1271:A:H2'   | 4:3:1272:A:C8    | 2.54                     | 0.42              |
| 4:3:1321:C:H2'   | 4:3:1322:A:O4'   | 2.19                     | 0.42              |
| 4:3:1691:U:H5''  | 35:b:139:TYR:O   | 2.19                     | 0.42              |
| 4:3:1765:G:OP1   | 4:3:1767:A:N6    | 2.52                     | 0.42              |
| 4:3:2052:C:O2    | 58:y:19:HIS:NE2  | 2.50                     | 0.42              |
| 4:3:2151:G:H4'   | 4:3:2152:C:C5    | 2.54                     | 0.42              |
| 6:5:68:C:O2'     | 6:5:157:A:H1'    | 2.19                     | 0.42              |
| 6:5:395:G:H2'    | 6:5:396:C:C6     | 2.54                     | 0.42              |
| 6:5:927:C:P      | 16:F:3:LYS:HZ1   | 2.42                     | 0.42              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 11:A:17:LEU:HD23 | 11:A:62:ARG:HG3   | 2.01                     | 0.42              |
| 11:A:30:VAL:HG22 | 11:A:55:HIS:CD2   | 2.55                     | 0.42              |
| 15:E:43:LYS:HE3  | 15:E:43:LYS:HB3   | 1.95                     | 0.42              |
| 22:L:94:ASN:HA   | 22:L:109:ARG:HH21 | 1.83                     | 0.42              |
| 25:O:36:ILE:HG23 | 25:O:51:ASP:CG    | 2.44                     | 0.42              |
| 30:T:44:GLU:O    | 30:T:48:ILE:HG23  | 2.19                     | 0.42              |
| 35:b:229:ALA:HA  | 48:o:21:TYR:CE2   | 2.54                     | 0.42              |
| 41:h:72:VAL:O    | 41:h:73:SER:OG    | 2.30                     | 0.42              |
| 49:p:79:ILE:HD13 | 49:p:91:ARG:HH21  | 1.84                     | 0.42              |
| 53:t:57:LYS:C    | 53:t:58:GLN:HG3   | 2.45                     | 0.42              |
| 54:u:45:ILE:HD11 | 54:u:49:GLN:HB2   | 2.00                     | 0.42              |
| 56:w:16:VAL:O    | 56:w:20:ILE:HG12  | 2.20                     | 0.42              |
| 57:x:90:LYS:HG3  | 57:x:91:HIS:H     | 1.85                     | 0.42              |
| 2:1:3:VAL:HG23   | 4:3:246:G:H3'     | 2.00                     | 0.42              |
| 4:3:764:G:OP1    | 34:a:10:SER:OG    | 2.37                     | 0.42              |
| 4:3:1119:A:H5'   | 40:g:52:LYS:NZ    | 2.33                     | 0.42              |
| 4:3:1992:C:H2'   | 4:3:1993:U:C6     | 2.54                     | 0.42              |
| 4:3:2310:C:H2'   | 4:3:2311:G:C8     | 2.54                     | 0.42              |
| 5:4:104:C:H2'    | 5:4:105:A:H8      | 1.84                     | 0.42              |
| 6:5:190:A:H2'    | 6:5:191:A:C8      | 2.52                     | 0.42              |
| 6:5:352:A:N3     | 6:5:364:U:O2'     | 2.47                     | 0.42              |
| 6:5:403:A:H2'    | 6:5:404:A:H8      | 1.84                     | 0.42              |
| 6:5:1045:C:H42   | 32:Y:76:G:N2      | 2.18                     | 0.42              |
| 6:5:1121:U:H3'   | 6:5:1122:U:H5''   | 2.02                     | 0.42              |
| 11:A:214:ILE:O   | 11:A:215:ILE:HD13 | 2.19                     | 0.42              |
| 12:B:20:SER:HB2  | 23:M:52:ALA:O     | 2.19                     | 0.42              |
| 14:D:110:GLU:HB3 | 14:D:112:PRO:HD2  | 2.01                     | 0.42              |
| 16:F:140:THR:HA  | 16:F:143:MET:HG3  | 2.01                     | 0.42              |
| 24:N:80:LYS:HA   | 24:N:85:ARG:NH1   | 2.34                     | 0.42              |
| 34:a:135:SER:HA  | 34:a:199:THR:HA   | 2.00                     | 0.42              |
| 38:e:87:GLU:OE2  | 38:e:135:THR:OG1  | 2.31                     | 0.42              |
| 39:f:83:GLU:HA   | 39:f:149:LYS:H    | 1.85                     | 0.42              |
| 46:m:80:ASP:O    | 46:m:84:SER:HB3   | 2.18                     | 0.42              |
| 46:m:92:LYS:HA   | 46:m:92:LYS:HD2   | 1.93                     | 0.42              |
| 4:3:755:C:H2'    | 4:3:756:A:C8      | 2.54                     | 0.42              |
| 4:3:867:G:H5'    | 44:k:39:GLN:HG2   | 2.01                     | 0.42              |
| 4:3:1005:G:H2'   | 4:3:1006:U:C6     | 2.55                     | 0.42              |
| 4:3:1605:A:H2'   | 4:3:1606:A:H8     | 1.84                     | 0.42              |
| 4:3:1697:C:O2'   | 4:3:2694:A:H4'    | 2.20                     | 0.42              |
| 4:3:1893:C:H2'   | 4:3:1894:U:H6     | 1.85                     | 0.42              |
| 4:3:2190:G:O2'   | 4:3:2191:G:H5'    | 2.19                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:3:2200:U:H2'    | 4:3:2201:G:H5'    | 2.02                     | 0.42              |
| 6:5:56:A:OP2      | 6:5:348:C:N4      | 2.52                     | 0.42              |
| 6:5:840:C:C4      | 6:5:841:C:C2      | 3.07                     | 0.42              |
| 6:5:1201:C:OP2    | 22:L:90:ARG:NH1   | 2.52                     | 0.42              |
| 9:8:27:A:H61      | 9:8:43:U:H3       | 1.67                     | 0.42              |
| 10:9:199:PRO:HB2  | 10:9:202:VAL:HG23 | 2.01                     | 0.42              |
| 11:A:208:PRO:HA   | 11:A:214:ILE:HD11 | 2.01                     | 0.42              |
| 14:D:64:SER:HB2   | 14:D:66:PHE:CD2   | 2.54                     | 0.42              |
| 21:K:4:ILE:HD13   | 21:K:7:LEU:HD21   | 2.02                     | 0.42              |
| 21:K:28:LEU:HG    | 21:K:30:LEU:HD12  | 2.02                     | 0.42              |
| 32:Y:64:A:O5'     | 32:Y:64:A:H8      | 2.02                     | 0.42              |
| 32:Y:95:C:H1'     | 32:Y:96:U:C2      | 2.53                     | 0.42              |
| 35:b:3:ILE:O      | 35:b:87:MET:HG2   | 2.20                     | 0.42              |
| 37:d:63:GLN:NE2   | 37:d:95:ARG:HD2   | 2.32                     | 0.42              |
| 37:d:104:ILE:HG23 | 37:d:105:TYR:CD1  | 2.53                     | 0.42              |
| 40:g:74:THR:HG22  | 40:g:110:CYS:HB2  | 2.02                     | 0.42              |
| 45:l:103:MET:HG3  | 45:l:104:PHE:CD2  | 2.54                     | 0.42              |
| 49:p:42:ALA:CB    | 50:q:71:ILE:HG22  | 2.50                     | 0.42              |
| 49:p:78:PHE:O     | 49:p:82:LEU:HD23  | 2.19                     | 0.42              |
| 52:s:48:TYR:CD2   | 52:s:91:ILE:HD13  | 2.54                     | 0.42              |
| 54:u:38:LYS:HG3   | 54:u:53:ARG:HE    | 1.84                     | 0.42              |
| 4:3:230:G:H2'     | 4:3:231:A:C8      | 2.55                     | 0.42              |
| 4:3:1229:U:H2'    | 4:3:1230:U:C6     | 2.55                     | 0.42              |
| 4:3:1836:A:H3'    | 4:3:1837:C:H6     | 1.84                     | 0.42              |
| 4:3:2106:G:H1     | 4:3:2198:G:H1     | 1.66                     | 0.42              |
| 4:3:2642:G:O2'    | 35:b:81:LEU:HD11  | 2.20                     | 0.42              |
| 4:3:2681:G:H2'    | 4:3:2682:A:H8     | 1.84                     | 0.42              |
| 6:5:304:U:H2'     | 6:5:305:A:C8      | 2.52                     | 0.42              |
| 6:5:573:G:O2'     | 6:5:818:A:H5'     | 2.19                     | 0.42              |
| 6:5:954:A:H62     | 28:R:78:ARG:HH11  | 1.66                     | 0.42              |
| 6:5:1320:A:C8     | 6:5:1322:U:C4     | 3.07                     | 0.42              |
| 8:7:17:G:H4'      | 8:7:18:G:H5''     | 2.01                     | 0.42              |
| 12:B:217:ARG:HE   | 19:I:23:LEU:HD13  | 1.85                     | 0.42              |
| 15:E:104:LYS:O    | 15:E:107:LEU:HG   | 2.20                     | 0.42              |
| 15:E:114:LYS:O    | 15:E:115:TYR:C    | 2.59                     | 0.42              |
| 15:E:164:GLY:O    | 15:E:166:PHE:CD2  | 2.73                     | 0.42              |
| 18:H:58:ASP:HB2   | 18:H:61:LYS:NZ    | 2.35                     | 0.42              |
| 18:H:78:ALA:HA    | 18:H:81:ILE:HG12  | 2.02                     | 0.42              |
| 20:J:8:ASN:CG     | 20:J:9:VAL:H      | 2.27                     | 0.42              |
| 21:K:113:GLY:HA2  | 21:K:117:THR:O    | 2.20                     | 0.42              |
| 24:N:79:VAL:CG2   | 24:N:85:ARG:HD2   | 2.48                     | 0.42              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 28:R:78:ARG:HG3   | 28:R:79:ASN:N    | 2.35                     | 0.42              |
| 31:X:40:ILE:HD11  | 31:X:56:TYR:CB   | 2.50                     | 0.42              |
| 36:c:43:ALA:C     | 36:c:45:TRP:H    | 2.26                     | 0.42              |
| 39:f:54:GLN:HA    | 39:f:57:HIS:CD2  | 2.54                     | 0.42              |
| 47:n:32:VAL:HG11  | 47:n:105:LEU:CD1 | 2.49                     | 0.42              |
| 48:o:100:TYR:O    | 48:o:100:TYR:CG  | 2.73                     | 0.42              |
| 49:p:9:THR:HB     | 49:p:12:ARG:NH2  | 2.34                     | 0.42              |
| 51:r:72:PHE:H     | 51:r:107:LEU:HA  | 1.84                     | 0.42              |
| 4:3:159:G:H2'     | 4:3:160:A:C8     | 2.55                     | 0.42              |
| 4:3:716:G:H1      | 4:3:831:U:H3     | 1.68                     | 0.42              |
| 4:3:1926:A:N1     | 6:5:1470:U:O2'   | 2.46                     | 0.42              |
| 4:3:2036:G:N1     | 4:3:2040:A:OP2   | 2.27                     | 0.42              |
| 4:3:2228:U:H2'    | 4:3:2229:C:C6    | 2.55                     | 0.42              |
| 4:3:2847:C:H2'    | 4:3:2848:A:C8    | 2.51                     | 0.42              |
| 5:4:6:U:H2'       | 5:4:7:G:C8       | 2.54                     | 0.42              |
| 6:5:561:A:H2'     | 6:5:565:G:C8     | 2.54                     | 0.42              |
| 6:5:1098:C:OP1    | 12:B:176:MET:N   | 2.52                     | 0.42              |
| 15:E:45:LEU:HD23  | 15:E:53:LEU:HA   | 2.02                     | 0.42              |
| 15:E:144:SER:HA   | 15:E:147:GLU:HG3 | 2.01                     | 0.42              |
| 15:E:178:PHE:O    | 15:E:179:LYS:HD3 | 2.19                     | 0.42              |
| 17:G:26:ARG:HG3   | 17:G:82:PRO:HG3  | 2.02                     | 0.42              |
| 20:J:9:VAL:HG22   | 20:J:10:SER:N    | 2.35                     | 0.42              |
| 20:J:98:LEU:H     | 20:J:98:LEU:HD12 | 1.85                     | 0.42              |
| 22:L:9:ILE:HB     | 22:L:13:LYS:NZ   | 2.35                     | 0.42              |
| 26:P:83:ARG:NH1   | 26:P:83:ARG:HB2  | 2.35                     | 0.42              |
| 34:a:173:GLN:HE22 | 34:a:180:VAL:HB  | 1.85                     | 0.42              |
| 39:f:61:ASN:O     | 39:f:64:LEU:HG   | 2.19                     | 0.42              |
| 40:g:93:LEU:HA    | 40:g:96:VAL:HG22 | 2.02                     | 0.42              |
| 43:j:27:SER:OG    | 43:j:28:THR:N    | 2.53                     | 0.42              |
| 50:q:5:VAL:CG1    | 50:q:55:VAL:HG21 | 2.50                     | 0.42              |
| 51:r:24:ILE:HG23  | 51:r:32:ALA:HB1  | 2.01                     | 0.42              |
| 51:r:65:ASN:OD1   | 51:r:66:GLY:N    | 2.52                     | 0.42              |
| 51:r:82:MET:HE2   | 51:r:84:ARG:NH1  | 2.34                     | 0.42              |
| 56:w:49:ARG:HH11  | 56:w:52:ALA:HB3  | 1.85                     | 0.42              |
| 57:x:77:THR:HB    | 57:x:79:LYS:NZ   | 2.35                     | 0.42              |
| 2:1:2:LYS:HA      | 4:3:246:G:H2'    | 2.01                     | 0.42              |
| 2:1:54:ARG:NH2    | 4:3:868:C:H4'    | 2.34                     | 0.42              |
| 2:1:54:ARG:NH2    | 44:k:52:GLU:HG2  | 2.33                     | 0.42              |
| 4:3:67:C:O2'      | 4:3:492:C:N3     | 2.48                     | 0.42              |
| 4:3:235:U:H2'     | 4:3:236:G:O4'    | 2.20                     | 0.42              |
| 4:3:356:A:OP2     | 36:c:174:ASN:HB2 | 2.20                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:3:1476:C:H2'    | 4:3:1477:A:C8     | 2.55                     | 0.42              |
| 4:3:1585:A:N3     | 4:3:1585:A:H2'    | 2.34                     | 0.42              |
| 4:3:1709:C:H2'    | 4:3:1710:A:O4'    | 2.20                     | 0.42              |
| 4:3:1761:C:H1'    | 48:o:103:TYR:CZ   | 2.54                     | 0.42              |
| 4:3:2069:A:H2     | 33:Z:36:ASP:OD1   | 2.03                     | 0.42              |
| 4:3:2126:A:OP1    | 4:3:2126:A:H2'    | 2.19                     | 0.42              |
| 4:3:2130:A:C2     | 4:3:2184:A:H1'    | 2.55                     | 0.42              |
| 4:3:2179:A:H1'    | 4:3:2180:U:C6     | 2.55                     | 0.42              |
| 4:3:2372:C:H2'    | 4:3:2373:G:O4'    | 2.19                     | 0.42              |
| 4:3:2541:C:H2'    | 4:3:2542:A:O4'    | 2.20                     | 0.42              |
| 4:3:2687:A:H2'    | 4:3:2688:C:C6     | 2.55                     | 0.42              |
| 4:3:2825:A:O2'    | 4:3:2830:A:N1     | 2.47                     | 0.42              |
| 4:3:2863:G:H8     | 4:3:2863:G:OP2    | 2.02                     | 0.42              |
| 6:5:516:C:H2'     | 6:5:528:G:C4      | 2.55                     | 0.42              |
| 6:5:640:C:OP1     | 17:G:40:LEU:HD21  | 2.20                     | 0.42              |
| 11:A:158:ARG:HA   | 11:A:161:LYS:HG2  | 2.01                     | 0.42              |
| 12:B:159:ARG:NH2  | 12:B:196:TYR:O    | 2.52                     | 0.42              |
| 13:C:47:MET:CG    | 13:C:52:GLN:HB3   | 2.50                     | 0.42              |
| 14:D:150:LEU:HD12 | 14:D:150:LEU:O    | 2.19                     | 0.42              |
| 17:G:101:PHE:HA   | 17:G:104:LEU:HG   | 2.02                     | 0.42              |
| 18:H:89:LEU:HD23  | 18:H:96:LEU:HD21  | 2.01                     | 0.42              |
| 18:H:90:LEU:HA    | 18:H:97:LYS:HB3   | 2.02                     | 0.42              |
| 20:J:79:VAL:O     | 20:J:105:GLU:HA   | 2.20                     | 0.42              |
| 25:O:83:VAL:HA    | 25:O:86:LYS:HE3   | 2.02                     | 0.42              |
| 32:Y:83:A:C2      | 32:Y:84:A:H2'     | 2.55                     | 0.42              |
| 34:a:57:HIS:CE1   | 34:a:227:THR:HA   | 2.54                     | 0.42              |
| 35:b:227:GLU:OE2  | 48:o:20:ALA:N     | 2.53                     | 0.42              |
| 38:e:106:LEU:HD23 | 38:e:126:VAL:HG11 | 2.02                     | 0.42              |
| 47:n:29:VAL:HG23  | 47:n:90:VAL:HG23  | 2.01                     | 0.42              |
| 47:n:47:SER:HG    | 47:n:48:GLN:CD    | 2.23                     | 0.42              |
| 48:o:93:ARG:NE    | 48:o:118:LYS:HB3  | 2.35                     | 0.42              |
| 48:o:116:GLU:CD   | 48:o:117:ARG:H    | 2.27                     | 0.42              |
| 51:r:52:ASN:HA    | 51:r:55:ILE:HG12  | 2.02                     | 0.42              |
| 53:t:32:GLN:HG2   | 53:t:71:LEU:HD12  | 2.01                     | 0.42              |
| 55:v:7:LEU:HD11   | 55:v:54:THR:HB    | 2.01                     | 0.42              |
| 4:3:696:U:H2'     | 4:3:697:U:C6      | 2.55                     | 0.42              |
| 4:3:1063:A:H2'    | 4:3:1064:A:C8     | 2.55                     | 0.42              |
| 4:3:1313:G:N2     | 4:3:1356:G:H5''   | 2.35                     | 0.42              |
| 4:3:1816:A:H2'    | 4:3:1817:A:C8     | 2.55                     | 0.42              |
| 4:3:1931:C:H2'    | 4:3:1932:C:C6     | 2.54                     | 0.42              |
| 4:3:2054:C:H2'    | 4:3:2055:A:H8     | 1.85                     | 0.42              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 4:3:2140:G:H3'    | 4:3:2164:G:H1    | 1.85                     | 0.42              |
| 4:3:2157:A:H2'    | 4:3:2158:C:O4'   | 2.19                     | 0.42              |
| 4:3:2743:U:H2'    | 4:3:2744:A:H8    | 1.83                     | 0.42              |
| 4:3:2825:A:H2'    | 4:3:2826:G:O4'   | 2.20                     | 0.42              |
| 4:3:2893:C:H2'    | 4:3:2894:G:O4'   | 2.19                     | 0.42              |
| 6:5:61:A:N1       | 6:5:92:G:O2'     | 2.38                     | 0.42              |
| 6:5:348:C:H4'     | 6:5:350:G:OP1    | 2.20                     | 0.42              |
| 6:5:404:A:OP1     | 13:C:111:ARG:NH1 | 2.53                     | 0.42              |
| 6:5:470:U:O4      | 6:5:471:A:N6     | 2.53                     | 0.42              |
| 6:5:515:G:N2      | 6:5:531:A:OP2    | 2.35                     | 0.42              |
| 6:5:818:A:H2'     | 6:5:819:G:C8     | 2.55                     | 0.42              |
| 6:5:998:G:H2'     | 6:5:998:G:N3     | 2.35                     | 0.42              |
| 6:5:1279:G:O2'    | 6:5:1280:A:O4'   | 2.38                     | 0.42              |
| 11:A:41:MET:HE1   | 11:A:208:PRO:HB3 | 2.02                     | 0.42              |
| 11:A:292:THR:OG1  | 30:T:54:ARG:NH2  | 2.53                     | 0.42              |
| 13:C:7:ILE:H      | 13:C:7:ILE:HD12  | 1.84                     | 0.42              |
| 13:C:112:SER:O    | 13:C:116:LEU:HG  | 2.20                     | 0.42              |
| 17:G:40:LEU:O     | 17:G:44:ILE:HG12 | 2.20                     | 0.42              |
| 17:G:100:PRO:HB2  | 17:G:102:GLU:CD  | 2.45                     | 0.42              |
| 21:K:42:LEU:HD13  | 21:K:94:LEU:HD11 | 2.01                     | 0.42              |
| 22:L:75:LEU:HD12  | 22:L:76:ASN:N    | 2.35                     | 0.42              |
| 25:O:69:VAL:HG12  | 25:O:73:PHE:HE2  | 1.84                     | 0.42              |
| 30:T:27:ARG:HA    | 30:T:30:GLN:NE2  | 2.35                     | 0.42              |
| 35:b:225:GLN:HE22 | 48:o:84:PRO:HA   | 1.85                     | 0.42              |
| 36:c:64:LYS:HE2   | 36:c:64:LYS:HB3  | 1.94                     | 0.42              |
| 37:d:108:LEU:HB3  | 37:d:109:PRO:HD3 | 2.02                     | 0.42              |
| 47:n:66:ASN:HB2   | 47:n:68:ASP:OD1  | 2.19                     | 0.42              |
| 53:t:14:THR:CG2   | 53:t:73:LYS:HG3  | 2.49                     | 0.42              |
| 55:v:36:CYS:SG    | 55:v:55:LEU:HD12 | 2.60                     | 0.42              |
| 4:3:999:U:H1'     | 4:3:2258:G:O6    | 2.20                     | 0.41              |
| 4:3:2224:A:H2'    | 4:3:2225:G:C8    | 2.55                     | 0.41              |
| 4:3:2352:U:C2'    | 59:z:34:LEU:HD11 | 2.47                     | 0.41              |
| 6:5:943:C:OP1     | 22:L:106:ALA:HA  | 2.20                     | 0.41              |
| 6:5:1026:A:H3'    | 6:5:1027:A:H8    | 1.84                     | 0.41              |
| 6:5:1261:A:N3     | 6:5:1327:G:O2'   | 2.41                     | 0.41              |
| 6:5:1438:U:OP2    | 48:o:113:LYS:NZ  | 2.42                     | 0.41              |
| 13:C:101:VAL:O    | 13:C:104:MET:HB3 | 2.20                     | 0.41              |
| 14:D:170:ILE:HG23 | 14:D:175:TYR:HB2 | 2.02                     | 0.41              |
| 15:E:107:LEU:O    | 15:E:111:LYS:HG2 | 2.20                     | 0.41              |
| 18:H:45:LEU:HD12  | 18:H:48:GLN:HB3  | 2.02                     | 0.41              |
| 18:H:98:LYS:C     | 18:H:100:LEU:H   | 2.28                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:N:26:VAL:O     | 24:N:30:THR:HG23  | 2.19                     | 0.41              |
| 30:T:5:GLU:HG3    | 30:T:7:LYS:N      | 2.33                     | 0.41              |
| 34:a:233:MET:HG3  | 34:a:234:ASN:N    | 2.35                     | 0.41              |
| 35:b:38:GLY:HA2   | 35:b:92:MET:HE1   | 2.01                     | 0.41              |
| 35:b:115:LYS:HE2  | 35:b:117:ARG:NH2  | 2.34                     | 0.41              |
| 38:e:87:GLU:CD    | 38:e:135:THR:HG1  | 2.27                     | 0.41              |
| 43:j:64:ARG:CG    | 43:j:83:ALA:HB3   | 2.50                     | 0.41              |
| 48:o:102:SER:HA   | 48:o:105:ARG:CZ   | 2.50                     | 0.41              |
| 49:p:27:ARG:HB3   | 49:p:37:THR:HG21  | 2.01                     | 0.41              |
| 49:p:42:ALA:HB3   | 50:q:71:ILE:HG22  | 2.01                     | 0.41              |
| 50:q:59:VAL:HG22  | 50:q:92:LEU:HD21  | 2.02                     | 0.41              |
| 4:3:194:A:H5''    | 4:3:208:A:N1      | 2.35                     | 0.41              |
| 4:3:984:C:H2'     | 4:3:985:A:H8      | 1.84                     | 0.41              |
| 4:3:1149:G:H2'    | 4:3:1150:U:C6     | 2.55                     | 0.41              |
| 4:3:1280:G:OP2    | 44:k:22:ARG:NE    | 2.31                     | 0.41              |
| 4:3:1558:A:P      | 4:3:1571:G:H22    | 2.43                     | 0.41              |
| 4:3:2631:G:OP1    | 4:3:2830:A:O2'    | 2.24                     | 0.41              |
| 4:3:2675:C:H1'    | 38:e:112:TYR:HD2  | 1.85                     | 0.41              |
| 4:3:2841:A:H2'    | 4:3:2842:G:C8     | 2.55                     | 0.41              |
| 6:5:381:C:H2'     | 6:5:382:U:C6      | 2.55                     | 0.41              |
| 6:5:474:G:O2'     | 6:5:475:U:H5'     | 2.20                     | 0.41              |
| 6:5:655:G:H2'     | 6:5:656:U:C6      | 2.55                     | 0.41              |
| 12:B:61:THR:HG22  | 12:B:62:GLN:N     | 2.28                     | 0.41              |
| 12:B:72:ALA:HA    | 12:B:109:ILE:HG22 | 2.02                     | 0.41              |
| 15:E:129:ASP:O    | 15:E:130:VAL:HB   | 2.20                     | 0.41              |
| 19:I:69:GLU:OE2   | 23:M:45:ARG:NE    | 2.53                     | 0.41              |
| 21:K:96:ARG:HG2   | 21:K:111:VAL:HG23 | 2.02                     | 0.41              |
| 27:Q:35:LYS:HG3   | 27:Q:36:ARG:N     | 2.25                     | 0.41              |
| 35:b:63:ASN:HB3   | 35:b:66:GLN:OE1   | 2.20                     | 0.41              |
| 36:c:31:GLN:HG2   | 44:k:1:MET:SD     | 2.60                     | 0.41              |
| 37:d:103:LEU:HD12 | 37:d:107:ALA:HB3  | 2.02                     | 0.41              |
| 39:f:29:PHE:O     | 39:f:33:LYS:HG2   | 2.20                     | 0.41              |
| 39:f:84:HIS:CB    | 39:f:148:VAL:HG22 | 2.40                     | 0.41              |
| 41:h:60:ASP:O     | 41:h:61:LYS:HB3   | 2.20                     | 0.41              |
| 43:j:71:ARG:NH1   | 43:j:104:ARG:HH11 | 2.18                     | 0.41              |
| 48:o:100:TYR:O    | 48:o:100:TYR:CD2  | 2.73                     | 0.41              |
| 49:p:68:LEU:HD11  | 49:p:78:PHE:CD1   | 2.55                     | 0.41              |
| 51:r:28:LYS:HA    | 51:r:28:LYS:HD2   | 1.70                     | 0.41              |
| 52:s:17:TYR:O     | 52:s:21:MET:HG2   | 2.20                     | 0.41              |
| 53:t:66:GLU:OE1   | 53:t:66:GLU:N     | 2.53                     | 0.41              |
| 57:x:21:ASN:HB3   | 57:x:23:PHE:CZ    | 2.55                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:3:401:G:H2'     | 4:3:402:A:C8      | 2.55                     | 0.41              |
| 4:3:402:A:H8      | 4:3:402:A:OP2     | 2.04                     | 0.41              |
| 4:3:1230:U:H2'    | 4:3:1231:G:C8     | 2.55                     | 0.41              |
| 4:3:1780:A:N7     | 4:3:1836:A:H1'    | 2.35                     | 0.41              |
| 4:3:2170:A:O2'    | 4:3:2181:A:H5'    | 2.19                     | 0.41              |
| 11:A:110:GLN:HG3  | 11:A:161:LYS:O    | 2.21                     | 0.41              |
| 11:A:177:ILE:HG12 | 11:A:199:VAL:CG2  | 2.51                     | 0.41              |
| 11:A:223:GLN:HG2  | 11:A:224:SER:H    | 1.86                     | 0.41              |
| 12:B:137:MET:C    | 12:B:137:MET:SD   | 3.03                     | 0.41              |
| 13:C:141:LYS:HE3  | 13:C:175:GLU:HG3  | 2.03                     | 0.41              |
| 15:E:25:GLN:CG    | 15:E:35:LEU:HD22  | 2.44                     | 0.41              |
| 19:I:85:VAL:HG23  | 19:I:86:ASN:N     | 2.35                     | 0.41              |
| 23:M:7:LYS:HE2    | 23:M:28:GLY:HA3   | 2.03                     | 0.41              |
| 26:P:17:LYS:O     | 26:P:17:LYS:HD2   | 2.20                     | 0.41              |
| 34:a:266:LYS:HD3  | 34:a:266:LYS:HA   | 1.78                     | 0.41              |
| 38:e:12:ASP:OD1   | 38:e:12:ASP:N     | 2.44                     | 0.41              |
| 46:m:99:ARG:O     | 46:m:116:LEU:HA   | 2.19                     | 0.41              |
| 50:q:91:LYS:C     | 50:q:92:LEU:HD12  | 2.45                     | 0.41              |
| 59:z:8:ARG:NE     | 59:z:17:ILE:HG21  | 2.35                     | 0.41              |
| 59:z:12:ASN:OD1   | 59:z:46:VAL:HG13  | 2.20                     | 0.41              |
| 4:3:117:C:H2'     | 4:3:118:G:O4'     | 2.20                     | 0.41              |
| 4:3:159:G:H2'     | 4:3:160:A:H8      | 1.85                     | 0.41              |
| 4:3:739:G:N2      | 4:3:761:G:O2'     | 2.52                     | 0.41              |
| 4:3:1104:A:H4'    | 4:3:1105:A:H2'    | 2.01                     | 0.41              |
| 4:3:2119:A:N6     | 4:3:2177:G:OP1    | 2.54                     | 0.41              |
| 4:3:2149:U:H2'    | 4:3:2156:G:H22    | 1.86                     | 0.41              |
| 4:3:2641:A:H2     | 35:b:69:PHE:HZ    | 1.69                     | 0.41              |
| 4:3:2815:G:H5''   | 35:b:63:ASN:HD21  | 1.85                     | 0.41              |
| 5:4:49:G:H2'      | 5:4:50:C:C6       | 2.55                     | 0.41              |
| 5:4:93:U:H2'      | 5:4:94:A:H8       | 1.84                     | 0.41              |
| 6:5:885:U:H2'     | 6:5:886:A:H8      | 1.86                     | 0.41              |
| 6:5:1482:A:H2'    | 6:5:1483:C:C6     | 2.54                     | 0.41              |
| 11:A:156:ILE:HD13 | 11:A:156:ILE:HA   | 1.91                     | 0.41              |
| 12:B:155:LEU:HB2  | 12:B:202:LYS:HB2  | 2.02                     | 0.41              |
| 13:C:96:ARG:HH21  | 13:C:135:ILE:HD13 | 1.84                     | 0.41              |
| 15:E:88:ILE:HG23  | 15:E:88:ILE:O     | 2.21                     | 0.41              |
| 20:J:106:LYS:NZ   | 27:Q:104:ASP:OXT  | 2.53                     | 0.41              |
| 25:O:50:ILE:HG13  | 25:O:51:ASP:N     | 2.35                     | 0.41              |
| 27:Q:34:PHE:CG    | 27:Q:35:LYS:N     | 2.88                     | 0.41              |
| 35:b:6:ILE:O      | 35:b:206:LEU:HD12 | 2.19                     | 0.41              |
| 36:c:129:ASP:O    | 36:c:133:PHE:CD2  | 2.74                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 36:c:159:PHE:HB2 | 36:c:180:VAL:HB   | 2.01                     | 0.41              |
| 39:f:25:TYR:CE1  | 39:f:29:PHE:CE2   | 3.08                     | 0.41              |
| 39:f:51:LEU:HD13 | 39:f:51:LEU:HA    | 1.89                     | 0.41              |
| 40:g:99:VAL:O    | 40:g:103:LYS:HG3  | 2.21                     | 0.41              |
| 44:k:134:GLN:HG3 | 44:k:137:LYS:HE3  | 2.02                     | 0.41              |
| 47:n:60:LEU:HD12 | 47:n:73:VAL:HG22  | 2.03                     | 0.41              |
| 47:n:102:ILE:O   | 47:n:105:LEU:HG   | 2.19                     | 0.41              |
| 4:3:205:C:O2'    | 4:3:255:A:N1      | 2.42                     | 0.41              |
| 4:3:411:U:H2'    | 4:3:412:A:C8      | 2.54                     | 0.41              |
| 4:3:1003:U:H2'   | 4:3:1004:U:C6     | 2.55                     | 0.41              |
| 4:3:1127:C:H2'   | 4:3:1128:G:O4'    | 2.20                     | 0.41              |
| 4:3:1456:C:O2'   | 4:3:1603:A:OP2    | 2.20                     | 0.41              |
| 4:3:1701:G:N1    | 4:3:1999:G:OP2    | 2.49                     | 0.41              |
| 4:3:1798:A:P     | 4:3:1798:A:H8     | 2.43                     | 0.41              |
| 4:3:2101:A:H2'   | 4:3:2102:U:C6     | 2.55                     | 0.41              |
| 4:3:2243:G:H2'   | 4:3:2244:U:C6     | 2.56                     | 0.41              |
| 4:3:2299:U:H1'   | 4:3:2382:A:H1'    | 2.02                     | 0.41              |
| 4:3:2623:U:H2'   | 4:3:2624:C:C6     | 2.56                     | 0.41              |
| 5:4:46:C:OP1     | 47:n:96:SER:HB3   | 2.20                     | 0.41              |
| 6:5:712:A:H2'    | 6:5:713:A:C8      | 2.55                     | 0.41              |
| 6:5:747:C:O2     | 24:N:20:GLY:HA3   | 2.20                     | 0.41              |
| 6:5:824:U:H2'    | 6:5:864:U:O4      | 2.21                     | 0.41              |
| 6:5:955:U:C4     | 28:R:78:ARG:NH2   | 2.89                     | 0.41              |
| 6:5:1225:A:N3    | 6:5:1345:G:O2'    | 2.41                     | 0.41              |
| 13:C:63:MET:HE3  | 13:C:64:TYR:CE1   | 2.55                     | 0.41              |
| 15:E:121:ARG:HB3 | 15:E:124:ASN:CB   | 2.46                     | 0.41              |
| 21:K:49:ARG:HG2  | 21:K:67:LYS:HB3   | 2.03                     | 0.41              |
| 24:N:80:LYS:HA   | 24:N:85:ARG:HH12  | 1.86                     | 0.41              |
| 25:O:38:HIS:O    | 25:O:39:LEU:HD12  | 2.20                     | 0.41              |
| 27:Q:68:ALA:HB2  | 27:Q:100:PRO:HB2  | 2.02                     | 0.41              |
| 27:Q:73:ARG:NH1  | 27:Q:78:ASN:O     | 2.54                     | 0.41              |
| 34:a:57:HIS:CE1  | 34:a:227:THR:HG23 | 2.55                     | 0.41              |
| 35:b:177:GLN:CD  | 35:b:212:LYS:HZ3  | 2.27                     | 0.41              |
| 36:c:119:LYS:HA  | 36:c:119:LYS:HD3  | 1.88                     | 0.41              |
| 38:e:30:PRO:HD2  | 38:e:82:VAL:O     | 2.21                     | 0.41              |
| 38:e:34:ILE:HG21 | 38:e:78:ALA:HB1   | 2.03                     | 0.41              |
| 41:h:20:LYS:H    | 41:h:20:LYS:HD2   | 1.84                     | 0.41              |
| 41:h:28:VAL:HG11 | 41:h:57:ALA:HB1   | 2.02                     | 0.41              |
| 48:o:95:LYS:HD3  | 48:o:118:LYS:HA   | 2.01                     | 0.41              |
| 49:p:50:ARG:H    | 49:p:50:ARG:HG2   | 1.68                     | 0.41              |
| 56:w:49:ARG:HA   | 56:w:49:ARG:HD3   | 1.37                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 58:y:37:LYS:HD3  | 58:y:43:CYS:HB3   | 2.01                     | 0.41              |
| 58:y:51:LEU:HD22 | 58:y:53:VAL:HG12  | 2.03                     | 0.41              |
| 4:3:153:U:H2'    | 4:3:154:U:C6      | 2.55                     | 0.41              |
| 4:3:269:A:N1     | 4:3:463:U:O2'     | 2.52                     | 0.41              |
| 4:3:752:C:H3'    | 4:3:753:A:H8      | 1.84                     | 0.41              |
| 4:3:1441:A:H2'   | 4:3:1442:G:H8     | 1.85                     | 0.41              |
| 6:5:883:A:N1     | 6:5:901:A:H5''    | 2.36                     | 0.41              |
| 8:7:5:C:H2'      | 8:7:6:C:H6        | 1.85                     | 0.41              |
| 10:9:30:VAL:O    | 10:9:33:THR:HG22  | 2.21                     | 0.41              |
| 11:A:118:THR:HA  | 11:A:194:LEU:HD11 | 2.02                     | 0.41              |
| 12:B:49:ARG:C    | 12:B:51:ALA:H     | 2.29                     | 0.41              |
| 17:G:101:PHE:CE1 | 17:G:132:LYS:HA   | 2.56                     | 0.41              |
| 19:I:11:GLU:CD   | 19:I:81:ILE:HD11  | 2.45                     | 0.41              |
| 35:b:186:GLU:HG2 | 35:b:187:ALA:N    | 2.36                     | 0.41              |
| 39:f:15:ARG:NH1  | 39:f:54:GLN:HE22  | 2.19                     | 0.41              |
| 42:i:93:ARG:HG3  | 42:i:97:LYS:HE3   | 2.01                     | 0.41              |
| 44:k:18:LYS:HB3  | 44:k:18:LYS:HE2   | 1.93                     | 0.41              |
| 44:k:52:GLU:HB3  | 44:k:55:GLN:HG2   | 2.02                     | 0.41              |
| 45:l:65:TRP:HB2  | 45:l:105:GLU:CG   | 2.51                     | 0.41              |
| 45:l:129:TRP:CD1 | 45:l:129:TRP:H    | 2.39                     | 0.41              |
| 48:o:60:ILE:HD12 | 48:o:82:HIS:HB2   | 2.02                     | 0.41              |
| 50:q:81:LYS:HD2  | 50:q:82:LYS:H     | 1.84                     | 0.41              |
| 52:s:37:LYS:HE2  | 52:s:57:THR:HG23  | 2.01                     | 0.41              |
| 53:t:26:LYS:NZ   | 53:t:28:MET:SD    | 2.76                     | 0.41              |
| 56:w:24:GLY:O    | 56:w:28:GLU:HG2   | 2.20                     | 0.41              |
| 58:y:10:LYS:HZ2  | 58:y:13:ARG:NH1   | 2.18                     | 0.41              |
| 4:3:230:G:O2'    | 4:3:232:A:N6      | 2.53                     | 0.41              |
| 4:3:583:U:C4     | 42:i:3:LYS:HD3    | 2.55                     | 0.41              |
| 4:3:960:A:H2'    | 4:3:961:U:C6      | 2.56                     | 0.41              |
| 4:3:1031:U:C5    | 49:p:52:LYS:HD2   | 2.55                     | 0.41              |
| 4:3:1275:C:H5''  | 44:k:13:ARG:HH12  | 1.85                     | 0.41              |
| 4:3:2342:U:C4    | 47:n:10:LEU:HD21  | 2.56                     | 0.41              |
| 4:3:2605:G:H8    | 4:3:2605:G:OP2    | 2.04                     | 0.41              |
| 6:5:650:A:C6     | 17:G:67:LYS:HG2   | 2.56                     | 0.41              |
| 6:5:677:C:H2'    | 6:5:678:A:H8      | 1.86                     | 0.41              |
| 6:5:734:A:H5'    | 15:E:87:ILE:O     | 2.20                     | 0.41              |
| 6:5:768:G:H2'    | 6:5:769:U:C6      | 2.55                     | 0.41              |
| 6:5:823:C:H2'    | 6:5:824:U:C6      | 2.55                     | 0.41              |
| 7:6:48:U:H2'     | 7:6:59:G:H1'      | 2.02                     | 0.41              |
| 8:7:18:G:H1      | 8:7:54:U:H1'      | 1.85                     | 0.41              |
| 11:A:228:LEU:HA  | 11:A:231:LEU:HD12 | 2.03                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 15:E:86:LEU:HD22 | 27:Q:96:LEU:CD2   | 2.50                     | 0.41              |
| 16:F:107:ALA:HB1 | 16:F:119:ILE:HG22 | 2.02                     | 0.41              |
| 17:G:49:VAL:HG11 | 17:G:57:PHE:CE1   | 2.54                     | 0.41              |
| 20:J:78:PHE:HA   | 20:J:104:ASN:O    | 2.20                     | 0.41              |
| 22:L:24:GLY:H    | 22:L:66:GLU:CB    | 2.34                     | 0.41              |
| 26:P:9:LEU:HB2   | 26:P:63:ILE:HG22  | 2.02                     | 0.41              |
| 28:R:40:ILE:HG21 | 28:R:66:MET:O     | 2.19                     | 0.41              |
| 28:R:45:VAL:HG11 | 28:R:64:ASP:OD1   | 2.19                     | 0.41              |
| 29:S:43:ASN:O    | 29:S:44:LEU:C     | 2.63                     | 0.41              |
| 31:X:45:LYS:NZ   | 31:X:46:GLY:H     | 2.18                     | 0.41              |
| 32:Y:84:A:H1'    | 32:Y:85:A:O4'     | 2.21                     | 0.41              |
| 34:a:37:LEU:O    | 34:a:38:LEU:HD23  | 2.21                     | 0.41              |
| 35:b:211:LYS:HG3 | 35:b:212:LYS:HD2  | 2.03                     | 0.41              |
| 36:c:200:GLU:HB3 | 36:c:203:VAL:HG23 | 2.02                     | 0.41              |
| 38:e:50:ASP:O    | 38:e:52:ASN:ND2   | 2.54                     | 0.41              |
| 38:e:60:GLU:OE1  | 38:e:60:GLU:N     | 2.53                     | 0.41              |
| 40:g:91:GLU:HA   | 40:g:94:LYS:HE3   | 2.02                     | 0.41              |
| 41:h:118:GLU:O   | 41:h:122:LYS:HG2  | 2.21                     | 0.41              |
| 42:i:93:ARG:HA   | 42:i:96:LEU:HG    | 2.02                     | 0.41              |
| 43:j:8:LEU:HD22  | 43:j:82:ASN:O     | 2.21                     | 0.41              |
| 51:r:88:ARG:HA   | 51:r:88:ARG:HD2   | 1.93                     | 0.41              |
| 54:u:38:LYS:HD3  | 54:u:38:LYS:HA    | 1.84                     | 0.41              |
| 56:w:58:LEU:HD23 | 56:w:65:TRP:HB3   | 2.01                     | 0.41              |
| 4:3:827:G:N3     | 4:3:2079:G:O2'    | 2.45                     | 0.41              |
| 4:3:1094:G:H2'   | 4:3:1095:U:C5     | 2.55                     | 0.41              |
| 4:3:1406:A:O2'   | 4:3:1408:G:OP2    | 2.38                     | 0.41              |
| 4:3:1487:U:H2'   | 4:3:1488:U:C6     | 2.56                     | 0.41              |
| 4:3:1827:U:C4    | 34:a:165:GLY:HA3  | 2.56                     | 0.41              |
| 4:3:2092:U:H2'   | 4:3:2093:U:C6     | 2.56                     | 0.41              |
| 4:3:2117:G:N2    | 4:3:2127:G:H1'    | 2.36                     | 0.41              |
| 4:3:2148:U:H2'   | 4:3:2149:U:C6     | 2.55                     | 0.41              |
| 4:3:2376:C:H2'   | 4:3:2377:A:C8     | 2.56                     | 0.41              |
| 4:3:2657:C:H2'   | 4:3:2658:U:C6     | 2.55                     | 0.41              |
| 6:5:199:A:N1     | 6:5:216:G:O2'     | 2.51                     | 0.41              |
| 6:5:659:U:P      | 15:E:101:ASN:HD21 | 2.43                     | 0.41              |
| 6:5:1433:G:H5''  | 29:S:22:LYS:HZ1   | 1.86                     | 0.41              |
| 9:8:43:U:H2'     | 9:8:44:G:C8       | 2.55                     | 0.41              |
| 12:B:39:LYS:HZ3  | 12:B:95:ILE:HG13  | 1.86                     | 0.41              |
| 17:G:51:GLU:CD   | 17:G:113:ILE:HD13 | 2.46                     | 0.41              |
| 35:b:54:PHE:O    | 35:b:78:THR:HB    | 2.21                     | 0.41              |
| 36:c:60:GLY:HA3  | 36:c:80:ARG:CG    | 2.51                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 37:d:104:ILE:HG23 | 37:d:105:TYR:HD1  | 1.86                     | 0.41              |
| 39:f:52:LYS:HD3   | 39:f:55:GLN:HE21  | 1.86                     | 0.41              |
| 39:f:111:PHE:HB2  | 39:f:114:LYS:HD2  | 2.03                     | 0.41              |
| 41:h:57:ALA:HA    | 41:h:63:PHE:CE2   | 2.56                     | 0.41              |
| 48:o:103:TYR:HA   | 48:o:106:GLU:CD   | 2.46                     | 0.41              |
| 49:p:9:THR:HB     | 49:p:12:ARG:HH21  | 1.85                     | 0.41              |
| 50:q:81:LYS:HD2   | 50:q:82:LYS:N     | 2.35                     | 0.41              |
| 51:r:24:ILE:HG22  | 51:r:71:VAL:HG21  | 2.03                     | 0.41              |
| 56:w:10:LYS:NZ    | 56:w:14:GLU:HB2   | 2.35                     | 0.41              |
| 1:0:11:LYS:NZ     | 4:3:721:G:O5'     | 2.54                     | 0.41              |
| 2:1:6:ALA:O       | 44:k:59:TYR:CZ    | 2.74                     | 0.41              |
| 4:3:24:U:H2'      | 4:3:25:G:H8       | 1.85                     | 0.41              |
| 4:3:45:U:H2'      | 4:3:46:A:O4'      | 2.20                     | 0.41              |
| 4:3:431:U:O2'     | 4:3:432:G:N7      | 2.53                     | 0.41              |
| 4:3:488:G:C8      | 36:c:59:ARG:HD2   | 2.56                     | 0.41              |
| 4:3:597:C:H5'     | 49:p:36:GLN:HE22  | 1.86                     | 0.41              |
| 4:3:849:C:H1'     | 4:3:1255:G:H21    | 1.86                     | 0.41              |
| 4:3:1275:C:H5''   | 44:k:13:ARG:NH1   | 2.35                     | 0.41              |
| 4:3:1327:G:O2'    | 4:3:1674:A:N6     | 2.54                     | 0.41              |
| 4:3:1536:C:H2'    | 4:3:1537:A:H8     | 1.85                     | 0.41              |
| 4:3:1605:A:H2'    | 4:3:1606:A:C8     | 2.56                     | 0.41              |
| 4:3:1619:A:H2'    | 4:3:1620:A:H8     | 1.80                     | 0.41              |
| 4:3:1755:A:H2'    | 4:3:1756:A:H8     | 1.86                     | 0.41              |
| 4:3:1797:C:O2'    | 34:a:216:ALA:HB2  | 2.21                     | 0.41              |
| 4:3:2031:C:H2'    | 4:3:2032:G:C8     | 2.55                     | 0.41              |
| 4:3:2116:U:H5''   | 4:3:2156:G:N2     | 2.34                     | 0.41              |
| 4:3:2175:U:H2'    | 4:3:2176:G:O4'    | 2.21                     | 0.41              |
| 4:3:2401:U:C2'    | 44:k:60:ARG:HH21  | 2.34                     | 0.41              |
| 4:3:2725:G:H1'    | 48:o:98:ARG:NH2   | 2.36                     | 0.41              |
| 4:3:2760:C:H2'    | 4:3:2761:A:O4'    | 2.20                     | 0.41              |
| 4:3:2798:A:OP1    | 4:3:2798:A:H4'    | 2.19                     | 0.41              |
| 6:5:399:C:OP1     | 13:C:133:SER:HB3  | 2.20                     | 0.41              |
| 6:5:578:C:H2'     | 6:5:579:G:O4'     | 2.21                     | 0.41              |
| 6:5:616:C:H5''    | 6:5:617:U:H5''    | 2.02                     | 0.41              |
| 6:5:1056:U:H5''   | 6:5:1165:G:N2     | 2.36                     | 0.41              |
| 6:5:1076:U:H3'    | 6:5:1077:U:C6     | 2.55                     | 0.41              |
| 6:5:1270:C:H5'    | 22:L:14:ARG:NH1   | 2.36                     | 0.41              |
| 7:6:63:C:H5'      | 10:9:54:LYS:HE2   | 2.03                     | 0.41              |
| 11:A:58:LEU:HD13  | 11:A:61:GLN:OE1   | 2.20                     | 0.41              |
| 12:B:18:TRP:CZ3   | 12:B:215:LEU:HD21 | 2.55                     | 0.41              |
| 12:B:121:ARG:HA   | 12:B:190:GLU:OE1  | 2.21                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:D:160:ILE:HG12 | 14:D:176:SER:O    | 2.20                     | 0.41              |
| 15:E:42:LEU:HD11  | 15:E:54:SER:HB2   | 2.03                     | 0.41              |
| 15:E:181:PHE:O    | 15:E:182:ASN:C    | 2.63                     | 0.41              |
| 17:G:24:ASN:HA    | 17:G:27:LYS:HG2   | 2.02                     | 0.41              |
| 18:H:20:TYR:HB2   | 18:H:66:ASN:HB2   | 2.02                     | 0.41              |
| 18:H:32:VAL:HA    | 18:H:67:VAL:HB    | 2.02                     | 0.41              |
| 19:I:106:PHE:HE1  | 57:x:93:SER:H     | 1.68                     | 0.41              |
| 22:L:96:PRO:HB3   | 22:L:100:GLN:HB2  | 2.02                     | 0.41              |
| 27:Q:56:ASP:OD1   | 27:Q:56:ASP:N     | 2.54                     | 0.41              |
| 29:S:44:LEU:HD13  | 29:S:76:LEU:CD2   | 2.51                     | 0.41              |
| 29:S:48:TYR:CE2   | 29:S:69:LYS:HD2   | 2.56                     | 0.41              |
| 29:S:48:TYR:CD2   | 29:S:69:LYS:HD2   | 2.56                     | 0.41              |
| 30:T:41:ARG:HD3   | 30:T:41:ARG:HA    | 1.94                     | 0.41              |
| 31:X:40:ILE:HG13  | 31:X:41:LYS:H     | 1.86                     | 0.41              |
| 35:b:177:GLN:NE2  | 35:b:212:LYS:HZ3  | 2.18                     | 0.41              |
| 35:b:211:LYS:HB2  | 35:b:211:LYS:HE2  | 1.78                     | 0.41              |
| 36:c:194:ALA:O    | 36:c:195:ASN:HB2  | 2.21                     | 0.41              |
| 38:e:9:ILE:O      | 38:e:9:ILE:HG22   | 2.20                     | 0.41              |
| 39:f:69:LYS:HG3   | 39:f:140:VAL:HG22 | 2.03                     | 0.41              |
| 39:f:75:THR:OG1   | 39:f:76:GLU:N     | 2.54                     | 0.41              |
| 42:i:11:GLN:OE1   | 42:i:11:GLN:HA    | 2.21                     | 0.41              |
| 44:k:112:ILE:CG2  | 44:k:128:VAL:HA   | 2.49                     | 0.41              |
| 44:k:123:PRO:HB3  | 44:k:143:ASN:OD1  | 2.21                     | 0.41              |
| 45:l:7:THR:HG21   | 45:l:93:TRP:HH2   | 1.86                     | 0.41              |
| 46:m:17:THR:O     | 46:m:21:GLN:HG3   | 2.21                     | 0.41              |
| 47:n:27:ARG:HB2   | 47:n:90:VAL:HG13  | 2.03                     | 0.41              |
| 49:p:107:LEU:HD23 | 49:p:111:LYS:HE2  | 2.02                     | 0.41              |
| 50:q:48:PRO:HG2   | 50:q:49:TYR:H     | 1.86                     | 0.41              |
| 51:r:83:LYS:HB3   | 51:r:95:MET:SD    | 2.61                     | 0.41              |
| 53:t:99:LYS:HD3   | 53:t:99:LYS:HA    | 1.91                     | 0.41              |
| 54:u:86:PHE:CE1   | 54:u:92:LYS:HB3   | 2.55                     | 0.41              |
| 1:0:2:LYS:NZ      | 4:3:1654:G:O3'    | 2.54                     | 0.41              |
| 1:0:26:SER:O      | 1:0:29:LYS:HG2    | 2.21                     | 0.41              |
| 4:3:158:U:H2'     | 4:3:159:G:H8      | 1.86                     | 0.41              |
| 4:3:332:G:O2'     | 4:3:356:A:N1      | 2.44                     | 0.41              |
| 4:3:454:G:H2'     | 4:3:455:G:H8      | 1.86                     | 0.41              |
| 4:3:671:C:O2'     | 4:3:675:U:OP1     | 2.37                     | 0.41              |
| 4:3:784:A:H4'     | 4:3:1301:G:N3     | 2.36                     | 0.41              |
| 4:3:1036:A:H2'    | 4:3:1037:A:C8     | 2.55                     | 0.41              |
| 4:3:1140:U:H2'    | 4:3:1141:U:C6     | 2.56                     | 0.41              |
| 4:3:1309:G:H2'    | 4:3:1310:U:C6     | 2.56                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:3:1457:A:H2'    | 4:3:1458:A:C8     | 2.56                     | 0.41              |
| 4:3:1691:U:H4'    | 35:b:139:TYR:CE2  | 2.56                     | 0.41              |
| 4:3:2358:U:H2'    | 4:3:2359:G:O4'    | 2.20                     | 0.41              |
| 6:5:328:G:OP2     | 29:S:3:ASN:HA     | 2.20                     | 0.41              |
| 6:5:498:G:H2'     | 6:5:499:U:C6      | 2.55                     | 0.41              |
| 6:5:1283:G:OP1    | 22:L:87:ARG:NE    | 2.50                     | 0.41              |
| 8:7:28:C:H5''     | 28:R:87:ARG:HH11  | 1.86                     | 0.41              |
| 12:B:184:ASP:HB2  | 12:B:210:ILE:HD11 | 2.03                     | 0.41              |
| 14:D:177:ASP:C    | 14:D:178:ILE:HG12 | 2.46                     | 0.41              |
| 17:G:46:GLU:OE2   | 17:G:50:LYS:NZ    | 2.34                     | 0.41              |
| 20:J:5:LYS:HZ2    | 20:J:7:ILE:HG13   | 1.85                     | 0.41              |
| 34:a:207:ASP:OD1  | 34:a:210:LEU:HB2  | 2.21                     | 0.41              |
| 36:c:128:VAL:HB   | 36:c:198:LEU:CG   | 2.50                     | 0.41              |
| 37:d:30:ARG:N     | 37:d:159:SER:OG   | 2.50                     | 0.41              |
| 37:d:110:ARG:HD3  | 37:d:137:ILE:O    | 2.20                     | 0.41              |
| 40:g:99:VAL:HG12  | 40:g:103:LYS:HE2  | 2.02                     | 0.41              |
| 44:k:59:TYR:O     | 44:k:62:LEU:HD23  | 2.21                     | 0.41              |
| 48:o:31:VAL:HG12  | 48:o:32:ASN:N     | 2.36                     | 0.41              |
| 51:r:33:GLN:HG3   | 51:r:51:LEU:HD22  | 2.02                     | 0.41              |
| 51:r:115:GLN:HE21 | 51:r:116:GLU:CD   | 2.29                     | 0.41              |
| 52:s:2:ASP:CG     | 52:s:3:VAL:N      | 2.79                     | 0.41              |
| 52:s:23:GLU:CD    | 52:s:24:THR:N     | 2.79                     | 0.41              |
| 52:s:62:PRO:HD3   | 52:s:77:LEU:HD13  | 2.02                     | 0.41              |
| 53:t:32:GLN:NE2   | 53:t:71:LEU:HB2   | 2.35                     | 0.41              |
| 57:x:29:LEU:HD12  | 57:x:30:LYS:O     | 2.21                     | 0.41              |
| 3:2:4:ARG:HB3     | 4:3:2474:C:OP1    | 2.21                     | 0.40              |
| 4:3:709:G:H1'     | 36:c:75:ARG:HD3   | 2.03                     | 0.40              |
| 4:3:815:G:H2'     | 4:3:817:A:C5      | 2.56                     | 0.40              |
| 4:3:1441:A:H2'    | 4:3:1442:G:C8     | 2.56                     | 0.40              |
| 4:3:1619:A:H5''   | 4:3:1619:A:H8     | 1.85                     | 0.40              |
| 4:3:2140:G:H2'    | 4:3:2165:A:H62    | 1.86                     | 0.40              |
| 4:3:2582:G:H2'    | 4:3:2583:U:O4'    | 2.21                     | 0.40              |
| 5:4:7:G:H2'       | 5:4:8:C:H6        | 1.85                     | 0.40              |
| 6:5:62:G:OP2      | 29:S:5:LYS:NZ     | 2.54                     | 0.40              |
| 13:C:131:THR:HA   | 13:C:132:PRO:HD3  | 1.89                     | 0.40              |
| 15:E:1:MET:CG     | 15:E:2:GLN:N      | 2.80                     | 0.40              |
| 20:J:48:SER:O     | 20:J:51:LYS:HG2   | 2.22                     | 0.40              |
| 37:d:118:SER:C    | 37:d:120:LYS:N    | 2.77                     | 0.40              |
| 39:f:115:ASP:HA   | 39:f:132:GLU:HG2  | 2.03                     | 0.40              |
| 40:g:97:ASP:HA    | 40:g:100:VAL:HG22 | 2.02                     | 0.40              |
| 41:h:61:LYS:HA    | 41:h:63:PHE:CE1   | 2.56                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 43:j:43:VAL:O     | 43:j:44:LYS:HE2   | 2.20                     | 0.40              |
| 44:k:2:GLU:HG3    | 44:k:4:ASN:H      | 1.86                     | 0.40              |
| 46:m:16:MET:SD    | 46:m:17:THR:N     | 2.95                     | 0.40              |
| 46:m:64:LYS:HA    | 46:m:67:LEU:CD2   | 2.50                     | 0.40              |
| 49:p:35:LYS:NZ    | 49:p:36:GLN:OE1   | 2.29                     | 0.40              |
| 53:t:52:THR:HG22  | 53:t:53:LYS:N     | 2.36                     | 0.40              |
| 56:w:18:LEU:HD22  | 56:w:21:LYS:NZ    | 2.36                     | 0.40              |
| 1:0:4:THR:O       | 4:3:721:G:O2'     | 2.38                     | 0.40              |
| 4:3:164:A:OP2     | 4:3:165:U:O2'     | 2.23                     | 0.40              |
| 4:3:706:C:H5      | 44:k:34:ARG:HH12  | 1.67                     | 0.40              |
| 4:3:1031:U:H5     | 49:p:52:LYS:HD2   | 1.87                     | 0.40              |
| 4:3:1099:C:H4'    | 41:h:84:LYS:HD3   | 2.04                     | 0.40              |
| 4:3:1697:C:HO2'   | 4:3:1698:A:H8     | 1.68                     | 0.40              |
| 4:3:1994:U:H2'    | 4:3:1995:G:H8     | 1.85                     | 0.40              |
| 4:3:2071:C:H2'    | 4:3:2072:C:C6     | 2.55                     | 0.40              |
| 4:3:2166:U:N3     | 4:3:2167:G:H1'    | 2.36                     | 0.40              |
| 4:3:2408:G:O2'    | 59:z:40:ARG:NH2   | 2.53                     | 0.40              |
| 4:3:2888:U:C5     | 58:y:40:HIS:HD2   | 2.39                     | 0.40              |
| 5:4:32:G:H4'      | 5:4:33:U:H5       | 1.85                     | 0.40              |
| 6:5:91:C:H2'      | 6:5:92:G:C8       | 2.57                     | 0.40              |
| 6:5:381:C:H2'     | 6:5:382:U:H6      | 1.86                     | 0.40              |
| 6:5:508:A:N3      | 6:5:541:C:H1'     | 2.36                     | 0.40              |
| 6:5:855:G:O2'     | 6:5:868:G:O2'     | 2.27                     | 0.40              |
| 6:5:896:G:H2'     | 6:5:897:A:H8      | 1.87                     | 0.40              |
| 6:5:1068:G:O2'    | 6:5:1070:G:O6     | 2.40                     | 0.40              |
| 11:A:223:GLN:O    | 11:A:227:LEU:HD23 | 2.21                     | 0.40              |
| 14:D:130:GLU:OE1  | 14:D:132:HIS:CE1  | 2.75                     | 0.40              |
| 19:I:27:THR:O     | 19:I:31:ILE:HG12  | 2.22                     | 0.40              |
| 20:J:5:LYS:HD3    | 20:J:7:ILE:HB     | 2.02                     | 0.40              |
| 26:P:12:ILE:HD12  | 26:P:60:LYS:HA    | 2.03                     | 0.40              |
| 30:T:23:LEU:HD12  | 30:T:24:GLU:N     | 2.36                     | 0.40              |
| 37:d:33:LYS:HD3   | 37:d:92:ARG:NH2   | 2.36                     | 0.40              |
| 38:e:50:ASP:O     | 38:e:50:ASP:OD1   | 2.38                     | 0.40              |
| 39:f:8:ASP:OD1    | 39:f:9:VAL:N      | 2.54                     | 0.40              |
| 39:f:66:HIS:ND1   | 39:f:138:LEU:HD11 | 2.35                     | 0.40              |
| 43:j:35:LEU:HD23  | 43:j:69:GLN:HG2   | 2.03                     | 0.40              |
| 44:k:42:ARG:HD3   | 44:k:42:ARG:HA    | 1.92                     | 0.40              |
| 45:l:74:LYS:HZ1   | 45:l:94:VAL:CG2   | 2.31                     | 0.40              |
| 46:m:103:LEU:HD12 | 46:m:113:MET:CB   | 2.50                     | 0.40              |
| 47:n:64:ASN:CG    | 47:n:65:GLY:N     | 2.79                     | 0.40              |
| 51:r:106:LYS:HE2  | 51:r:106:LYS:HB3  | 1.85                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 53:t:88:LYS:O    | 53:t:104:PHE:HA  | 2.21                     | 0.40              |
| 2:1:30:ALA:N     | 2:1:31:PRO:HD2   | 2.36                     | 0.40              |
| 4:3:474:U:H2'    | 4:3:475:A:H8     | 1.87                     | 0.40              |
| 4:3:881:A:H1'    | 4:3:882:C:C5'    | 2.49                     | 0.40              |
| 4:3:1015:G:H2'   | 4:3:1018:G:O6    | 2.22                     | 0.40              |
| 4:3:1092:A:N7    | 4:3:1121:A:H2'   | 2.36                     | 0.40              |
| 4:3:1573:A:H2'   | 4:3:1574:G:O4'   | 2.20                     | 0.40              |
| 4:3:2155:G:H8    | 4:3:2155:G:O5'   | 2.04                     | 0.40              |
| 4:3:2300:A:H2'   | 4:3:2301:C:C6    | 2.57                     | 0.40              |
| 4:3:2551:G:H21   | 4:3:2654:U:H5''  | 1.87                     | 0.40              |
| 4:3:2584:G:H5'   | 4:3:2586:G:N7    | 2.36                     | 0.40              |
| 5:4:65:G:H2'     | 5:4:66:A:C8      | 2.55                     | 0.40              |
| 5:4:96:G:H2'     | 5:4:97:A:O4'     | 2.21                     | 0.40              |
| 6:5:305:A:H2'    | 6:5:306:G:H8     | 1.87                     | 0.40              |
| 6:5:763:A:OP2    | 6:5:809:G:N2     | 2.54                     | 0.40              |
| 6:5:1027:A:H2'   | 6:5:1028:C:O4'   | 2.22                     | 0.40              |
| 6:5:1038:G:H5''  | 23:M:4:LYS:HE2   | 2.03                     | 0.40              |
| 7:6:59:G:H2'     | 7:6:59:G:N3      | 2.36                     | 0.40              |
| 8:7:50:G:H2'     | 8:7:51:G:C8      | 2.56                     | 0.40              |
| 10:9:71:LYS:HG3  | 10:9:175:ARG:NH2 | 2.37                     | 0.40              |
| 10:9:198:LYS:HZ1 | 10:9:206:TYR:HB2 | 1.85                     | 0.40              |
| 11:A:30:VAL:HA   | 11:A:55:HIS:HD2  | 1.83                     | 0.40              |
| 11:A:84:PHE:CE2  | 11:A:99:ILE:HG21 | 2.57                     | 0.40              |
| 12:B:137:MET:HG3 | 12:B:171:TYR:CE2 | 2.57                     | 0.40              |
| 15:E:99:SER:OG   | 27:Q:50:ARG:NH1  | 2.54                     | 0.40              |
| 20:J:64:ALA:HA   | 20:J:67:VAL:HG12 | 2.03                     | 0.40              |
| 20:J:119:ARG:HD3 | 30:T:34:TYR:HB2  | 2.03                     | 0.40              |
| 21:K:127:ARG:HB2 | 21:K:132:ALA:HB3 | 2.04                     | 0.40              |
| 22:L:49:THR:O    | 22:L:52:GLU:HG2  | 2.21                     | 0.40              |
| 35:b:6:ILE:HG22  | 35:b:207:ILE:HB  | 2.03                     | 0.40              |
| 36:c:6:LEU:H     | 36:c:14:GLU:CD   | 2.29                     | 0.40              |
| 36:c:37:ALA:HA   | 36:c:40:VAL:HG22 | 2.03                     | 0.40              |
| 41:h:20:LYS:N    | 41:h:21:PRO:HD2  | 2.36                     | 0.40              |
| 45:l:20:LYS:O    | 45:l:98:LYS:HB3  | 2.21                     | 0.40              |
| 45:l:111:GLU:HA  | 45:l:114:MET:CE  | 2.51                     | 0.40              |
| 49:p:93:VAL:HA   | 49:p:96:GLU:HB2  | 2.04                     | 0.40              |
| 53:t:64:GLN:H    | 53:t:64:GLN:CD   | 2.29                     | 0.40              |
| 57:x:7:PHE:O     | 57:x:7:PHE:CD2   | 2.74                     | 0.40              |
| 2:1:10:ARG:NH2   | 4:3:2402:C:H5'   | 2.37                     | 0.40              |
| 4:3:287:G:N2     | 39:f:42:LYS:NZ   | 2.69                     | 0.40              |
| 4:3:2080:C:HO2'  | 4:3:2606:A:HO2'  | 1.68                     | 0.40              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 4:3:2204:C:H2'    | 4:3:2205:U:O4'   | 2.21                     | 0.40              |
| 6:5:195:U:H2'     | 6:5:196:G:C8     | 2.55                     | 0.40              |
| 6:5:595:G:H4'     | 26:P:29:ARG:NH2  | 2.36                     | 0.40              |
| 6:5:906:C:H2'     | 6:5:907:A:C8     | 2.57                     | 0.40              |
| 6:5:1220:A:H2'    | 6:5:1221:A:C8    | 2.56                     | 0.40              |
| 6:5:1329:G:H2'    | 6:5:1330:A:C8    | 2.56                     | 0.40              |
| 6:5:1440:U:H2'    | 6:5:1441:C:O4'   | 2.22                     | 0.40              |
| 7:6:36:C:H2'      | 7:6:37:A:O4'     | 2.21                     | 0.40              |
| 11:A:33:VAL:CG2   | 11:A:281:ARG:H   | 2.34                     | 0.40              |
| 12:B:95:ILE:HD12  | 12:B:95:ILE:HA   | 1.99                     | 0.40              |
| 13:C:123:LEU:HD21 | 13:C:145:LYS:HE2 | 2.02                     | 0.40              |
| 19:I:44:GLY:HA2   | 19:I:45:PRO:HD3  | 1.86                     | 0.40              |
| 20:J:9:VAL:CG1    | 20:J:72:MET:HB3  | 2.48                     | 0.40              |
| 36:c:142:VAL:O    | 36:c:145:GLN:NE2 | 2.54                     | 0.40              |
| 39:f:109:GLN:HG2  | 39:f:110:LYS:N   | 2.37                     | 0.40              |
| 44:k:51:PHE:CZ    | 44:k:53:GLY:HA2  | 2.56                     | 0.40              |
| 46:m:30:LYS:HA    | 46:m:116:LEU:O   | 2.22                     | 0.40              |
| 52:s:32:ASN:OD1   | 52:s:34:LYS:HG2  | 2.21                     | 0.40              |
| 54:u:99:LYS:HE3   | 54:u:101:LYS:HE2 | 2.02                     | 0.40              |
| 55:v:51:SER:OG    | 55:v:53:ARG:CZ   | 2.70                     | 0.40              |
| 57:x:7:PHE:O      | 57:x:7:PHE:CG    | 2.74                     | 0.40              |
| 2:1:16:SER:OG     | 4:3:687:G:OP1    | 2.29                     | 0.40              |
| 4:3:358:A:H62     | 4:3:372:G:H21    | 1.69                     | 0.40              |
| 4:3:622:U:C4'     | 36:c:94:LYS:HE3  | 2.49                     | 0.40              |
| 4:3:931:G:H2'     | 4:3:932:U:O4'    | 2.21                     | 0.40              |
| 4:3:954:A:H3'     | 4:3:2276:A:H61   | 1.86                     | 0.40              |
| 4:3:1131:A:H2'    | 4:3:1132:C:O4'   | 2.22                     | 0.40              |
| 4:3:2128:G:H3'    | 4:3:2129:U:C6    | 2.57                     | 0.40              |
| 4:3:2268:C:H6     | 4:3:2268:C:O5'   | 2.04                     | 0.40              |
| 4:3:2625:U:H2'    | 4:3:2626:A:H8    | 1.86                     | 0.40              |
| 4:3:2638:G:O4'    | 4:3:2897:G:H1'   | 2.21                     | 0.40              |
| 6:5:251:G:H2'     | 6:5:252:U:C6     | 2.57                     | 0.40              |
| 6:5:260:C:H2'     | 6:5:261:G:O4'    | 2.20                     | 0.40              |
| 6:5:266:A:H2'     | 6:5:267:C:C6     | 2.57                     | 0.40              |
| 6:5:383:U:H5''    | 6:5:384:G:OP1    | 2.22                     | 0.40              |
| 6:5:571:A:H2'     | 6:5:572:A:C8     | 2.56                     | 0.40              |
| 6:5:615:G:H2'     | 6:5:616:C:O4'    | 2.21                     | 0.40              |
| 6:5:690:G:H4'     | 32:Y:66:U:OP2    | 2.22                     | 0.40              |
| 6:5:1078:G:H5'    | 6:5:1078:G:C8    | 2.56                     | 0.40              |
| 6:5:1289:U:H2'    | 6:5:1290:G:O4'   | 2.22                     | 0.40              |
| 11:A:38:ASN:HB2   | 11:A:205:ASN:HA  | 2.03                     | 0.40              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 13:C:106:PHE:HA  | 13:C:157:ALA:HA   | 2.02                     | 0.40              |
| 16:F:12:LEU:HB3  | 16:F:20:THR:CG2   | 2.52                     | 0.40              |
| 16:F:137:LYS:HA  | 16:F:140:THR:HG22 | 2.04                     | 0.40              |
| 19:I:17:GLU:O    | 19:I:103:THR:HB   | 2.22                     | 0.40              |
| 21:K:136:LYS:HB2 | 21:K:136:LYS:HE3  | 1.89                     | 0.40              |
| 24:N:32:GLN:CD   | 24:N:56:LYS:HD3   | 2.47                     | 0.40              |
| 25:O:50:ILE:HG23 | 25:O:52:GLU:HG3   | 2.03                     | 0.40              |
| 34:a:252:ASP:OD1 | 34:a:252:ASP:N    | 2.54                     | 0.40              |
| 34:a:256:THR:HG1 | 34:a:260:LYS:H    | 1.68                     | 0.40              |
| 46:m:102:LYS:O   | 46:m:102:LYS:HD2  | 2.21                     | 0.40              |
| 46:m:103:LEU:N   | 46:m:113:MET:O    | 2.39                     | 0.40              |
| 46:m:105:PRO:HB2 | 46:m:110:ALA:HA   | 2.04                     | 0.40              |
| 48:o:28:GLY:HA3  | 48:o:96:VAL:CG1   | 2.52                     | 0.40              |
| 50:q:6:VAL:HG21  | 50:q:49:TYR:HE1   | 1.87                     | 0.40              |
| 51:r:83:LYS:O    | 51:r:84:ARG:HD2   | 2.21                     | 0.40              |
| 56:w:107:ASP:OD1 | 56:w:108:ALA:N    | 2.55                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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   | 0     | 45/48 (94%)   | 45 (100%) | 0        | 0        | 100         | 100 |
| 2   | 1     | 57/59 (97%)   | 57 (100%) | 0        | 0        | 100         | 100 |
| 3   | 2     | 35/37 (95%)   | 35 (100%) | 0        | 0        | 100         | 100 |
| 10  | 9     | 224/226 (99%) | 218 (97%) | 5 (2%)   | 1 (0%)   | 30          | 67  |
| 11  | A     | 264/294 (90%) | 233 (88%) | 28 (11%) | 3 (1%)   | 11          | 46  |
| 12  | B     | 222/273 (81%) | 198 (89%) | 21 (10%) | 3 (1%)   | 9           | 40  |
| 13  | C     | 202/205 (98%) | 168 (83%) | 33 (16%) | 1 (0%)   | 24          | 63  |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 14  | D     | 156/219 (71%) | 147 (94%) | 7 (4%)   | 2 (1%)   | 9           | 42  |
| 15  | E     | 213/215 (99%) | 171 (80%) | 33 (16%) | 9 (4%)   | 2           | 17  |
| 16  | F     | 153/155 (99%) | 132 (86%) | 17 (11%) | 4 (3%)   | 4           | 25  |
| 17  | G     | 140/142 (99%) | 131 (94%) | 9 (6%)   | 0        | 100         | 100 |
| 18  | H     | 127/132 (96%) | 115 (91%) | 10 (8%)  | 2 (2%)   | 7           | 38  |
| 19  | I     | 102/108 (94%) | 89 (87%)  | 12 (12%) | 1 (1%)   | 12          | 49  |
| 20  | J     | 118/121 (98%) | 103 (87%) | 9 (8%)   | 6 (5%)   | 1           | 15  |
| 21  | K     | 133/139 (96%) | 113 (85%) | 16 (12%) | 4 (3%)   | 3           | 23  |
| 22  | L     | 119/124 (96%) | 109 (92%) | 10 (8%)  | 0        | 100         | 100 |
| 23  | M     | 58/61 (95%)   | 56 (97%)  | 2 (3%)   | 0        | 100         | 100 |
| 24  | N     | 84/86 (98%)   | 78 (93%)  | 6 (7%)   | 0        | 100         | 100 |
| 25  | O     | 85/94 (90%)   | 78 (92%)  | 5 (6%)   | 2 (2%)   | 4           | 27  |
| 26  | P     | 83/85 (98%)   | 71 (86%)  | 11 (13%) | 1 (1%)   | 10          | 44  |
| 27  | Q     | 71/104 (68%)  | 63 (89%)  | 6 (8%)   | 2 (3%)   | 4           | 24  |
| 28  | R     | 84/87 (97%)   | 79 (94%)  | 5 (6%)   | 0        | 100         | 100 |
| 29  | S     | 77/87 (88%)   | 74 (96%)  | 2 (3%)   | 1 (1%)   | 9           | 42  |
| 30  | T     | 57/60 (95%)   | 56 (98%)  | 1 (2%)   | 0        | 100         | 100 |
| 31  | X     | 28/444 (6%)   | 24 (86%)  | 4 (14%)  | 0        | 100         | 100 |
| 33  | Z     | 3/36 (8%)     | 3 (100%)  | 0        | 0        | 100         | 100 |
| 34  | a     | 283/287 (99%) | 268 (95%) | 14 (5%)  | 1 (0%)   | 30          | 67  |
| 35  | b     | 227/287 (79%) | 220 (97%) | 7 (3%)   | 0        | 100         | 100 |
| 36  | c     | 209/212 (99%) | 199 (95%) | 10 (5%)  | 0        | 100         | 100 |
| 37  | d     | 177/180 (98%) | 168 (95%) | 9 (5%)   | 0        | 100         | 100 |
| 38  | e     | 174/184 (95%) | 162 (93%) | 12 (7%)  | 0        | 100         | 100 |
| 39  | f     | 147/149 (99%) | 113 (77%) | 29 (20%) | 5 (3%)   | 3           | 21  |
| 40  | g     | 123/161 (76%) | 115 (94%) | 8 (6%)   | 0        | 100         | 100 |
| 41  | h     | 126/137 (92%) | 121 (96%) | 5 (4%)   | 0        | 100         | 100 |
| 42  | i     | 142/146 (97%) | 133 (94%) | 9 (6%)   | 0        | 100         | 100 |
| 43  | j     | 120/122 (98%) | 115 (96%) | 5 (4%)   | 0        | 100         | 100 |
| 44  | k     | 148/151 (98%) | 137 (93%) | 11 (7%)  | 0        | 100         | 100 |
| 45  | l     | 134/139 (96%) | 130 (97%) | 4 (3%)   | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 46  | m     | 117/124 (94%)   | 111 (95%)  | 6 (5%)   | 0        | 100         | 100 |
| 47  | n     | 114/116 (98%)   | 111 (97%)  | 3 (3%)   | 0        | 100         | 100 |
| 48  | o     | 116/119 (98%)   | 107 (92%)  | 9 (8%)   | 0        | 100         | 100 |
| 49  | p     | 116/127 (91%)   | 114 (98%)  | 2 (2%)   | 0        | 100         | 100 |
| 50  | q     | 97/100 (97%)    | 93 (96%)   | 4 (4%)   | 0        | 100         | 100 |
| 51  | r     | 140/159 (88%)   | 137 (98%)  | 3 (2%)   | 0        | 100         | 100 |
| 52  | s     | 93/237 (39%)    | 89 (96%)   | 4 (4%)   | 0        | 100         | 100 |
| 53  | t     | 109/111 (98%)   | 102 (94%)  | 7 (6%)   | 0        | 100         | 100 |
| 54  | u     | 86/104 (83%)    | 82 (95%)   | 4 (5%)   | 0        | 100         | 100 |
| 55  | v     | 62/65 (95%)     | 61 (98%)   | 1 (2%)   | 0        | 100         | 100 |
| 56  | w     | 108/111 (97%)   | 103 (95%)  | 5 (5%)   | 0        | 100         | 100 |
| 57  | x     | 85/97 (88%)     | 63 (74%)   | 21 (25%) | 1 (1%)   | 10          | 44  |
| 58  | y     | 54/57 (95%)     | 52 (96%)   | 2 (4%)   | 0        | 100         | 100 |
| 59  | z     | 48/53 (91%)     | 47 (98%)   | 1 (2%)   | 0        | 100         | 100 |
| All | All   | 6295/7376 (85%) | 5799 (92%) | 447 (7%) | 49 (1%)  | 18          | 54  |

All (49) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 14  | D     | 216 | LEU  |
| 15  | E     | 121 | ARG  |
| 15  | E     | 143 | LEU  |
| 18  | H     | 102 | SER  |
| 20  | J     | 32  | GLY  |
| 26  | P     | 54  | LEU  |
| 39  | f     | 34  | LYS  |
| 13  | C     | 81  | GLN  |
| 16  | F     | 9   | ARG  |
| 16  | F     | 15  | PRO  |
| 20  | J     | 9   | VAL  |
| 20  | J     | 33  | ASN  |
| 27  | Q     | 39  | LYS  |
| 29  | S     | 37  | LYS  |
| 39  | f     | 27  | ILE  |
| 39  | f     | 95  | LYS  |
| 10  | 9     | 221 | LYS  |
| 11  | A     | 52  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11  | A     | 219 | ASN  |
| 12  | B     | 221 | HIS  |
| 16  | F     | 12  | LEU  |
| 16  | F     | 79  | ILE  |
| 21  | K     | 56  | LYS  |
| 11  | A     | 17  | LEU  |
| 14  | D     | 66  | PHE  |
| 15  | E     | 133 | THR  |
| 15  | E     | 182 | ASN  |
| 19  | I     | 100 | VAL  |
| 20  | J     | 10  | SER  |
| 25  | O     | 47  | LYS  |
| 25  | O     | 49  | LYS  |
| 27  | Q     | 35  | LYS  |
| 34  | a     | 128 | ILE  |
| 39  | f     | 12  | LEU  |
| 15  | E     | 42  | LEU  |
| 15  | E     | 139 | THR  |
| 15  | E     | 169 | VAL  |
| 15  | E     | 185 | HIS  |
| 18  | H     | 93  | ASN  |
| 21  | K     | 72  | ASN  |
| 12  | B     | 216 | ASN  |
| 15  | E     | 163 | MET  |
| 57  | x     | 18  | SER  |
| 12  | B     | 46  | VAL  |
| 20  | J     | 7   | ILE  |
| 21  | K     | 57  | LYS  |
| 20  | J     | 30  | PRO  |
| 39  | f     | 93  | ILE  |
| 21  | K     | 55  | 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.

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| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 1   | 0     | 40/41 (98%)    | 40 (100%)  | 0        | 100         | 100 |
| 2   | 1     | 51/51 (100%)   | 51 (100%)  | 0        | 100         | 100 |
| 3   | 2     | 35/35 (100%)   | 35 (100%)  | 0        | 100         | 100 |
| 10  | 9     | 186/186 (100%) | 186 (100%) | 0        | 100         | 100 |
| 11  | A     | 239/262 (91%)  | 239 (100%) | 0        | 100         | 100 |
| 12  | B     | 187/232 (81%)  | 187 (100%) | 0        | 100         | 100 |
| 13  | C     | 182/183 (100%) | 182 (100%) | 0        | 100         | 100 |
| 14  | D     | 128/178 (72%)  | 128 (100%) | 0        | 100         | 100 |
| 15  | E     | 196/196 (100%) | 195 (100%) | 1 (0%)   | 81          | 83  |
| 16  | F     | 132/132 (100%) | 132 (100%) | 0        | 100         | 100 |
| 17  | G     | 124/124 (100%) | 124 (100%) | 0        | 100         | 100 |
| 18  | H     | 112/115 (97%)  | 112 (100%) | 0        | 100         | 100 |
| 19  | I     | 97/99 (98%)    | 97 (100%)  | 0        | 100         | 100 |
| 20  | J     | 96/97 (99%)    | 96 (100%)  | 0        | 100         | 100 |
| 21  | K     | 117/120 (98%)  | 117 (100%) | 0        | 100         | 100 |
| 22  | L     | 102/105 (97%)  | 102 (100%) | 0        | 100         | 100 |
| 23  | M     | 47/48 (98%)    | 47 (100%)  | 0        | 100         | 100 |
| 24  | N     | 78/78 (100%)   | 78 (100%)  | 0        | 100         | 100 |
| 25  | O     | 76/82 (93%)    | 76 (100%)  | 0        | 100         | 100 |
| 26  | P     | 75/75 (100%)   | 75 (100%)  | 0        | 100         | 100 |
| 27  | Q     | 64/94 (68%)    | 64 (100%)  | 0        | 100         | 100 |
| 28  | R     | 76/77 (99%)    | 76 (100%)  | 0        | 100         | 100 |
| 29  | S     | 71/77 (92%)    | 71 (100%)  | 0        | 100         | 100 |
| 30  | T     | 55/56 (98%)    | 55 (100%)  | 0        | 100         | 100 |
| 31  | X     | 27/406 (7%)    | 27 (100%)  | 0        | 100         | 100 |
| 33  | Z     | 2/2 (100%)     | 2 (100%)   | 0        | 100         | 100 |
| 34  | a     | 241/243 (99%)  | 240 (100%) | 1 (0%)   | 84          | 84  |
| 35  | b     | 186/233 (80%)  | 186 (100%) | 0        | 100         | 100 |
| 36  | c     | 183/184 (100%) | 183 (100%) | 0        | 100         | 100 |
| 37  | d     | 153/154 (99%)  | 153 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Rotameric   | Outliers | Percentiles |     |
|-----|-------|-----------------|-------------|----------|-------------|-----|
| 38  | e     | 153/159 (96%)   | 152 (99%)   | 1 (1%)   | 76          | 81  |
| 39  | f     | 134/134 (100%)  | 128 (96%)   | 6 (4%)   | 24          | 46  |
| 40  | g     | 100/129 (78%)   | 100 (100%)  | 0        | 100         | 100 |
| 41  | h     | 102/110 (93%)   | 102 (100%)  | 0        | 100         | 100 |
| 42  | i     | 126/128 (98%)   | 126 (100%)  | 0        | 100         | 100 |
| 43  | j     | 103/103 (100%)  | 103 (100%)  | 0        | 100         | 100 |
| 44  | k     | 125/126 (99%)   | 125 (100%)  | 0        | 100         | 100 |
| 45  | l     | 113/115 (98%)   | 113 (100%)  | 0        | 100         | 100 |
| 46  | m     | 105/109 (96%)   | 105 (100%)  | 0        | 100         | 100 |
| 47  | n     | 99/99 (100%)    | 99 (100%)   | 0        | 100         | 100 |
| 48  | o     | 104/105 (99%)   | 104 (100%)  | 0        | 100         | 100 |
| 49  | p     | 104/108 (96%)   | 103 (99%)   | 1 (1%)   | 68          | 78  |
| 50  | q     | 90/91 (99%)     | 90 (100%)   | 0        | 100         | 100 |
| 51  | r     | 118/132 (89%)   | 118 (100%)  | 0        | 100         | 100 |
| 52  | s     | 84/208 (40%)    | 84 (100%)   | 0        | 100         | 100 |
| 53  | t     | 96/96 (100%)    | 96 (100%)   | 0        | 100         | 100 |
| 54  | u     | 70/85 (82%)     | 70 (100%)   | 0        | 100         | 100 |
| 55  | v     | 59/60 (98%)     | 59 (100%)   | 0        | 100         | 100 |
| 56  | w     | 97/98 (99%)     | 97 (100%)   | 0        | 100         | 100 |
| 57  | x     | 79/86 (92%)     | 79 (100%)   | 0        | 100         | 100 |
| 58  | y     | 48/49 (98%)     | 48 (100%)   | 0        | 100         | 100 |
| 59  | z     | 47/50 (94%)     | 47 (100%)   | 0        | 100         | 100 |
| All | All   | 5514/6345 (87%) | 5504 (100%) | 10 (0%)  | 85          | 87  |

All (10) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 15  | E     | 114 | LYS  |
| 34  | a     | 29  | ASN  |
| 38  | e     | 51  | ASN  |
| 39  | f     | 47  | ARG  |
| 39  | f     | 51  | LEU  |
| 39  | f     | 62  | LYS  |
| 39  | f     | 77  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 39  | f     | 89  | TYR  |
| 39  | f     | 92  | ILE  |
| 49  | p     | 2   | ARG  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (77) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | 1     | 18  | GLN  |
| 3   | 2     | 32  | HIS  |
| 3   | 2     | 34  | GLN  |
| 11  | A     | 51  | HIS  |
| 11  | A     | 55  | HIS  |
| 11  | A     | 81  | GLN  |
| 11  | A     | 174 | ASN  |
| 11  | A     | 287 | ASN  |
| 12  | B     | 6   | ASN  |
| 12  | B     | 86  | GLN  |
| 12  | B     | 150 | ASN  |
| 12  | B     | 216 | ASN  |
| 12  | B     | 221 | HIS  |
| 13  | C     | 81  | GLN  |
| 13  | C     | 88  | ASN  |
| 13  | C     | 115 | GLN  |
| 14  | D     | 123 | HIS  |
| 15  | E     | 25  | GLN  |
| 15  | E     | 101 | ASN  |
| 16  | F     | 18  | ASN  |
| 16  | F     | 83  | ASN  |
| 18  | H     | 52  | GLN  |
| 18  | H     | 93  | ASN  |
| 20  | J     | 8   | ASN  |
| 21  | K     | 29  | ASN  |
| 24  | N     | 15  | HIS  |
| 26  | P     | 25  | GLN  |
| 26  | P     | 42  | HIS  |
| 26  | P     | 46  | GLN  |
| 26  | P     | 49  | ASN  |
| 28  | R     | 14  | HIS  |
| 28  | R     | 23  | ASN  |
| 29  | S     | 31  | ASN  |
| 30  | T     | 30  | GLN  |
| 34  | a     | 31  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 34  | a     | 159 | GLN  |
| 34  | a     | 240 | HIS  |
| 35  | b     | 21  | ASN  |
| 35  | b     | 34  | ASN  |
| 35  | b     | 59  | ASN  |
| 35  | b     | 157 | GLN  |
| 35  | b     | 168 | HIS  |
| 36  | c     | 42  | GLN  |
| 37  | d     | 7   | HIS  |
| 37  | d     | 63  | GLN  |
| 38  | e     | 59  | ASN  |
| 39  | f     | 57  | HIS  |
| 39  | f     | 61  | ASN  |
| 39  | f     | 100 | GLN  |
| 40  | g     | 87  | ASN  |
| 41  | h     | 13  | ASN  |
| 41  | h     | 38  | GLN  |
| 41  | h     | 40  | ASN  |
| 41  | h     | 47  | GLN  |
| 42  | i     | 64  | GLN  |
| 42  | i     | 138 | GLN  |
| 43  | j     | 56  | GLN  |
| 44  | k     | 39  | GLN  |
| 44  | k     | 75  | GLN  |
| 44  | k     | 81  | ASN  |
| 45  | l     | 13  | HIS  |
| 46  | m     | 58  | ASN  |
| 46  | m     | 62  | GLN  |
| 47  | n     | 7   | GLN  |
| 47  | n     | 66  | ASN  |
| 47  | n     | 69  | ASN  |
| 48  | o     | 85  | ASN  |
| 49  | p     | 40  | GLN  |
| 49  | p     | 65  | ASN  |
| 49  | p     | 90  | ASN  |
| 49  | p     | 110 | GLN  |
| 53  | t     | 33  | GLN  |
| 54  | u     | 90  | GLN  |
| 56  | w     | 35  | HIS  |
| 56  | w     | 42  | HIS  |
| 57  | x     | 31  | GLN  |
| 57  | x     | 98  | ASN  |

## 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 32  | Y     | 39/40 (97%)     | 25 (64%)          | 6 (15%)         |
| 4   | 3     | 2892/2907 (99%) | 532 (18%)         | 20 (0%)         |
| 5   | 4     | 107/108 (99%)   | 29 (27%)          | 0               |
| 6   | 5     | 1505/1520 (99%) | 252 (16%)         | 8 (0%)          |
| 7   | 6     | 76/76 (100%)    | 22 (28%)          | 6 (7%)          |
| 8   | 7     | 74/75 (98%)     | 20 (27%)          | 2 (2%)          |
| 9   | 8     | 75/76 (98%)     | 23 (30%)          | 0               |
| All | All   | 4768/4802 (99%) | 903 (18%)         | 42 (0%)         |

All (903) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | 3     | 11  | U    |
| 4   | 3     | 12  | A    |
| 4   | 3     | 13  | C    |
| 4   | 3     | 14  | U    |
| 4   | 3     | 28  | G    |
| 4   | 3     | 37  | G    |
| 4   | 3     | 48  | G    |
| 4   | 3     | 64  | U    |
| 4   | 3     | 65  | A    |
| 4   | 3     | 73  | A    |
| 4   | 3     | 76  | A    |
| 4   | 3     | 77  | G    |
| 4   | 3     | 102 | A    |
| 4   | 3     | 103 | G    |
| 4   | 3     | 119 | A    |
| 4   | 3     | 121 | U    |
| 4   | 3     | 126 | C    |
| 4   | 3     | 132 | G    |
| 4   | 3     | 141 | A    |
| 4   | 3     | 142 | A    |
| 4   | 3     | 163 | A    |
| 4   | 3     | 180 | A    |
| 4   | 3     | 184 | A    |
| 4   | 3     | 187 | C    |
| 4   | 3     | 200 | A    |
| 4   | 3     | 203 | A    |
| 4   | 3     | 219 | G    |
| 4   | 3     | 220 | A    |
| 4   | 3     | 225 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | 3     | 226 | A    |
| 4   | 3     | 232 | A    |
| 4   | 3     | 234 | G    |
| 4   | 3     | 237 | A    |
| 4   | 3     | 245 | U    |
| 4   | 3     | 246 | G    |
| 4   | 3     | 252 | G    |
| 4   | 3     | 269 | A    |
| 4   | 3     | 276 | A    |
| 4   | 3     | 284 | U    |
| 4   | 3     | 287 | G    |
| 4   | 3     | 295 | U    |
| 4   | 3     | 296 | U    |
| 4   | 3     | 297 | G    |
| 4   | 3     | 298 | U    |
| 4   | 3     | 299 | A    |
| 4   | 3     | 309 | A    |
| 4   | 3     | 310 | U    |
| 4   | 3     | 311 | G    |
| 4   | 3     | 315 | A    |
| 4   | 3     | 316 | C    |
| 4   | 3     | 317 | U    |
| 4   | 3     | 319 | G    |
| 4   | 3     | 325 | G    |
| 4   | 3     | 336 | C    |
| 4   | 3     | 345 | A    |
| 4   | 3     | 363 | G    |
| 4   | 3     | 364 | A    |
| 4   | 3     | 365 | U    |
| 4   | 3     | 402 | A    |
| 4   | 3     | 409 | A    |
| 4   | 3     | 410 | G    |
| 4   | 3     | 411 | U    |
| 4   | 3     | 418 | G    |
| 4   | 3     | 419 | A    |
| 4   | 3     | 424 | G    |
| 4   | 3     | 425 | U    |
| 4   | 3     | 426 | U    |
| 4   | 3     | 432 | G    |
| 4   | 3     | 437 | A    |
| 4   | 3     | 440 | C    |
| 4   | 3     | 460 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | 3     | 463 | U    |
| 4   | 3     | 483 | A    |
| 4   | 3     | 517 | G    |
| 4   | 3     | 539 | U    |
| 4   | 3     | 540 | A    |
| 4   | 3     | 548 | A    |
| 4   | 3     | 562 | C    |
| 4   | 3     | 565 | C    |
| 4   | 3     | 566 | G    |
| 4   | 3     | 567 | U    |
| 4   | 3     | 573 | A    |
| 4   | 3     | 581 | A    |
| 4   | 3     | 583 | U    |
| 4   | 3     | 596 | G    |
| 4   | 3     | 598 | G    |
| 4   | 3     | 607 | U    |
| 4   | 3     | 608 | A    |
| 4   | 3     | 610 | G    |
| 4   | 3     | 620 | G    |
| 4   | 3     | 636 | U    |
| 4   | 3     | 637 | U    |
| 4   | 3     | 638 | A    |
| 4   | 3     | 648 | G    |
| 4   | 3     | 649 | A    |
| 4   | 3     | 650 | G    |
| 4   | 3     | 663 | A    |
| 4   | 3     | 670 | G    |
| 4   | 3     | 673 | A    |
| 4   | 3     | 681 | A    |
| 4   | 3     | 682 | A    |
| 4   | 3     | 689 | U    |
| 4   | 3     | 691 | G    |
| 4   | 3     | 705 | A    |
| 4   | 3     | 712 | A    |
| 4   | 3     | 716 | G    |
| 4   | 3     | 721 | G    |
| 4   | 3     | 722 | C    |
| 4   | 3     | 765 | A    |
| 4   | 3     | 775 | C    |
| 4   | 3     | 782 | U    |
| 4   | 3     | 792 | G    |
| 4   | 3     | 797 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | 3     | 800 | C    |
| 4   | 3     | 810 | G    |
| 4   | 3     | 811 | G    |
| 4   | 3     | 817 | A    |
| 4   | 3     | 819 | U    |
| 4   | 3     | 820 | U    |
| 4   | 3     | 824 | A    |
| 4   | 3     | 828 | A    |
| 4   | 3     | 829 | A    |
| 4   | 3     | 840 | G    |
| 4   | 3     | 846 | U    |
| 4   | 3     | 847 | C    |
| 4   | 3     | 854 | A    |
| 4   | 3     | 862 | U    |
| 4   | 3     | 881 | A    |
| 4   | 3     | 882 | C    |
| 4   | 3     | 883 | A    |
| 4   | 3     | 901 | C    |
| 4   | 3     | 902 | U    |
| 4   | 3     | 903 | A    |
| 4   | 3     | 904 | C    |
| 4   | 3     | 906 | G    |
| 4   | 3     | 918 | G    |
| 4   | 3     | 924 | C    |
| 4   | 3     | 926 | U    |
| 4   | 3     | 927 | A    |
| 4   | 3     | 928 | G    |
| 4   | 3     | 930 | C    |
| 4   | 3     | 932 | U    |
| 4   | 3     | 933 | A    |
| 4   | 3     | 934 | C    |
| 4   | 3     | 935 | U    |
| 4   | 3     | 936 | G    |
| 4   | 3     | 944 | U    |
| 4   | 3     | 947 | A    |
| 4   | 3     | 949 | C    |
| 4   | 3     | 951 | C    |
| 4   | 3     | 952 | U    |
| 4   | 3     | 953 | G    |
| 4   | 3     | 970 | U    |
| 4   | 3     | 981 | A    |
| 4   | 3     | 982 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 4   | 3     | 994  | U    |
| 4   | 3     | 997  | G    |
| 4   | 3     | 998  | C    |
| 4   | 3     | 1008 | A    |
| 4   | 3     | 1010 | G    |
| 4   | 3     | 1016 | A    |
| 4   | 3     | 1019 | A    |
| 4   | 3     | 1026 | A    |
| 4   | 3     | 1032 | A    |
| 4   | 3     | 1039 | G    |
| 4   | 3     | 1045 | A    |
| 4   | 3     | 1049 | U    |
| 4   | 3     | 1058 | U    |
| 4   | 3     | 1060 | G    |
| 4   | 3     | 1061 | A    |
| 4   | 3     | 1068 | U    |
| 4   | 3     | 1074 | A    |
| 4   | 3     | 1080 | A    |
| 4   | 3     | 1082 | A    |
| 4   | 3     | 1084 | C    |
| 4   | 3     | 1096 | U    |
| 4   | 3     | 1097 | G    |
| 4   | 3     | 1098 | G    |
| 4   | 3     | 1099 | C    |
| 4   | 3     | 1102 | A    |
| 4   | 3     | 1104 | A    |
| 4   | 3     | 1105 | A    |
| 4   | 3     | 1106 | G    |
| 4   | 3     | 1107 | C    |
| 4   | 3     | 1110 | C    |
| 4   | 3     | 1111 | C    |
| 4   | 3     | 1113 | U    |
| 4   | 3     | 1114 | C    |
| 4   | 3     | 1115 | G    |
| 4   | 3     | 1120 | A    |
| 4   | 3     | 1122 | G    |
| 4   | 3     | 1123 | A    |
| 4   | 3     | 1125 | U    |
| 4   | 3     | 1130 | A    |
| 4   | 3     | 1132 | C    |
| 4   | 3     | 1138 | A    |
| 4   | 3     | 1144 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 4   | 3     | 1145 | G    |
| 4   | 3     | 1146 | A    |
| 4   | 3     | 1147 | G    |
| 4   | 3     | 1165 | U    |
| 4   | 3     | 1167 | U    |
| 4   | 3     | 1168 | A    |
| 4   | 3     | 1170 | C    |
| 4   | 3     | 1176 | U    |
| 4   | 3     | 1177 | A    |
| 4   | 3     | 1178 | A    |
| 4   | 3     | 1204 | A    |
| 4   | 3     | 1208 | A    |
| 4   | 3     | 1209 | U    |
| 4   | 3     | 1210 | A    |
| 4   | 3     | 1212 | C    |
| 4   | 3     | 1215 | G    |
| 4   | 3     | 1234 | U    |
| 4   | 3     | 1235 | U    |
| 4   | 3     | 1236 | G    |
| 4   | 3     | 1242 | G    |
| 4   | 3     | 1246 | U    |
| 4   | 3     | 1250 | A    |
| 4   | 3     | 1251 | G    |
| 4   | 3     | 1253 | G    |
| 4   | 3     | 1256 | A    |
| 4   | 3     | 1257 | G    |
| 4   | 3     | 1266 | G    |
| 4   | 3     | 1268 | U    |
| 4   | 3     | 1280 | G    |
| 4   | 3     | 1281 | A    |
| 4   | 3     | 1283 | A    |
| 4   | 3     | 1285 | U    |
| 4   | 3     | 1286 | G    |
| 4   | 3     | 1292 | A    |
| 4   | 3     | 1301 | G    |
| 4   | 3     | 1304 | U    |
| 4   | 3     | 1313 | G    |
| 4   | 3     | 1325 | C    |
| 4   | 3     | 1328 | A    |
| 4   | 3     | 1329 | U    |
| 4   | 3     | 1330 | U    |
| 4   | 3     | 1369 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 4   | 3     | 1378 | C    |
| 4   | 3     | 1380 | U    |
| 4   | 3     | 1388 | G    |
| 4   | 3     | 1393 | A    |
| 4   | 3     | 1406 | A    |
| 4   | 3     | 1407 | U    |
| 4   | 3     | 1412 | A    |
| 4   | 3     | 1423 | A    |
| 4   | 3     | 1424 | U    |
| 4   | 3     | 1431 | A    |
| 4   | 3     | 1444 | C    |
| 4   | 3     | 1445 | U    |
| 4   | 3     | 1446 | G    |
| 4   | 3     | 1448 | U    |
| 4   | 3     | 1456 | C    |
| 4   | 3     | 1463 | G    |
| 4   | 3     | 1467 | U    |
| 4   | 3     | 1480 | A    |
| 4   | 3     | 1481 | U    |
| 4   | 3     | 1483 | G    |
| 4   | 3     | 1486 | U    |
| 4   | 3     | 1487 | U    |
| 4   | 3     | 1502 | A    |
| 4   | 3     | 1504 | G    |
| 4   | 3     | 1508 | G    |
| 4   | 3     | 1510 | A    |
| 4   | 3     | 1513 | A    |
| 4   | 3     | 1514 | U    |
| 4   | 3     | 1515 | A    |
| 4   | 3     | 1519 | A    |
| 4   | 3     | 1522 | U    |
| 4   | 3     | 1534 | A    |
| 4   | 3     | 1535 | A    |
| 4   | 3     | 1541 | A    |
| 4   | 3     | 1546 | U    |
| 4   | 3     | 1550 | G    |
| 4   | 3     | 1569 | A    |
| 4   | 3     | 1570 | A    |
| 4   | 3     | 1571 | G    |
| 4   | 3     | 1580 | G    |
| 4   | 3     | 1582 | G    |
| 4   | 3     | 1584 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 4   | 3     | 1585 | A    |
| 4   | 3     | 1588 | A    |
| 4   | 3     | 1589 | A    |
| 4   | 3     | 1603 | A    |
| 4   | 3     | 1612 | U    |
| 4   | 3     | 1617 | U    |
| 4   | 3     | 1618 | U    |
| 4   | 3     | 1619 | A    |
| 4   | 3     | 1641 | A    |
| 4   | 3     | 1642 | G    |
| 4   | 3     | 1643 | A    |
| 4   | 3     | 1644 | A    |
| 4   | 3     | 1645 | C    |
| 4   | 3     | 1650 | A    |
| 4   | 3     | 1651 | C    |
| 4   | 3     | 1661 | A    |
| 4   | 3     | 1668 | G    |
| 4   | 3     | 1680 | A    |
| 4   | 3     | 1681 | G    |
| 4   | 3     | 1682 | C    |
| 4   | 3     | 1688 | A    |
| 4   | 3     | 1694 | A    |
| 4   | 3     | 1708 | G    |
| 4   | 3     | 1727 | U    |
| 4   | 3     | 1737 | G    |
| 4   | 3     | 1748 | U    |
| 4   | 3     | 1749 | A    |
| 4   | 3     | 1764 | U    |
| 4   | 3     | 1769 | A    |
| 4   | 3     | 1770 | A    |
| 4   | 3     | 1771 | C    |
| 4   | 3     | 1780 | A    |
| 4   | 3     | 1789 | C    |
| 4   | 3     | 1791 | A    |
| 4   | 3     | 1807 | C    |
| 4   | 3     | 1808 | C    |
| 4   | 3     | 1809 | A    |
| 4   | 3     | 1816 | A    |
| 4   | 3     | 1823 | U    |
| 4   | 3     | 1836 | A    |
| 4   | 3     | 1854 | A    |
| 4   | 3     | 1855 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 4   | 3     | 1866 | G    |
| 4   | 3     | 1869 | G    |
| 4   | 3     | 1878 | A    |
| 4   | 3     | 1886 | C    |
| 4   | 3     | 1910 | G    |
| 4   | 3     | 1913 | G    |
| 4   | 3     | 1920 | A    |
| 4   | 3     | 1936 | G    |
| 4   | 3     | 1937 | G    |
| 4   | 3     | 1938 | U    |
| 4   | 3     | 1943 | A    |
| 4   | 3     | 1944 | A    |
| 4   | 3     | 1962 | U    |
| 4   | 3     | 1974 | U    |
| 4   | 3     | 1977 | A    |
| 4   | 3     | 1978 | U    |
| 4   | 3     | 1979 | G    |
| 4   | 3     | 1998 | U    |
| 4   | 3     | 1999 | G    |
| 4   | 3     | 2000 | U    |
| 4   | 3     | 2004 | G    |
| 4   | 3     | 2028 | G    |
| 4   | 3     | 2030 | A    |
| 4   | 3     | 2038 | A    |
| 4   | 3     | 2040 | A    |
| 4   | 3     | 2041 | C    |
| 4   | 3     | 2042 | A    |
| 4   | 3     | 2050 | G    |
| 4   | 3     | 2057 | C    |
| 4   | 3     | 2062 | C    |
| 4   | 3     | 2063 | G    |
| 4   | 3     | 2067 | A    |
| 4   | 3     | 2068 | G    |
| 4   | 3     | 2069 | A    |
| 4   | 3     | 2076 | G    |
| 4   | 3     | 2084 | A    |
| 4   | 3     | 2099 | U    |
| 4   | 3     | 2100 | G    |
| 4   | 3     | 2106 | G    |
| 4   | 3     | 2107 | A    |
| 4   | 3     | 2108 | C    |
| 4   | 3     | 2109 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 4   | 3     | 2110 | U    |
| 4   | 3     | 2111 | U    |
| 4   | 3     | 2112 | A    |
| 4   | 3     | 2114 | C    |
| 4   | 3     | 2118 | U    |
| 4   | 3     | 2119 | A    |
| 4   | 3     | 2122 | G    |
| 4   | 3     | 2123 | A    |
| 4   | 3     | 2124 | A    |
| 4   | 3     | 2125 | U    |
| 4   | 3     | 2126 | A    |
| 4   | 3     | 2128 | G    |
| 4   | 3     | 2129 | U    |
| 4   | 3     | 2131 | G    |
| 4   | 3     | 2135 | C    |
| 4   | 3     | 2139 | C    |
| 4   | 3     | 2140 | G    |
| 4   | 3     | 2151 | G    |
| 4   | 3     | 2152 | C    |
| 4   | 3     | 2153 | U    |
| 4   | 3     | 2156 | G    |
| 4   | 3     | 2158 | C    |
| 4   | 3     | 2159 | U    |
| 4   | 3     | 2160 | U    |
| 4   | 3     | 2161 | G    |
| 4   | 3     | 2165 | A    |
| 4   | 3     | 2166 | U    |
| 4   | 3     | 2167 | G    |
| 4   | 3     | 2168 | C    |
| 4   | 3     | 2169 | G    |
| 4   | 3     | 2170 | A    |
| 4   | 3     | 2171 | A    |
| 4   | 3     | 2175 | U    |
| 4   | 3     | 2178 | A    |
| 4   | 3     | 2179 | A    |
| 4   | 3     | 2180 | U    |
| 4   | 3     | 2181 | A    |
| 4   | 3     | 2184 | A    |
| 4   | 3     | 2185 | C    |
| 4   | 3     | 2187 | C    |
| 4   | 3     | 2188 | U    |
| 4   | 3     | 2193 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 4   | 3     | 2194 | G    |
| 4   | 3     | 2195 | U    |
| 4   | 3     | 2196 | G    |
| 4   | 3     | 2198 | G    |
| 4   | 3     | 2199 | C    |
| 4   | 3     | 2200 | U    |
| 4   | 3     | 2201 | G    |
| 4   | 3     | 2202 | U    |
| 4   | 3     | 2207 | A    |
| 4   | 3     | 2211 | G    |
| 4   | 3     | 2212 | U    |
| 4   | 3     | 2219 | U    |
| 4   | 3     | 2220 | A    |
| 4   | 3     | 2221 | U    |
| 4   | 3     | 2227 | U    |
| 4   | 3     | 2228 | U    |
| 4   | 3     | 2233 | A    |
| 4   | 3     | 2246 | G    |
| 4   | 3     | 2247 | G    |
| 4   | 3     | 2259 | OMG  |
| 4   | 3     | 2274 | A    |
| 4   | 3     | 2276 | A    |
| 4   | 3     | 2287 | G    |
| 4   | 3     | 2291 | U    |
| 4   | 3     | 2295 | A    |
| 4   | 3     | 2298 | G    |
| 4   | 3     | 2305 | C    |
| 4   | 3     | 2311 | G    |
| 4   | 3     | 2313 | U    |
| 4   | 3     | 2316 | G    |
| 4   | 3     | 2319 | A    |
| 4   | 3     | 2327 | U    |
| 4   | 3     | 2329 | G    |
| 4   | 3     | 2333 | G    |
| 4   | 3     | 2335 | A    |
| 4   | 3     | 2336 | A    |
| 4   | 3     | 2342 | U    |
| 4   | 3     | 2343 | A    |
| 4   | 3     | 2344 | A    |
| 4   | 3     | 2353 | G    |
| 4   | 3     | 2355 | C    |
| 4   | 3     | 2358 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 4   | 3     | 2366 | A    |
| 4   | 3     | 2391 | G    |
| 4   | 3     | 2393 | C    |
| 4   | 3     | 2397 | G    |
| 4   | 3     | 2410 | C    |
| 4   | 3     | 2411 | C    |
| 4   | 3     | 2414 | U    |
| 4   | 3     | 2422 | G    |
| 4   | 3     | 2431 | U    |
| 4   | 3     | 2433 | A    |
| 4   | 3     | 2437 | G    |
| 4   | 3     | 2438 | A    |
| 4   | 3     | 2443 | A    |
| 4   | 3     | 2449 | U    |
| 4   | 3     | 2456 | A    |
| 4   | 3     | 2477 | A    |
| 4   | 3     | 2481 | U    |
| 4   | 3     | 2482 | U    |
| 4   | 3     | 2483 | C    |
| 4   | 3     | 2484 | A    |
| 4   | 3     | 2486 | A    |
| 4   | 3     | 2488 | C    |
| 4   | 3     | 2499 | U    |
| 4   | 3     | 2510 | G    |
| 4   | 3     | 2513 | G    |
| 4   | 3     | 2521 | A    |
| 4   | 3     | 2526 | A    |
| 4   | 3     | 2537 | G    |
| 4   | 3     | 2543 | G    |
| 4   | 3     | 2574 | A    |
| 4   | 3     | 2575 | G    |
| 4   | 3     | 2580 | A    |
| 4   | 3     | 2585 | A    |
| 4   | 3     | 2593 | U    |
| 4   | 3     | 2594 | C    |
| 4   | 3     | 2605 | G    |
| 4   | 3     | 2610 | A    |
| 4   | 3     | 2611 | G    |
| 4   | 3     | 2617 | U    |
| 4   | 3     | 2618 | C    |
| 4   | 3     | 2621 | U    |
| 4   | 3     | 2623 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 4   | 3     | 2637 | A    |
| 4   | 3     | 2638 | G    |
| 4   | 3     | 2654 | U    |
| 4   | 3     | 2668 | A    |
| 4   | 3     | 2669 | G    |
| 4   | 3     | 2697 | C    |
| 4   | 3     | 2698 | U    |
| 4   | 3     | 2722 | G    |
| 4   | 3     | 2734 | C    |
| 4   | 3     | 2737 | G    |
| 4   | 3     | 2741 | A    |
| 4   | 3     | 2752 | G    |
| 4   | 3     | 2756 | A    |
| 4   | 3     | 2760 | C    |
| 4   | 3     | 2764 | U    |
| 4   | 3     | 2765 | A    |
| 4   | 3     | 2773 | A    |
| 4   | 3     | 2786 | A    |
| 4   | 3     | 2798 | A    |
| 4   | 3     | 2799 | U    |
| 4   | 3     | 2804 | C    |
| 4   | 3     | 2806 | A    |
| 4   | 3     | 2807 | G    |
| 4   | 3     | 2808 | A    |
| 4   | 3     | 2810 | A    |
| 4   | 3     | 2813 | A    |
| 4   | 3     | 2822 | C    |
| 4   | 3     | 2824 | A    |
| 4   | 3     | 2829 | G    |
| 4   | 3     | 2839 | A    |
| 4   | 3     | 2853 | U    |
| 4   | 3     | 2862 | U    |
| 4   | 3     | 2863 | G    |
| 4   | 3     | 2871 | G    |
| 4   | 3     | 2876 | G    |
| 4   | 3     | 2884 | C    |
| 4   | 3     | 2887 | A    |
| 4   | 3     | 2888 | U    |
| 4   | 3     | 2895 | A    |
| 4   | 3     | 2896 | G    |
| 4   | 3     | 2899 | C    |
| 5   | 4     | 9    | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | 4     | 10  | C    |
| 5   | 4     | 11  | A    |
| 5   | 4     | 13  | G    |
| 5   | 4     | 14  | U    |
| 5   | 4     | 22  | G    |
| 5   | 4     | 23  | A    |
| 5   | 4     | 28  | C    |
| 5   | 4     | 33  | U    |
| 5   | 4     | 35  | C    |
| 5   | 4     | 39  | U    |
| 5   | 4     | 41  | C    |
| 5   | 4     | 48  | A    |
| 5   | 4     | 49  | G    |
| 5   | 4     | 54  | U    |
| 5   | 4     | 56  | A    |
| 5   | 4     | 60  | C    |
| 5   | 4     | 64  | G    |
| 5   | 4     | 65  | G    |
| 5   | 4     | 80  | G    |
| 5   | 4     | 82  | U    |
| 5   | 4     | 83  | U    |
| 5   | 4     | 84  | C    |
| 5   | 4     | 85  | A    |
| 5   | 4     | 88  | G    |
| 5   | 4     | 89  | A    |
| 5   | 4     | 99  | A    |
| 5   | 4     | 106 | A    |
| 5   | 4     | 108 | C    |
| 6   | 5     | 6   | C    |
| 6   | 5     | 10  | G    |
| 6   | 5     | 33  | A    |
| 6   | 5     | 40  | G    |
| 6   | 5     | 48  | C    |
| 6   | 5     | 49  | C    |
| 6   | 5     | 52  | A    |
| 6   | 5     | 57  | U    |
| 6   | 5     | 61  | A    |
| 6   | 5     | 106 | C    |
| 6   | 5     | 114 | C    |
| 6   | 5     | 115 | A    |
| 6   | 5     | 117 | U    |
| 6   | 5     | 120 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | 5     | 149 | G    |
| 6   | 5     | 154 | G    |
| 6   | 5     | 163 | G    |
| 6   | 5     | 167 | A    |
| 6   | 5     | 171 | A    |
| 6   | 5     | 173 | U    |
| 6   | 5     | 176 | G    |
| 6   | 5     | 180 | C    |
| 6   | 5     | 182 | C    |
| 6   | 5     | 185 | G    |
| 6   | 5     | 186 | A    |
| 6   | 5     | 189 | C    |
| 6   | 5     | 190 | A    |
| 6   | 5     | 197 | A    |
| 6   | 5     | 198 | A    |
| 6   | 5     | 199 | A    |
| 6   | 5     | 220 | U    |
| 6   | 5     | 223 | G    |
| 6   | 5     | 239 | A    |
| 6   | 5     | 241 | C    |
| 6   | 5     | 243 | G    |
| 6   | 5     | 247 | G    |
| 6   | 5     | 262 | G    |
| 6   | 5     | 263 | C    |
| 6   | 5     | 269 | A    |
| 6   | 5     | 275 | A    |
| 6   | 5     | 285 | G    |
| 6   | 5     | 301 | G    |
| 6   | 5     | 302 | A    |
| 6   | 5     | 324 | C    |
| 6   | 5     | 325 | A    |
| 6   | 5     | 326 | C    |
| 6   | 5     | 328 | G    |
| 6   | 5     | 341 | C    |
| 6   | 5     | 342 | G    |
| 6   | 5     | 344 | G    |
| 6   | 5     | 347 | G    |
| 6   | 5     | 348 | C    |
| 6   | 5     | 350 | G    |
| 6   | 5     | 359 | A    |
| 6   | 5     | 363 | U    |
| 6   | 5     | 368 | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | 5     | 369 | A    |
| 6   | 5     | 370 | A    |
| 6   | 5     | 374 | G    |
| 6   | 5     | 380 | G    |
| 6   | 5     | 383 | U    |
| 6   | 5     | 394 | U    |
| 6   | 5     | 408 | U    |
| 6   | 5     | 416 | U    |
| 6   | 5     | 418 | U    |
| 6   | 5     | 419 | A    |
| 6   | 5     | 422 | A    |
| 6   | 5     | 425 | G    |
| 6   | 5     | 426 | U    |
| 6   | 5     | 447 | G    |
| 6   | 5     | 449 | A    |
| 6   | 5     | 450 | U    |
| 6   | 5     | 452 | A    |
| 6   | 5     | 461 | G    |
| 6   | 5     | 462 | G    |
| 6   | 5     | 464 | A    |
| 6   | 5     | 468 | G    |
| 6   | 5     | 470 | U    |
| 6   | 5     | 475 | U    |
| 6   | 5     | 476 | U    |
| 6   | 5     | 477 | U    |
| 6   | 5     | 481 | U    |
| 6   | 5     | 482 | G    |
| 6   | 5     | 488 | U    |
| 6   | 5     | 489 | U    |
| 6   | 5     | 493 | A    |
| 6   | 5     | 494 | A    |
| 6   | 5     | 495 | U    |
| 6   | 5     | 507 | A    |
| 6   | 5     | 509 | C    |
| 6   | 5     | 510 | U    |
| 6   | 5     | 516 | C    |
| 6   | 5     | 517 | C    |
| 6   | 5     | 522 | G    |
| 6   | 5     | 525 | 7MG  |
| 6   | 5     | 530 | A    |
| 6   | 5     | 531 | A    |
| 6   | 5     | 545 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | 5     | 557 | A    |
| 6   | 5     | 560 | U    |
| 6   | 5     | 562 | U    |
| 6   | 5     | 570 | A    |
| 6   | 5     | 571 | A    |
| 6   | 5     | 572 | A    |
| 6   | 5     | 574 | C    |
| 6   | 5     | 575 | A    |
| 6   | 5     | 579 | G    |
| 6   | 5     | 586 | G    |
| 6   | 5     | 594 | A    |
| 6   | 5     | 595 | G    |
| 6   | 5     | 628 | A    |
| 6   | 5     | 650 | A    |
| 6   | 5     | 661 | G    |
| 6   | 5     | 662 | G    |
| 6   | 5     | 683 | G    |
| 6   | 5     | 700 | G    |
| 6   | 5     | 715 | A    |
| 6   | 5     | 719 | G    |
| 6   | 5     | 720 | U    |
| 6   | 5     | 721 | G    |
| 6   | 5     | 728 | G    |
| 6   | 5     | 745 | U    |
| 6   | 5     | 752 | G    |
| 6   | 5     | 768 | G    |
| 6   | 5     | 790 | U    |
| 6   | 5     | 791 | A    |
| 6   | 5     | 811 | A    |
| 6   | 5     | 812 | A    |
| 6   | 5     | 814 | C    |
| 6   | 5     | 818 | A    |
| 6   | 5     | 825 | A    |
| 6   | 5     | 829 | G    |
| 6   | 5     | 836 | C    |
| 6   | 5     | 838 | A    |
| 6   | 5     | 839 | U    |
| 6   | 5     | 867 | A    |
| 6   | 5     | 883 | A    |
| 6   | 5     | 885 | U    |
| 6   | 5     | 908 | A    |
| 6   | 5     | 910 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 6   | 5     | 911  | G    |
| 6   | 5     | 921  | G    |
| 6   | 5     | 922  | G    |
| 6   | 5     | 929  | C    |
| 6   | 5     | 930  | A    |
| 6   | 5     | 955  | U    |
| 6   | 5     | 964  | A    |
| 6   | 5     | 970  | A    |
| 6   | 5     | 971  | A    |
| 6   | 5     | 972  | A    |
| 6   | 5     | 982  | A    |
| 6   | 5     | 987  | U    |
| 6   | 5     | 988  | G    |
| 6   | 5     | 989  | A    |
| 6   | 5     | 994  | C    |
| 6   | 5     | 995  | U    |
| 6   | 5     | 996  | U    |
| 6   | 5     | 997  | G    |
| 6   | 5     | 998  | G    |
| 6   | 5     | 999  | C    |
| 6   | 5     | 1000 | A    |
| 6   | 5     | 1002 | A    |
| 6   | 5     | 1007 | U    |
| 6   | 5     | 1009 | G    |
| 6   | 5     | 1015 | U    |
| 6   | 5     | 1018 | U    |
| 6   | 5     | 1019 | G    |
| 6   | 5     | 1020 | G    |
| 6   | 5     | 1022 | G    |
| 6   | 5     | 1023 | G    |
| 6   | 5     | 1024 | U    |
| 6   | 5     | 1025 | U    |
| 6   | 5     | 1027 | A    |
| 6   | 5     | 1028 | C    |
| 6   | 5     | 1029 | C    |
| 6   | 5     | 1030 | G    |
| 6   | 5     | 1032 | G    |
| 6   | 5     | 1034 | G    |
| 6   | 5     | 1036 | C    |
| 6   | 5     | 1044 | G    |
| 6   | 5     | 1045 | C    |
| 6   | 5     | 1047 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 6   | 5     | 1056 | U    |
| 6   | 5     | 1072 | G    |
| 6   | 5     | 1076 | U    |
| 6   | 5     | 1078 | G    |
| 6   | 5     | 1083 | A    |
| 6   | 5     | 1085 | G    |
| 6   | 5     | 1086 | U    |
| 6   | 5     | 1092 | A    |
| 6   | 5     | 1118 | A    |
| 6   | 5     | 1121 | U    |
| 6   | 5     | 1122 | U    |
| 6   | 5     | 1123 | G    |
| 6   | 5     | 1124 | U    |
| 6   | 5     | 1134 | C    |
| 6   | 5     | 1135 | U    |
| 6   | 5     | 1141 | U    |
| 6   | 5     | 1142 | G    |
| 6   | 5     | 1158 | A    |
| 6   | 5     | 1159 | A    |
| 6   | 5     | 1170 | C    |
| 6   | 5     | 1171 | A    |
| 6   | 5     | 1172 | A    |
| 6   | 5     | 1188 | A    |
| 6   | 5     | 1189 | U    |
| 6   | 5     | 1202 | A    |
| 6   | 5     | 1203 | A    |
| 6   | 5     | 1215 | U    |
| 6   | 5     | 1231 | U    |
| 6   | 5     | 1232 | C    |
| 6   | 5     | 1233 | G    |
| 6   | 5     | 1235 | C    |
| 6   | 5     | 1255 | A    |
| 6   | 5     | 1260 | U    |
| 6   | 5     | 1271 | U    |
| 6   | 5     | 1274 | G    |
| 6   | 5     | 1279 | G    |
| 6   | 5     | 1291 | C    |
| 6   | 5     | 1294 | U    |
| 6   | 5     | 1296 | C    |
| 6   | 5     | 1297 | G    |
| 6   | 5     | 1306 | A    |
| 6   | 5     | 1312 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 6   | 5     | 1320 | A    |
| 6   | 5     | 1321 | G    |
| 6   | 5     | 1337 | U    |
| 6   | 5     | 1338 | A    |
| 6   | 5     | 1339 | U    |
| 6   | 5     | 1343 | G    |
| 6   | 5     | 1345 | G    |
| 6   | 5     | 1372 | C    |
| 6   | 5     | 1373 | A    |
| 6   | 5     | 1397 | G    |
| 6   | 5     | 1417 | U    |
| 6   | 5     | 1426 | U    |
| 6   | 5     | 1427 | U    |
| 6   | 5     | 1428 | A    |
| 6   | 5     | 1429 | G    |
| 6   | 5     | 1462 | G    |
| 6   | 5     | 1466 | U    |
| 6   | 5     | 1467 | A    |
| 6   | 5     | 1469 | G    |
| 6   | 5     | 1472 | G    |
| 6   | 5     | 1478 | A    |
| 6   | 5     | 1480 | G    |
| 6   | 5     | 1481 | U    |
| 6   | 5     | 1482 | A    |
| 6   | 5     | 1492 | G    |
| 6   | 5     | 1504 | G    |
| 6   | 5     | 1505 | G    |
| 6   | 5     | 1509 | A    |
| 7   | 6     | 2    | G    |
| 7   | 6     | 3    | G    |
| 7   | 6     | 13   | C    |
| 7   | 6     | 15   | A    |
| 7   | 6     | 16   | C    |
| 7   | 6     | 17   | U    |
| 7   | 6     | 18   | G    |
| 7   | 6     | 19   | A    |
| 7   | 6     | 20   | U    |
| 7   | 6     | 21   | A    |
| 7   | 6     | 33   | U    |
| 7   | 6     | 34   | U    |
| 7   | 6     | 46   | G    |
| 7   | 6     | 47   | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | 6     | 48  | U    |
| 7   | 6     | 59  | G    |
| 7   | 6     | 65  | U    |
| 7   | 6     | 70  | U    |
| 7   | 6     | 71  | C    |
| 7   | 6     | 72  | C    |
| 7   | 6     | 73  | A    |
| 7   | 6     | 75  | C    |
| 8   | 7     | 4   | U    |
| 8   | 7     | 11  | U    |
| 8   | 7     | 13  | U    |
| 8   | 7     | 15  | G    |
| 8   | 7     | 16  | U    |
| 8   | 7     | 17  | G    |
| 8   | 7     | 19  | A    |
| 8   | 7     | 20  | U    |
| 8   | 7     | 21  | A    |
| 8   | 7     | 22  | A    |
| 8   | 7     | 34  | G    |
| 8   | 7     | 44  | G    |
| 8   | 7     | 46  | U    |
| 8   | 7     | 47  | U    |
| 8   | 7     | 48  | G    |
| 8   | 7     | 51  | G    |
| 8   | 7     | 57  | A    |
| 8   | 7     | 71  | C    |
| 8   | 7     | 73  | C    |
| 8   | 7     | 75  | A    |
| 9   | 8     | 3   | A    |
| 9   | 8     | 9   | A    |
| 9   | 8     | 10  | G    |
| 9   | 8     | 15  | G    |
| 9   | 8     | 16  | U    |
| 9   | 8     | 17  | U    |
| 9   | 8     | 18  | G    |
| 9   | 8     | 19  | G    |
| 9   | 8     | 20  | U    |
| 9   | 8     | 21  | A    |
| 9   | 8     | 30  | G    |
| 9   | 8     | 31  | A    |
| 9   | 8     | 41  | A    |
| 9   | 8     | 46  | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9   | 8     | 47  | U    |
| 9   | 8     | 48  | C    |
| 9   | 8     | 58  | A    |
| 9   | 8     | 60  | C    |
| 9   | 8     | 71  | G    |
| 9   | 8     | 73  | A    |
| 9   | 8     | 74  | C    |
| 9   | 8     | 75  | C    |
| 9   | 8     | 76  | A    |
| 32  | Y     | 58  | A    |
| 32  | Y     | 59  | A    |
| 32  | Y     | 61  | A    |
| 32  | Y     | 62  | A    |
| 32  | Y     | 64  | A    |
| 32  | Y     | 65  | C    |
| 32  | Y     | 66  | U    |
| 32  | Y     | 67  | G    |
| 32  | Y     | 70  | G    |
| 32  | Y     | 77  | U    |
| 32  | Y     | 79  | U    |
| 32  | Y     | 80  | U    |
| 32  | Y     | 81  | C    |
| 32  | Y     | 82  | A    |
| 32  | Y     | 83  | A    |
| 32  | Y     | 84  | A    |
| 32  | Y     | 86  | A    |
| 32  | Y     | 87  | A    |
| 32  | Y     | 88  | A    |
| 32  | Y     | 89  | A    |
| 32  | Y     | 91  | A    |
| 32  | Y     | 92  | A    |
| 32  | Y     | 94  | A    |
| 32  | Y     | 95  | C    |
| 32  | Y     | 96  | U    |

All (42) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | 3     | 315 | A    |
| 4   | 3     | 410 | G    |
| 4   | 3     | 881 | A    |
| 4   | 3     | 901 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 4   | 3     | 902  | U    |
| 4   | 3     | 1124 | G    |
| 4   | 3     | 1209 | U    |
| 4   | 3     | 1583 | G    |
| 4   | 3     | 1618 | U    |
| 4   | 3     | 2106 | G    |
| 4   | 3     | 2118 | U    |
| 4   | 3     | 2139 | C    |
| 4   | 3     | 2152 | C    |
| 4   | 3     | 2164 | G    |
| 4   | 3     | 2167 | G    |
| 4   | 3     | 2169 | G    |
| 4   | 3     | 2180 | U    |
| 4   | 3     | 2194 | G    |
| 4   | 3     | 2410 | C    |
| 4   | 3     | 2764 | U    |
| 6   | 5     | 196  | G    |
| 6   | 5     | 571  | A    |
| 6   | 5     | 994  | C    |
| 6   | 5     | 995  | U    |
| 6   | 5     | 1024 | U    |
| 6   | 5     | 1123 | G    |
| 6   | 5     | 1158 | A    |
| 6   | 5     | 1338 | A    |
| 7   | 6     | 1    | G    |
| 7   | 6     | 15   | A    |
| 7   | 6     | 17   | U    |
| 7   | 6     | 33   | U    |
| 7   | 6     | 46   | G    |
| 7   | 6     | 74   | C    |
| 8   | 7     | 10   | G    |
| 8   | 7     | 46   | U    |
| 32  | Y     | 64   | A    |
| 32  | Y     | 65   | C    |
| 32  | Y     | 79   | U    |
| 32  | Y     | 81   | C    |
| 32  | Y     | 94   | A    |
| 32  | Y     | 95   | C    |

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

8 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 6   | B8T  | 5     | 1377 | 6    | 19,22,23     | 3.32 | 8 (42%)  | 25,31,34    | 0.85 | 1 (4%)   |
| 6   | MA6  | 5     | 1493 | 6    | 23,26,27     | 1.41 | 3 (13%)  | 33,38,41    | 3.17 | 14 (42%) |
| 6   | 7MG  | 5     | 525  | 6    | 23,26,27     | 3.64 | 11 (47%) | 27,39,42    | 2.16 | 9 (33%)  |
| 4   | 2MA  | 3     | 2511 | 4,63 | 22,25,26     | 4.13 | 10 (45%) | 32,37,40    | 3.53 | 12 (37%) |
| 4   | OMG  | 3     | 2259 | 4,8  | 23,26,27     | 2.60 | 7 (30%)  | 32,38,41    | 2.44 | 10 (31%) |
| 6   | 5MC  | 5     | 1375 | 6    | 19,22,23     | 4.56 | 8 (42%)  | 26,32,35    | 1.02 | 2 (7%)   |
| 6   | MA6  | 5     | 1494 | 6    | 23,26,27     | 1.40 | 3 (13%)  | 33,38,41    | 3.23 | 14 (42%) |
| 4   | 1MG  | 3     | 783  | 4    | 23,26,27     | 0.61 | 0        | 33,39,42    | 0.74 | 1 (3%)   |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|------|------|---------|------------|---------|
| 6   | B8T  | 5     | 1377 | 6    | -       | 2/7/27/28  | 0/2/2/2 |
| 6   | MA6  | 5     | 1493 | 6    | -       | 0/11/29/30 | 0/3/3/3 |
| 6   | 7MG  | 5     | 525  | 6    | -       | 2/7/37/38  | 0/3/3/3 |
| 4   | 2MA  | 3     | 2511 | 4,63 | -       | 1/7/25/26  | 0/3/3/3 |
| 4   | OMG  | 3     | 2259 | 4,8  | -       | 3/9/27/28  | 0/3/3/3 |
| 6   | 5MC  | 5     | 1375 | 6    | -       | 0/7/25/26  | 0/2/2/2 |
| 6   | MA6  | 5     | 1494 | 6    | -       | 2/11/29/30 | 0/3/3/3 |
| 4   | 1MG  | 3     | 783  | 4    | -       | 0/7/25/26  | 0/3/3/3 |

All (50) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 4   | 3     | 2511 | 2MA  | C4-N3 | 11.95 | 1.49        | 1.34     |
| 6   | 5     | 1375 | 5MC  | C6-C5 | 10.01 | 1.50        | 1.34     |
| 6   | 5     | 1375 | 5MC  | C5-C4 | 9.26  | 1.51        | 1.44     |
| 6   | 5     | 525  | 7MG  | C8-N9 | 8.71  | 1.51        | 1.45     |
| 4   | 3     | 2511 | 2MA  | C2-N3 | 8.09  | 1.47        | 1.34     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 6   | 5     | 1375 | 5MC  | C4-N3 | 7.98  | 1.46        | 1.34     |
| 4   | 3     | 2511 | 2MA  | C6-N1 | 7.49  | 1.45        | 1.35     |
| 6   | 5     | 1377 | B8T  | C4-N3 | 7.45  | 1.45        | 1.32     |
| 4   | 3     | 2259 | OMG  | C2-N2 | 7.27  | 1.51        | 1.34     |
| 6   | 5     | 525  | 7MG  | C5-N7 | 7.24  | 1.44        | 1.35     |
| 6   | 5     | 1375 | 5MC  | C2-N3 | 7.16  | 1.50        | 1.36     |
| 6   | 5     | 1377 | B8T  | C2-N3 | 6.64  | 1.49        | 1.36     |
| 4   | 3     | 2511 | 2MA  | C2-N1 | 6.43  | 1.45        | 1.34     |
| 4   | 3     | 2259 | OMG  | C4-N3 | 6.20  | 1.48        | 1.34     |
| 6   | 5     | 1377 | B8T  | C6-C5 | 6.12  | 1.49        | 1.35     |
| 6   | 5     | 525  | 7MG  | C2-N3 | 5.85  | 1.47        | 1.33     |
| 6   | 5     | 525  | 7MG  | C4-N3 | 5.81  | 1.47        | 1.34     |
| 6   | 5     | 1375 | 5MC  | C4-N4 | 5.79  | 1.48        | 1.34     |
| 6   | 5     | 1375 | 5MC  | C6-N1 | 5.63  | 1.47        | 1.38     |
| 6   | 5     | 525  | 7MG  | C4-N9 | 5.32  | 1.44        | 1.37     |
| 4   | 3     | 2511 | 2MA  | C5-C6 | 5.30  | 1.55        | 1.41     |
| 4   | 3     | 2259 | OMG  | C2-N3 | 5.13  | 1.45        | 1.33     |
| 6   | 5     | 525  | 7MG  | C2-N2 | 4.87  | 1.45        | 1.34     |
| 6   | 5     | 1375 | 5MC  | C2-N1 | 4.78  | 1.50        | 1.40     |
| 6   | 5     | 1377 | B8T  | C4-N4 | 4.68  | 1.45        | 1.36     |
| 6   | 5     | 1377 | B8T  | C2-N1 | 4.39  | 1.49        | 1.40     |
| 6   | 5     | 1493 | MA6  | C6-N6 | 4.21  | 1.48        | 1.36     |
| 6   | 5     | 1494 | MA6  | C6-N6 | 4.14  | 1.48        | 1.36     |
| 6   | 5     | 525  | 7MG  | C2-N1 | 3.95  | 1.47        | 1.37     |
| 6   | 5     | 525  | 7MG  | C5-C6 | 3.72  | 1.52        | 1.43     |
| 4   | 3     | 2511 | 2MA  | C5-N7 | -3.70 | 1.32        | 1.39     |
| 6   | 5     | 1377 | B8T  | C5-C4 | 3.66  | 1.49        | 1.41     |
| 4   | 3     | 2259 | OMG  | C2-N1 | 3.40  | 1.45        | 1.37     |
| 6   | 5     | 525  | 7MG  | C6-N1 | 3.38  | 1.45        | 1.38     |
| 4   | 3     | 2511 | 2MA  | C8-N7 | 3.38  | 1.38        | 1.31     |
| 6   | 5     | 1377 | B8T  | C6-N1 | 3.11  | 1.45        | 1.38     |
| 6   | 5     | 1377 | B8T  | O2-C2 | -2.67 | 1.18        | 1.23     |
| 6   | 5     | 525  | 7MG  | O6-C6 | -2.42 | 1.19        | 1.23     |
| 6   | 5     | 1494 | MA6  | C5-C4 | -2.39 | 1.34        | 1.39     |
| 4   | 3     | 2259 | OMG  | C5-C6 | 2.34  | 1.53        | 1.44     |
| 6   | 5     | 1493 | MA6  | C5-N7 | -2.32 | 1.34        | 1.39     |
| 6   | 5     | 1493 | MA6  | C5-C4 | -2.31 | 1.35        | 1.39     |
| 6   | 5     | 1494 | MA6  | C5-N7 | -2.24 | 1.35        | 1.39     |
| 4   | 3     | 2511 | 2MA  | C6-N6 | -2.15 | 1.28        | 1.34     |
| 6   | 5     | 1375 | 5MC  | O2-C2 | -2.15 | 1.19        | 1.23     |
| 4   | 3     | 2511 | 2MA  | C4-N9 | -2.10 | 1.33        | 1.37     |
| 6   | 5     | 525  | 7MG  | C5-C4 | 2.06  | 1.44        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 4   | 3     | 2259 | OMG  | C8-N7   | 2.05  | 1.38        | 1.32     |
| 4   | 3     | 2259 | OMG  | O2'-CM2 | -2.04 | 1.35        | 1.42     |
| 4   | 3     | 2511 | 2MA  | C8-N9   | -2.00 | 1.34        | 1.37     |

All (63) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|--------|-------------|----------|
| 4   | 3     | 2511 | 2MA  | C1'-N9-C8 | -12.43 | 99.51       | 127.09   |
| 4   | 3     | 2511 | 2MA  | C4-N9-C1' | 10.80  | 151.88      | 126.63   |
| 6   | 5     | 1494 | MA6  | N1-C6-N6  | -10.43 | 104.15      | 116.86   |
| 6   | 5     | 1493 | MA6  | N1-C6-N6  | -9.77  | 104.95      | 116.86   |
| 4   | 3     | 2259 | OMG  | C1'-N9-C8 | -6.83  | 107.32      | 126.73   |
| 6   | 5     | 1494 | MA6  | C5-C6-N6  | 6.74   | 136.00      | 125.33   |
| 6   | 5     | 1493 | MA6  | C5-C6-N6  | 6.40   | 135.47      | 125.33   |
| 4   | 3     | 2511 | 2MA  | C5-C4-N3  | -5.88  | 120.99      | 127.18   |
| 6   | 5     | 1494 | MA6  | N1-C2-N3  | -5.76  | 119.87      | 128.58   |
| 4   | 3     | 2259 | OMG  | C1'-N9-C4 | 5.64   | 143.15      | 126.49   |
| 6   | 5     | 1493 | MA6  | N1-C2-N3  | -5.57  | 120.15      | 128.58   |
| 6   | 5     | 1493 | MA6  | C1'-N9-C8 | -5.51  | 114.87      | 127.09   |
| 6   | 5     | 1494 | MA6  | C1'-N9-C8 | -5.09  | 115.79      | 127.09   |
| 6   | 5     | 525  | 7MG  | C5-C6-N1  | 4.98   | 119.70      | 110.94   |
| 6   | 5     | 1493 | MA6  | C5-C4-N3  | -4.73  | 120.21      | 126.72   |
| 4   | 3     | 2511 | 2MA  | N9-C8-N7  | -4.71  | 107.26      | 113.94   |
| 6   | 5     | 1494 | MA6  | C5-C4-N3  | -4.63  | 120.34      | 126.72   |
| 6   | 5     | 525  | 7MG  | C2-N3-C4  | 4.62   | 120.25      | 112.30   |
| 4   | 3     | 2259 | OMG  | C5-C4-N3  | -4.59  | 121.08      | 128.39   |
| 6   | 5     | 1494 | MA6  | N9-C8-N7  | -4.50  | 107.56      | 113.94   |
| 4   | 3     | 2259 | OMG  | C2-N3-C4  | 4.35   | 119.79      | 112.30   |
| 6   | 5     | 1493 | MA6  | C4-N9-C1' | 4.30   | 136.68      | 126.63   |
| 6   | 5     | 1493 | MA6  | N9-C8-N7  | -4.30  | 107.84      | 113.94   |
| 6   | 5     | 525  | 7MG  | C5-C4-N3  | -4.17  | 120.30      | 128.13   |
| 6   | 5     | 1493 | MA6  | C4-C5-C6  | 4.05   | 120.10      | 115.91   |
| 6   | 5     | 1494 | MA6  | C4-N9-C1' | 3.86   | 135.66      | 126.63   |
| 6   | 5     | 525  | 7MG  | C4-C5-N7  | 3.68   | 109.72      | 105.38   |
| 6   | 5     | 1494 | MA6  | C4-C5-C6  | 3.62   | 119.65      | 115.91   |
| 4   | 3     | 2259 | OMG  | N9-C8-N7  | -3.54  | 106.83      | 113.40   |
| 6   | 5     | 1494 | MA6  | C2-N1-C6  | 3.42   | 120.18      | 111.83   |
| 6   | 5     | 1493 | MA6  | C2-N1-C6  | 3.40   | 120.13      | 111.83   |
| 6   | 5     | 1494 | MA6  | C2-N3-C4  | 3.39   | 120.10      | 111.83   |
| 4   | 3     | 2511 | 2MA  | N3-C2-N1  | -3.29  | 119.96      | 125.77   |
| 6   | 5     | 1493 | MA6  | C2-N3-C4  | 3.27   | 119.82      | 111.83   |
| 6   | 5     | 525  | 7MG  | C5-C4-N9  | 3.19   | 110.42      | 106.33   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 4   | 3     | 2511 | 2MA  | C5-N7-C8  | 3.05  | 108.25      | 103.45   |
| 6   | 5     | 1494 | MA6  | C5-N7-C8  | 2.98  | 108.14      | 103.45   |
| 4   | 3     | 2259 | OMG  | C2-N1-C6  | -2.98 | 119.70      | 125.11   |
| 6   | 5     | 1493 | MA6  | N3-C4-N9  | 2.95  | 132.19      | 127.17   |
| 4   | 3     | 2511 | 2MA  | N3-C4-N9  | 2.95  | 130.73      | 126.99   |
| 6   | 5     | 1375 | 5MC  | C5-C6-N1  | -2.89 | 120.18      | 123.31   |
| 6   | 5     | 1493 | MA6  | C5-N7-C8  | 2.88  | 107.97      | 103.45   |
| 6   | 5     | 525  | 7MG  | C2-N1-C6  | -2.84 | 119.95      | 125.11   |
| 6   | 5     | 525  | 7MG  | O6-C6-C5  | -2.78 | 120.80      | 127.62   |
| 6   | 5     | 1494 | MA6  | N3-C4-N9  | 2.76  | 131.86      | 127.17   |
| 4   | 3     | 2259 | OMG  | N9-C4-N3  | 2.76  | 131.47      | 125.95   |
| 4   | 3     | 2511 | 2MA  | C4-N9-C8  | 2.72  | 108.59      | 105.74   |
| 4   | 3     | 2259 | OMG  | C5-C6-N1  | 2.67  | 120.04      | 113.25   |
| 6   | 5     | 1494 | MA6  | C4-N9-C8  | 2.66  | 108.53      | 105.74   |
| 4   | 3     | 2511 | 2MA  | CM2-C2-N1 | 2.64  | 121.09      | 117.13   |
| 6   | 5     | 525  | 7MG  | N9-C4-N3  | 2.61  | 129.28      | 125.46   |
| 4   | 3     | 2511 | 2MA  | C4-C5-N7  | -2.59 | 107.62      | 110.58   |
| 6   | 5     | 1493 | MA6  | C4-N9-C8  | 2.58  | 108.45      | 105.74   |
| 6   | 5     | 1377 | B8T  | C6-C5-C4  | 2.54  | 120.06      | 117.00   |
| 4   | 3     | 2259 | OMG  | O6-C6-C5  | -2.42 | 120.14      | 126.53   |
| 4   | 3     | 2259 | OMG  | C8-N7-C5  | 2.32  | 108.39      | 104.26   |
| 6   | 5     | 525  | 7MG  | N9-C8-N7  | 2.29  | 106.61      | 103.37   |
| 6   | 5     | 1494 | MA6  | C4-C5-N7  | -2.29 | 107.97      | 110.58   |
| 4   | 3     | 2511 | 2MA  | C5-C4-N9  | 2.26  | 108.28      | 105.81   |
| 4   | 3     | 2511 | 2MA  | N6-C6-N1  | 2.23  | 120.04      | 117.03   |
| 6   | 5     | 1375 | 5MC  | CM5-C5-C6 | -2.18 | 119.91      | 122.85   |
| 4   | 3     | 783  | 1MG  | N2-C2-N1  | -2.15 | 117.06      | 118.79   |
| 6   | 5     | 1493 | MA6  | C4-C5-N7  | -2.14 | 108.13      | 110.58   |

There are no chirality outliers.

All (10) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 4   | 3     | 2259 | OMG  | O4'-C4'-C5'-O5' |
| 4   | 3     | 2259 | OMG  | C1'-C2'-O2'-CM2 |
| 6   | 5     | 525  | 7MG  | O4'-C4'-C5'-O5' |
| 6   | 5     | 1494 | MA6  | O4'-C4'-C5'-O5' |
| 4   | 3     | 2259 | OMG  | C3'-C4'-C5'-O5' |
| 6   | 5     | 525  | 7MG  | C3'-C4'-C5'-O5' |
| 6   | 5     | 1494 | MA6  | C3'-C4'-C5'-O5' |
| 6   | 5     | 1377 | B8T  | O4'-C4'-C5'-O5' |
| 4   | 3     | 2511 | 2MA  | C4'-C5'-O5'-P   |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 6   | 5     | 1377 | B8T  | C3'-C4'-C5'-O5' |

There are no ring outliers.

4 monomers are involved in 6 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 6   | 5     | 1493 | MA6  | 1       | 0            |
| 6   | 5     | 525  | 7MG  | 1       | 0            |
| 4   | 3     | 2511 | 2MA  | 2       | 0            |
| 4   | 3     | 783  | 1MG  | 2       | 0            |

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 331 ligands modelled in this entry, 329 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res  | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |      |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 61  | CLM  | 3     | 3001 | -    | 20,20,20     | 2.09 | 2 (10%)     | 23,27,27    | 0.87 | 0           |
| 64  | LYS  | 8     | 102  | 9    | 7,8,9        | 0.88 | 0           | 3,8,10      | 0.29 | 0           |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|------|------|---------|------------|---------|
| 61  | CLM  | 3     | 3001 | -    | -       | 2/20/22/22 | 0/1/1/1 |
| 64  | LYS  | 8     | 102  | 9    | -       | 3/6/7/9    | -       |

All (2) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 61  | 3     | 3001 | CLM  | C2-N2  | 7.41  | 1.49        | 1.34     |
| 61  | 3     | 3001 | CLM  | O9B-N9 | -2.66 | 1.18        | 1.22     |

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

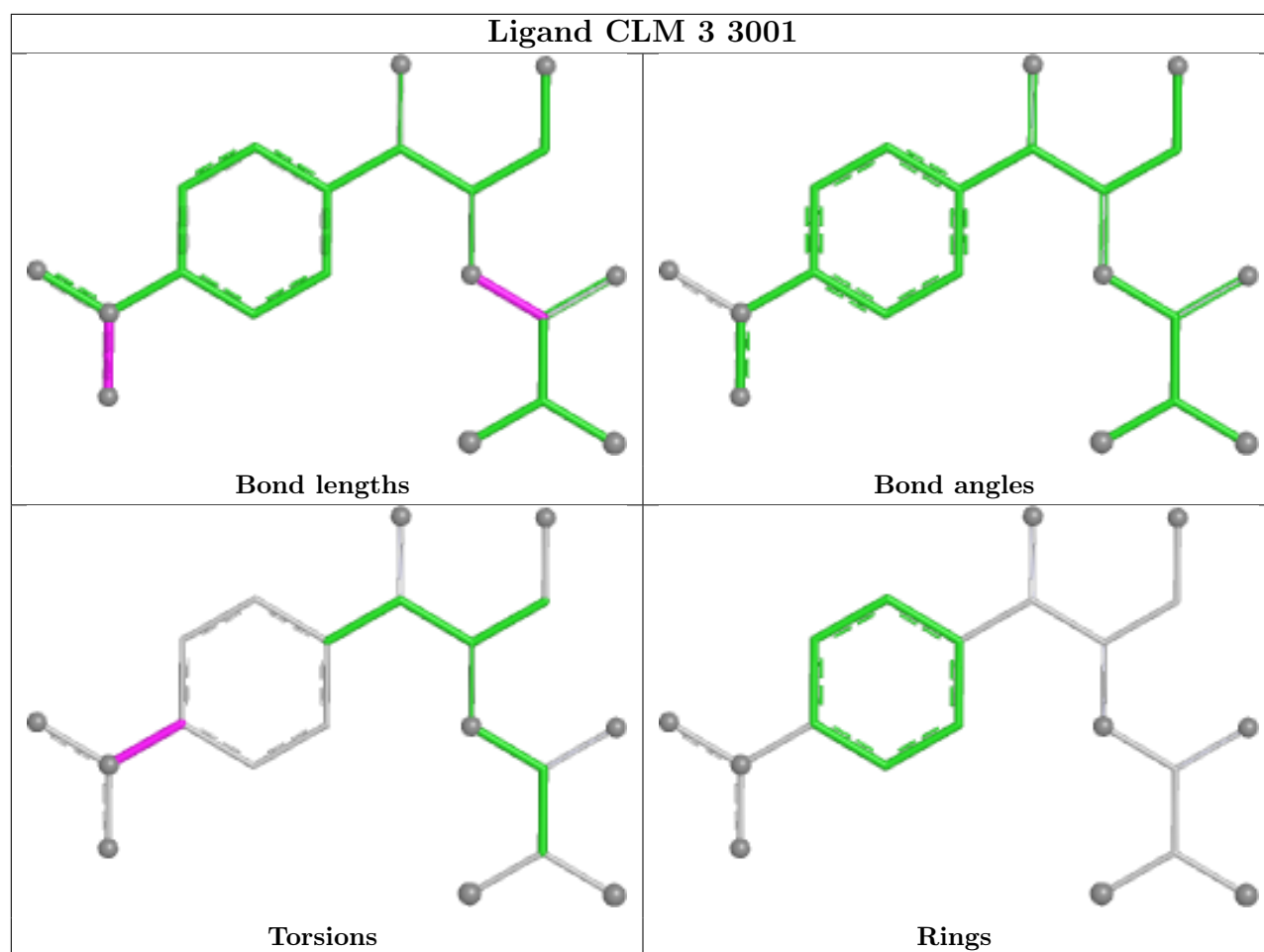
| Mol | Chain | Res  | Type | Atoms         |
|-----|-------|------|------|---------------|
| 64  | 8     | 102  | LYS  | O-C-CA-CB     |
| 64  | 8     | 102  | LYS  | N-CA-CB-CG    |
| 64  | 8     | 102  | LYS  | C-CA-CB-CG    |
| 61  | 3     | 3001 | CLM  | C8-C9-N9-O9B  |
| 61  | 3     | 3001 | CLM  | C10-C9-N9-O9B |

There are no ring outliers.

1 monomer is involved in 1 short contact:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 61  | 3     | 3001 | CLM  | 1       | 0            |

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

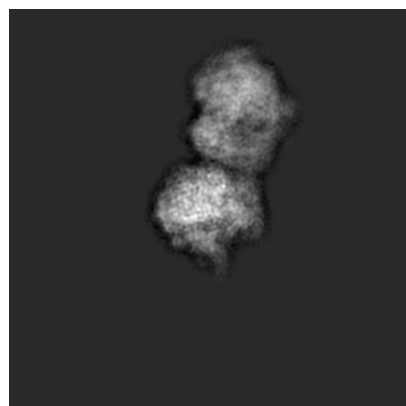
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17145. These allow visual inspection of the internal detail of the map and identification of artifacts.

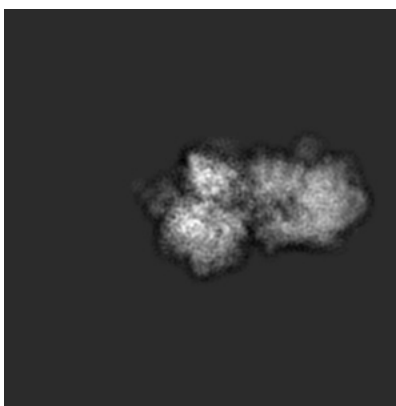
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

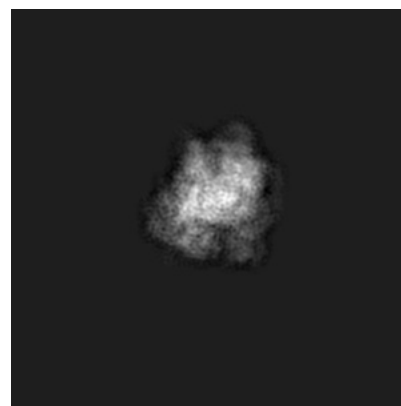
#### 6.1.1 Primary map



X

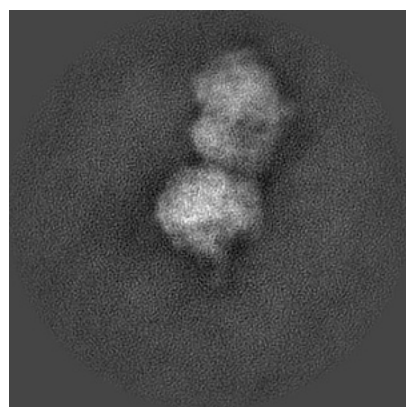


Y

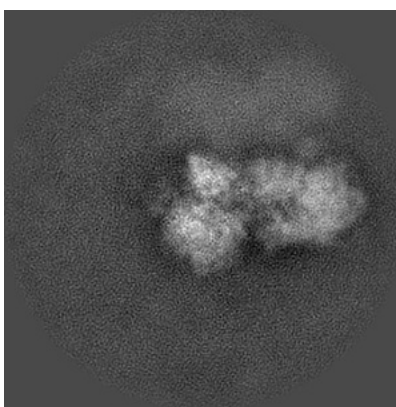


Z

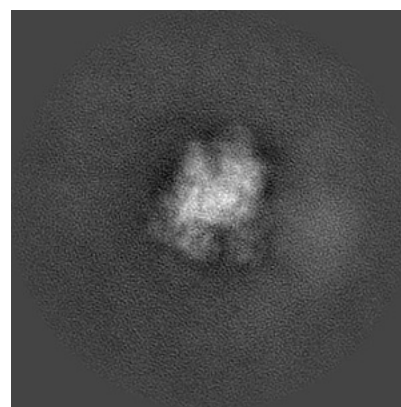
#### 6.1.2 Raw map



X



Y

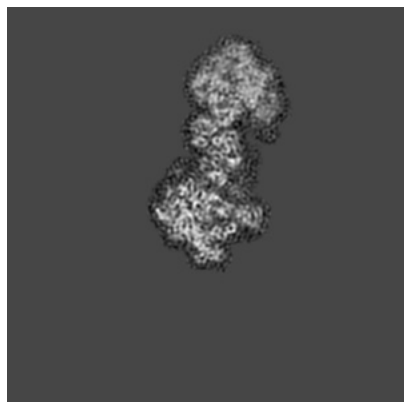


Z

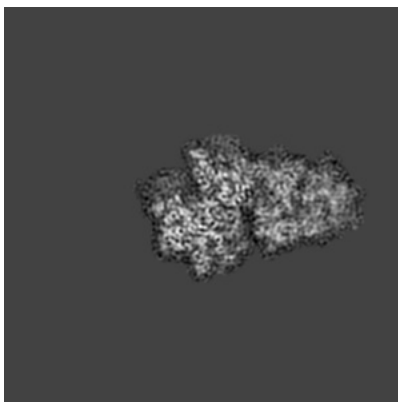
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

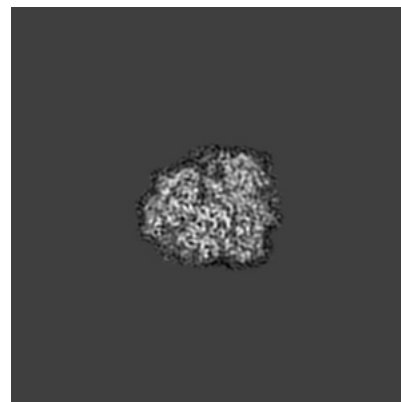
### 6.2.1 Primary map



X Index: 128

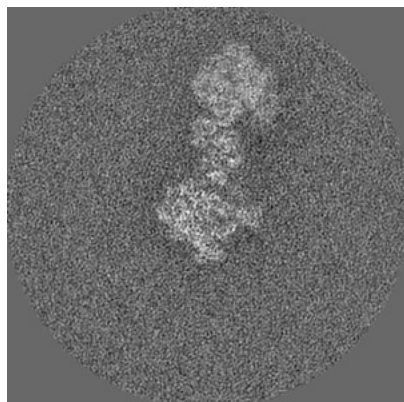


Y Index: 128

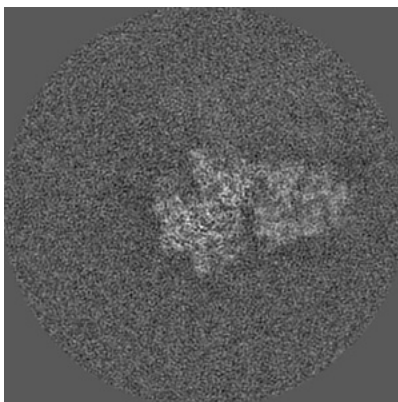


Z Index: 128

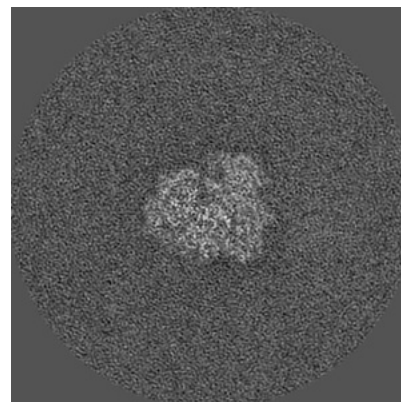
### 6.2.2 Raw map



X Index: 128



Y Index: 128

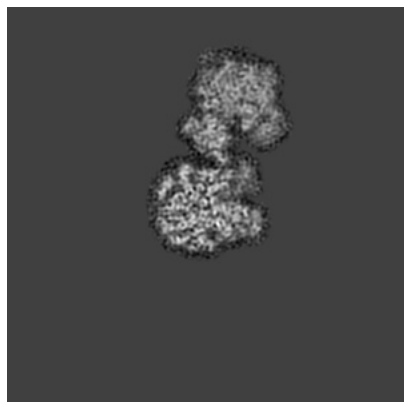


Z Index: 128

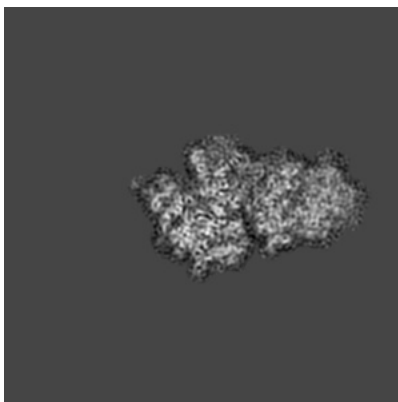
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

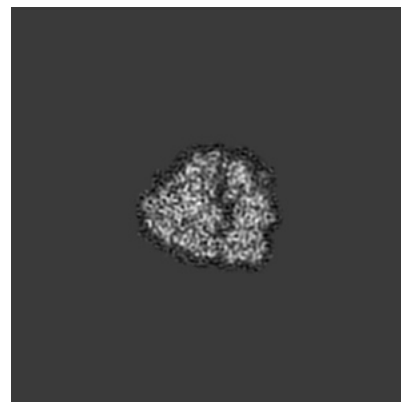
### 6.3.1 Primary map



X Index: 117

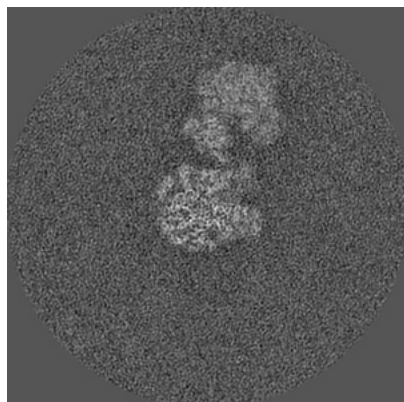


Y Index: 131

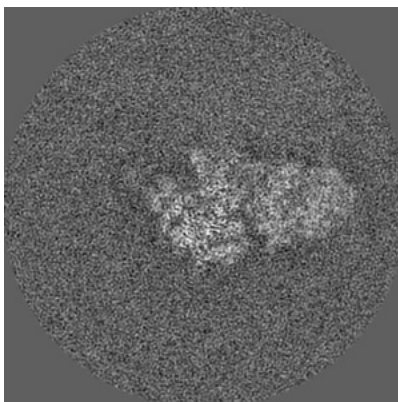


Z Index: 124

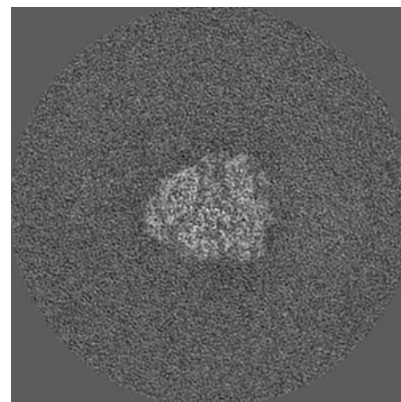
### 6.3.2 Raw map



X Index: 117



Y Index: 131

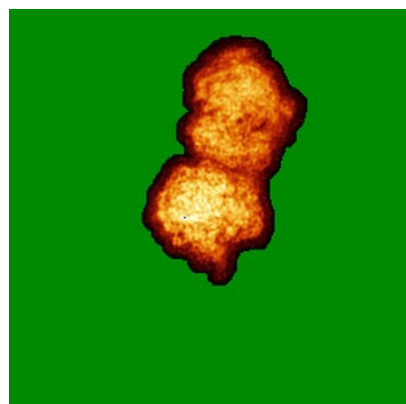


Z Index: 127

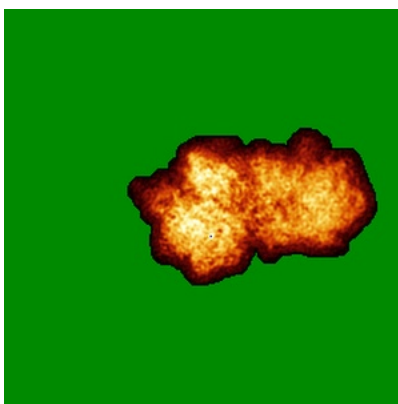
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

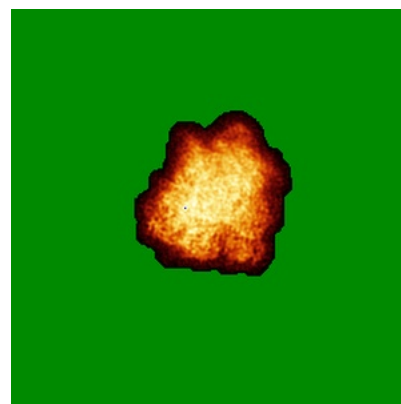
### 6.4.1 Primary map



X

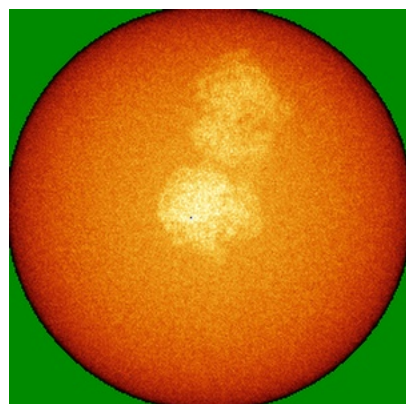


Y

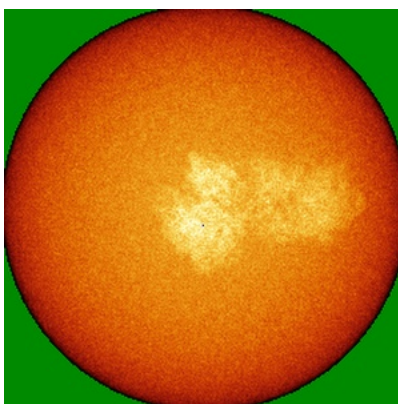


Z

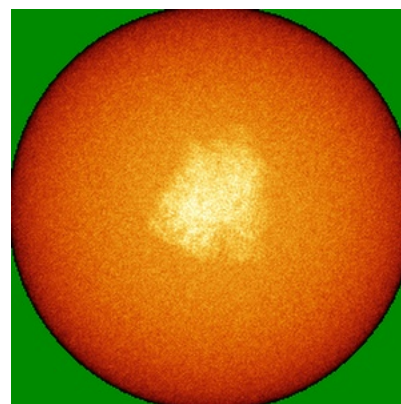
### 6.4.2 Raw map



X



Y



Z

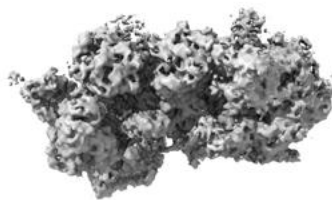
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views [i](#)

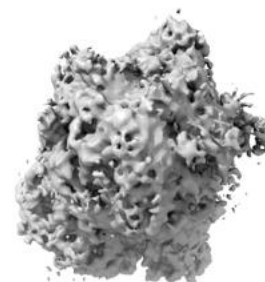
### 6.5.1 Primary map



X



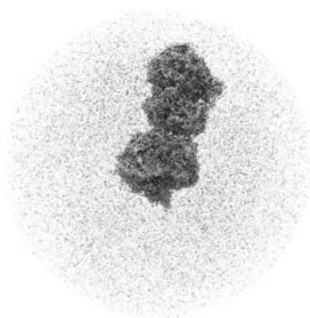
Y



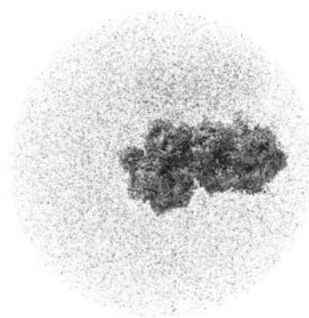
Z

The images above show the 3D surface view of the map at the recommended contour level 1.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

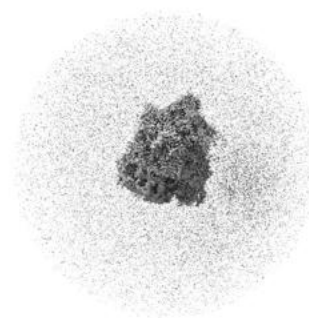
### 6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

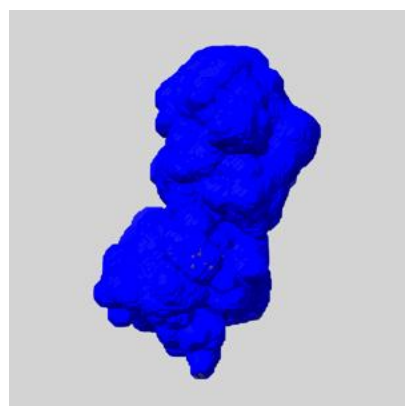
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

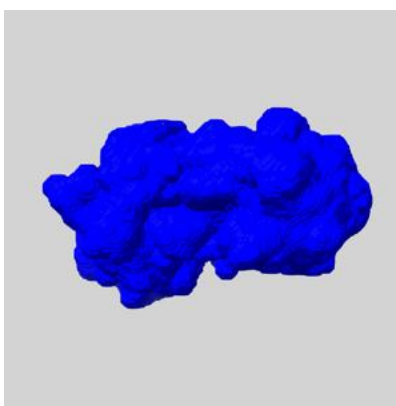
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

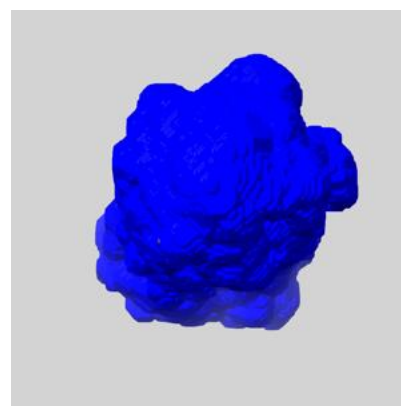
### 6.6.1 emd\_17145\_msk\_1.map [i](#)



X



Y

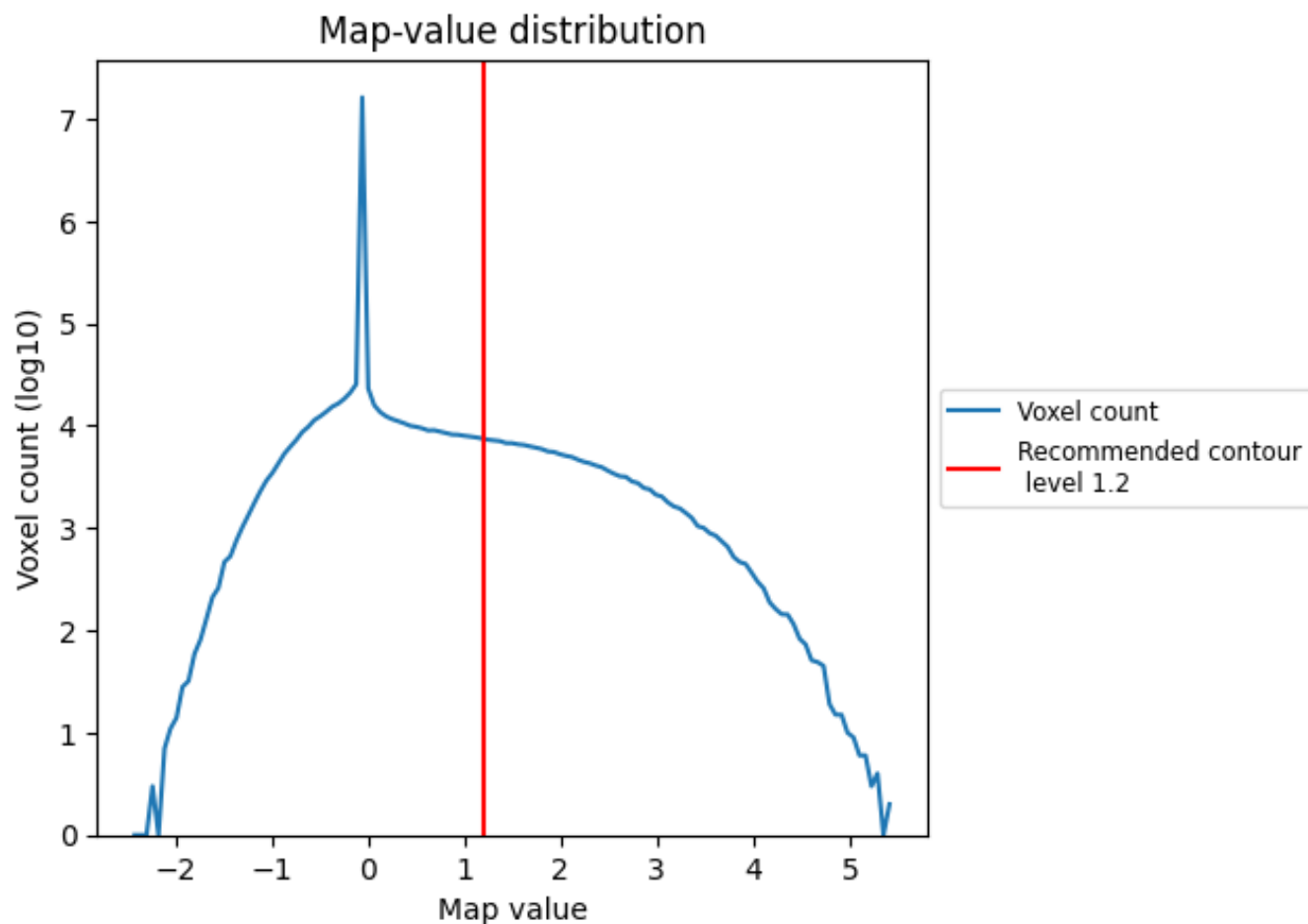


Z

## 7 Map analysis [i](#)

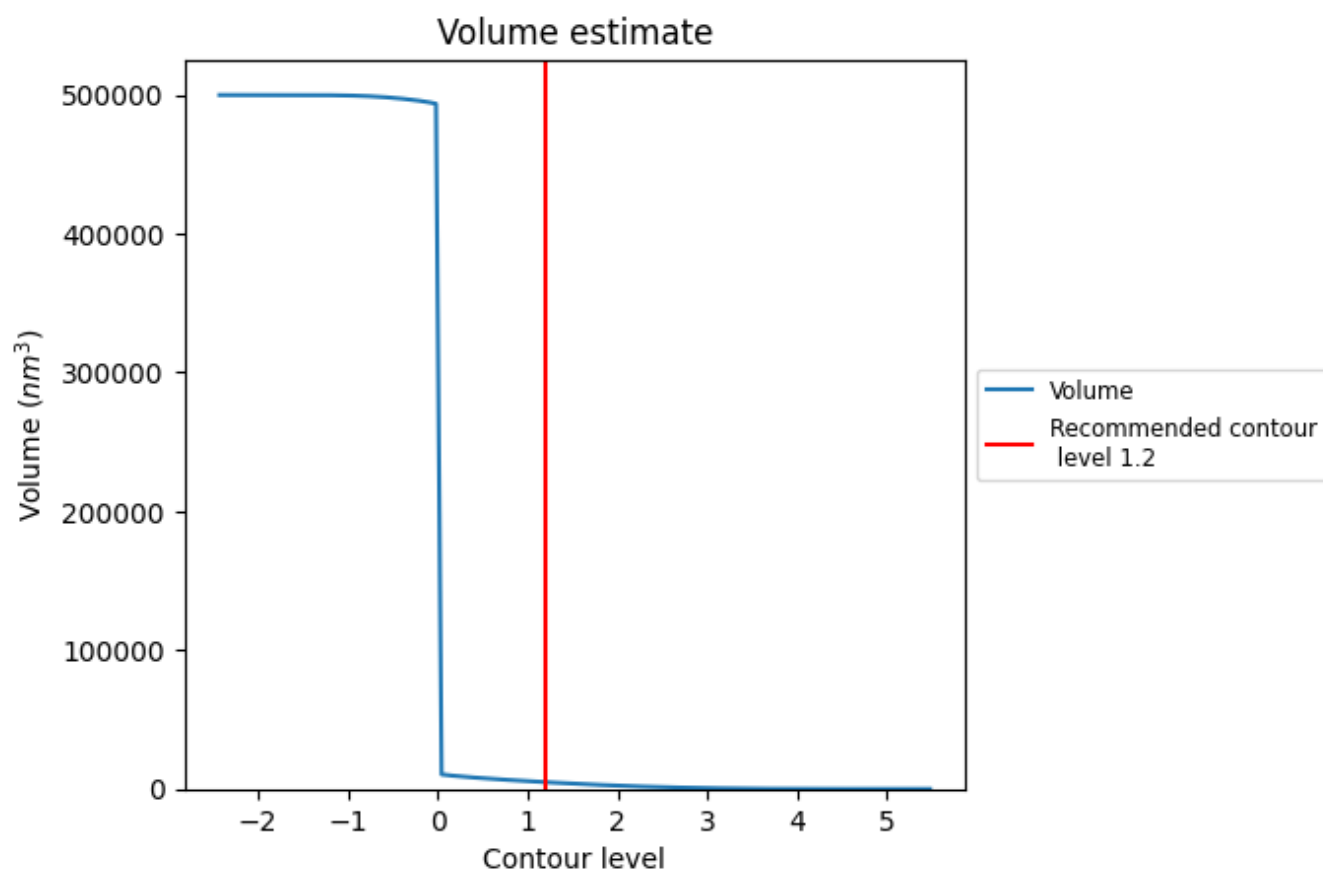
This section contains the results of statistical analysis of the map.

### 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.

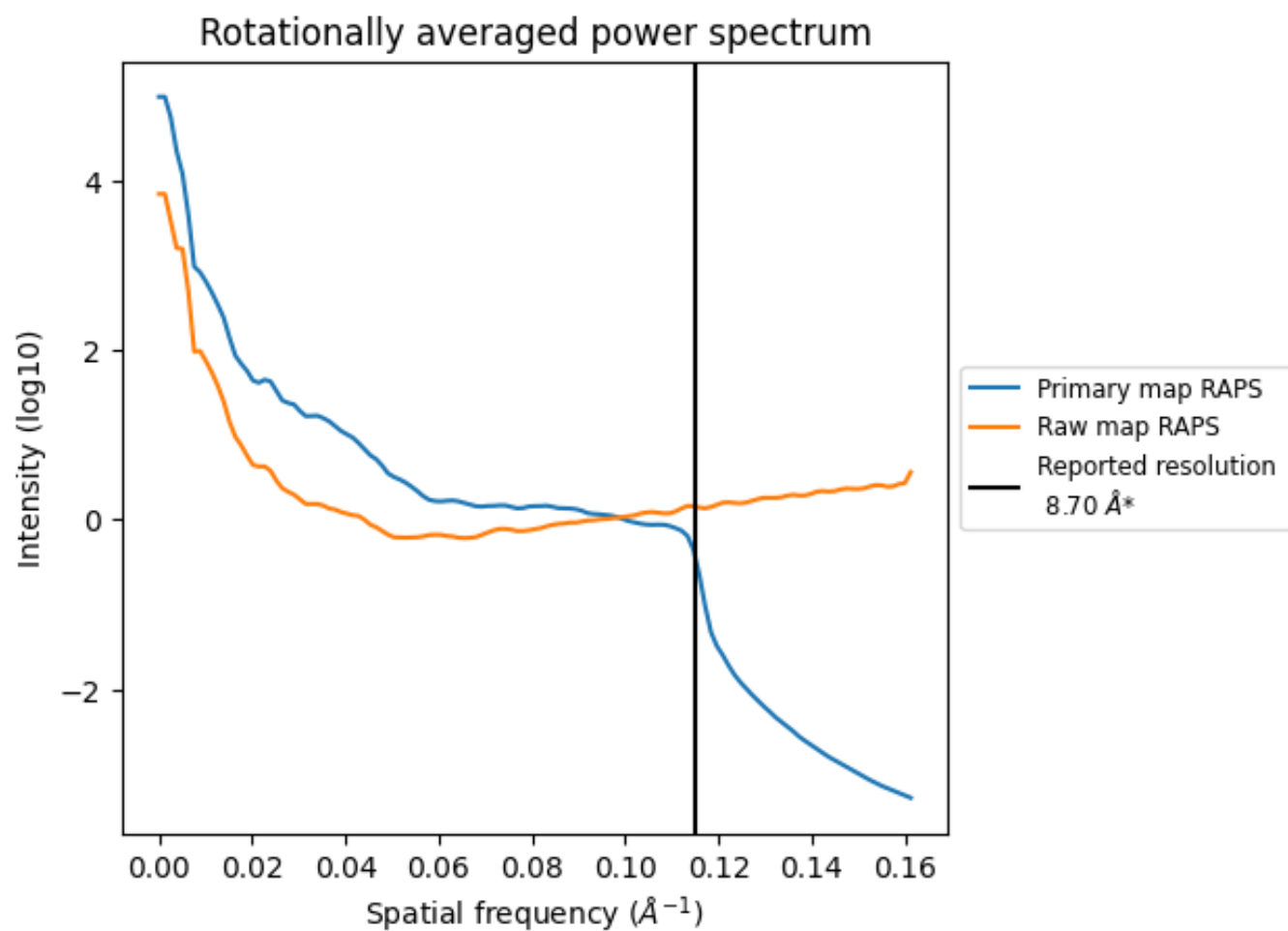
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 4893  $\text{nm}^3$ ; this corresponds to an approximate mass of 4420 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 ⓘ

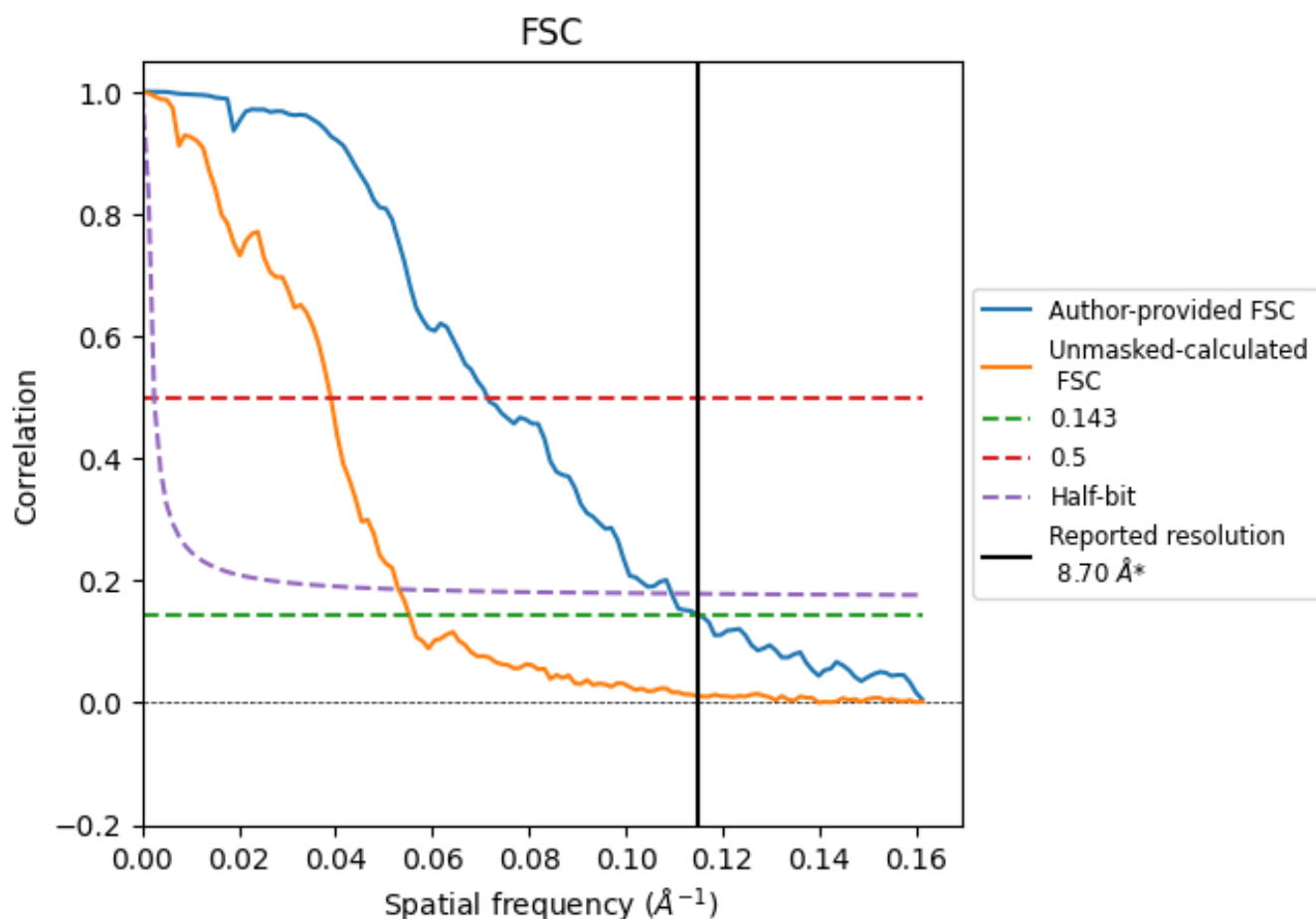


\*Reported resolution corresponds to spatial frequency of 0.115  $\text{\AA}^{-1}$

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.115  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

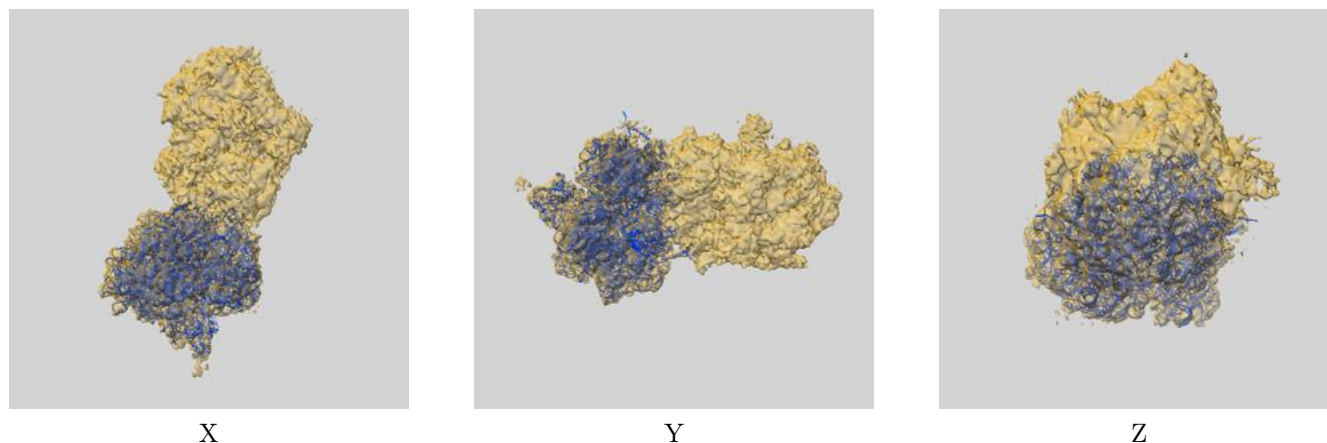
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |       |          |
|---------------------------|------------------------------------|-------|----------|
|                           | 0.143                              | 0.5   | Half-bit |
| Reported by author        | 8.70                               | -     | -        |
| Author-provided FSC curve | 8.68                               | 14.01 | 9.13     |
| Unmasked-calculated*      | 18.08                              | 25.71 | 18.83    |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 18.08 differs from the reported value 8.7 by more than 10 %

## 9 Map-model fit [i](#)

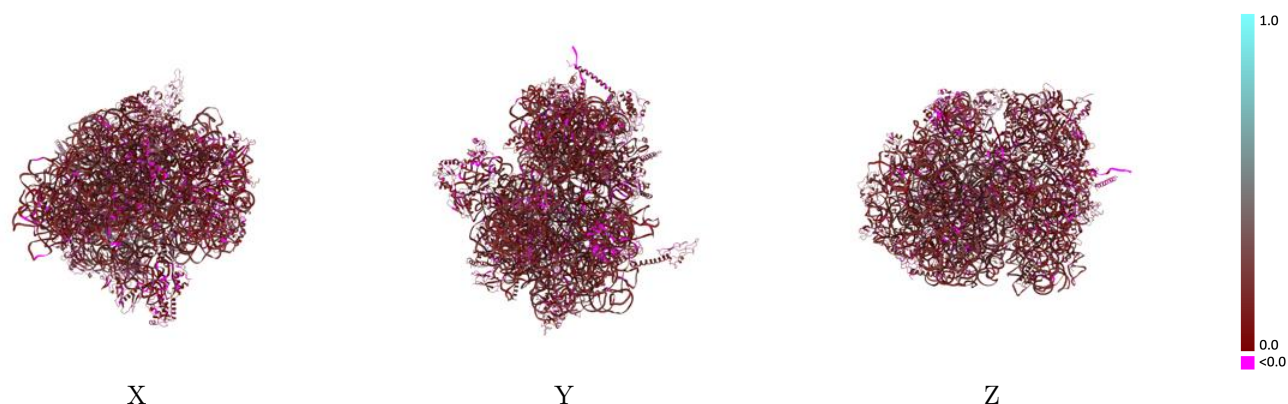
This section contains information regarding the fit between EMDB map EMD-17145 and PDB model 8P8V. Per-residue inclusion information can be found in section [3](#) on page [18](#).

### 9.1 Map-model overlay [i](#)



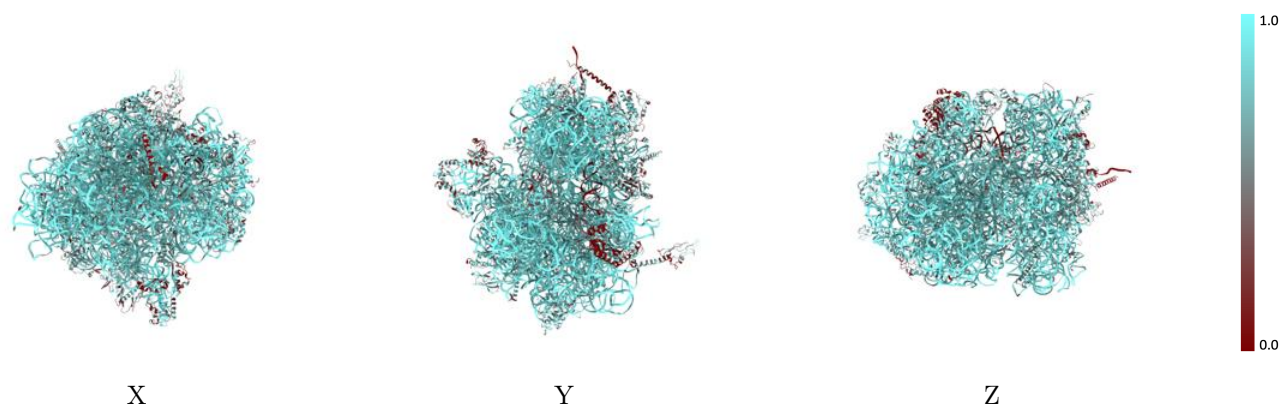
The images above show the 3D surface view of the map at the recommended contour level 1.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)



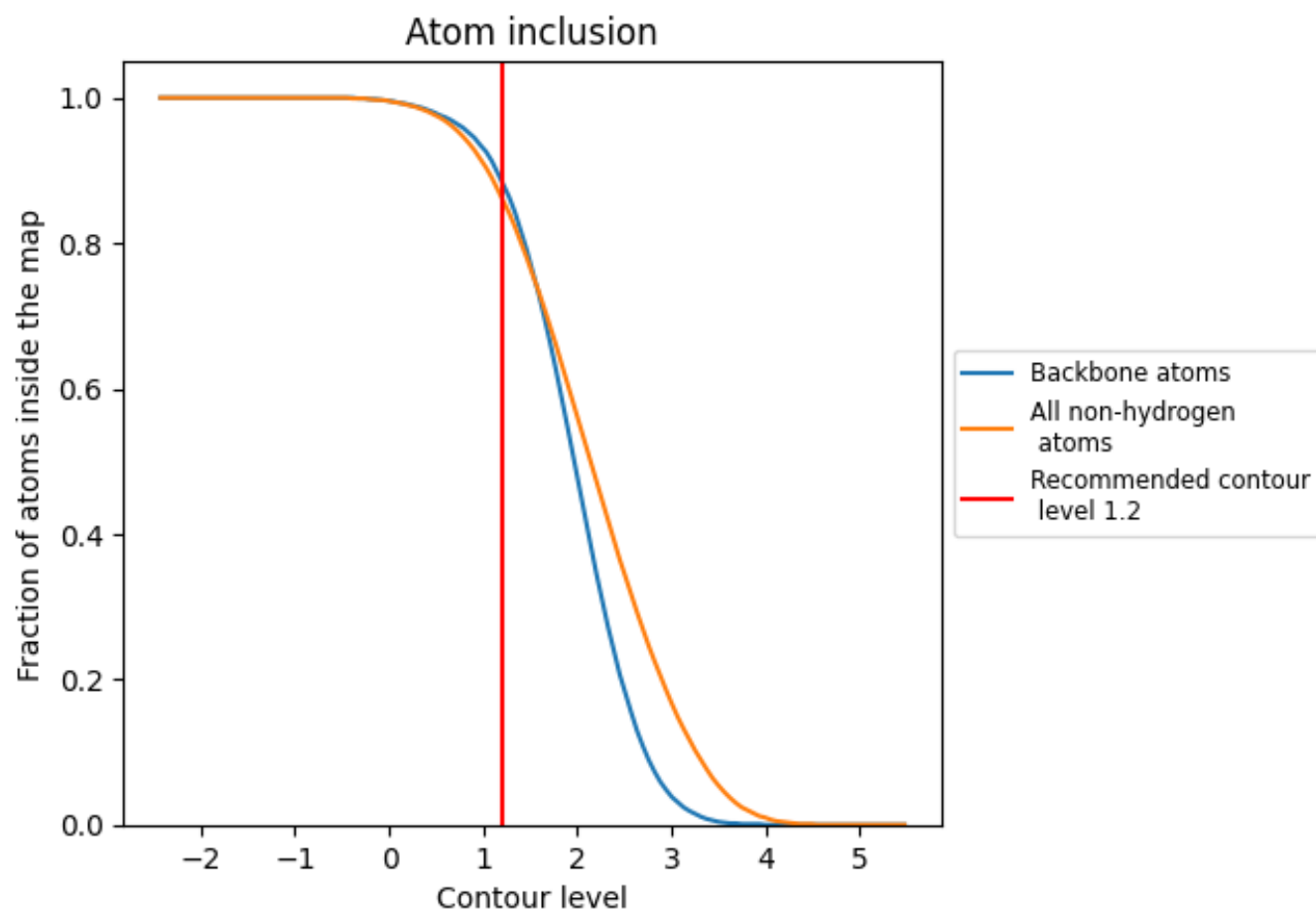
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.2).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 86% 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 (1.2) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.8620   |  0.1410   |
| 0     |  0.8790   |  0.1210   |
| 1     |  0.8050   |  0.1100   |
| 2     |  0.8250   |  0.0770   |
| 3     |  0.9670   |  0.1560   |
| 4     |  0.9660   |  0.1580   |
| 5     |  0.9610   |  0.1540   |
| 6     |  0.4120   |  0.0900   |
| 7     |  0.9360   |  0.1530   |
| 8     |  0.7940   |  0.1540   |
| 9     |  0.1110   |  0.0370   |
| A     |  0.6140   |  0.1390   |
| B     |  0.7110   |  0.1250   |
| C     |  0.6850   |  0.1130   |
| D     |  0.6690  |  0.1170  |
| E     |  0.5570 |  0.1310 |
| F     |  0.7200 |  0.1370 |
| G     |  0.7170 |  0.1230 |
| H     |  0.7390 |  0.0960 |
| I     |  0.6440 |  0.0920 |
| J     |  0.5920 |  0.0980 |
| K     |  0.7840 |  0.1280 |
| L     |  0.7260 |  0.1310 |
| M     |  0.8000 |  0.1130 |
| N     |  0.7850 |  0.1540 |
| O     |  0.7800 |  0.1100 |
| P     |  0.6880 |  0.1210 |
| Q     |  0.6090 |  0.1400 |
| R     |  0.7520 |  0.1000 |
| S     |  0.7930 |  0.1330 |
| T     |  0.6920 |  0.1580 |
| X     |  0.4890 |  0.1050 |
| Y     |  0.5720 |  0.0990 |
| Z     |  0.4330 |  0.0540 |
| a     |  0.7790 |  0.1030 |



*Continued on next page...*

*Continued from previous page...*

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| b     |  0.7210   |  0.0960   |
| c     |  0.7490   |  0.1230   |
| d     |  0.6910   |  0.1180   |
| e     |  0.6440   |  0.1270   |
| f     |  0.5230   |  0.1390   |
| g     |  0.6170   |  0.0990   |
| h     |  0.3690   |  0.0540   |
| i     |  0.7920   |  0.1160   |
| j     |  0.6980   |  0.1170   |
| k     |  0.7500   |  0.1210   |
| l     |  0.7860   |  0.1190   |
| m     |  0.8060   |  0.1090   |
| n     |  0.8000   |  0.1200   |
| o     |  0.7350   |  0.1280   |
| p     |  0.8070   |  0.1270   |
| q     |  0.7550   |  0.1180   |
| r     |  0.8050   |  0.1380   |
| s     |  0.7240  |  0.1220  |
| t     |  0.6840 |  0.1210 |
| u     |  0.7410 |  0.0790 |
| v     |  0.7970 |  0.1030 |
| w     |  0.6800 |  0.1620 |
| x     |  0.4950 |  0.1020 |
| y     |  0.8050 |  0.0930 |
| z     |  0.8440 |  0.1260 |