



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 02:46 AM UTC

PDB ID : 4V97 / pdb\_00004v97  
Title : Crystal structure of the bacterial ribosome ram mutation G299A.  
Authors : Fagan, C.E.; Dunkle, J.A.; Maehigashi, T.; Dunham, C.M.  
Deposited on : 2012-04-06  
Resolution : 3.52 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

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:

|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                                             |
| Mogul                          | : | 2022.3.0, CSD as543be (2022)                                     |
| Xtriage (Phenix)               | : | 2.0                                                              |
| EDS                            | : | 3.0                                                              |
| Buster-report                  | : | wwPDB partial adaption of 1.1.7 (2018)                           |
| Percentile statistics          | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| CCP4                           | : | 9.0.010 (Gargrove)                                               |
| Density-Fitness                | : | 1.0.12                                                           |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.49                                                             |

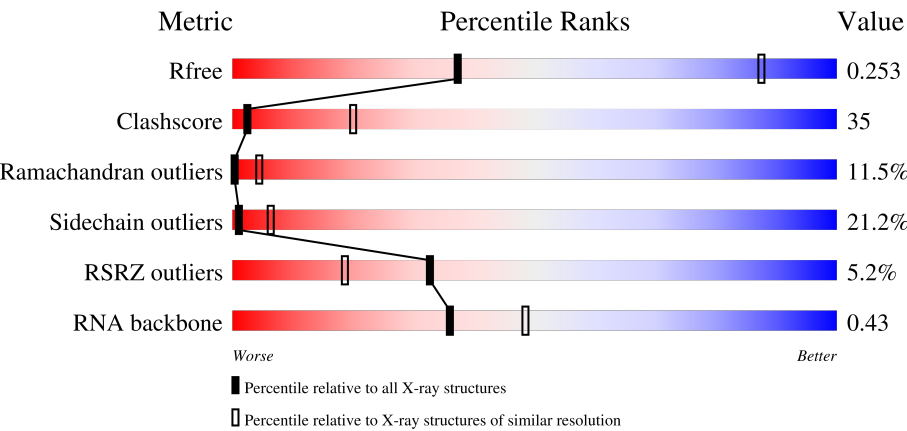
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.52 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.



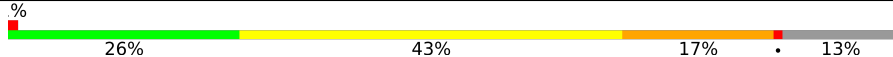
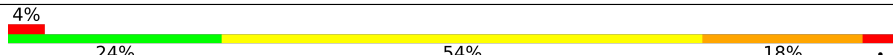
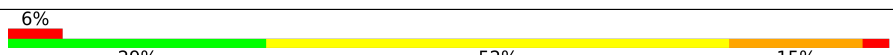
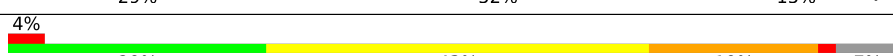
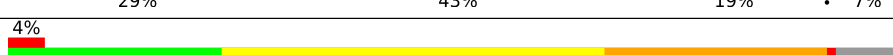
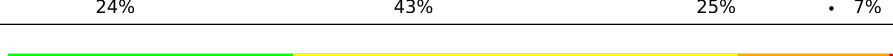
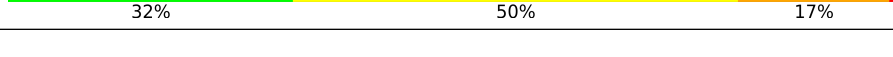
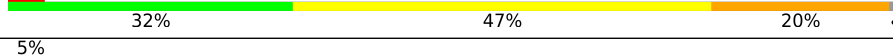
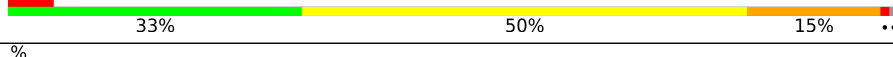
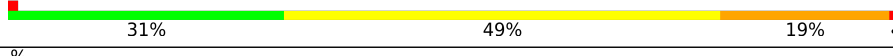
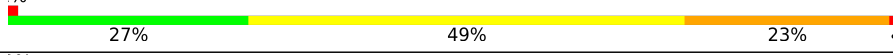
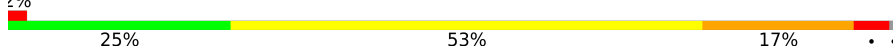
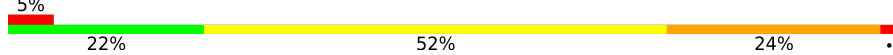
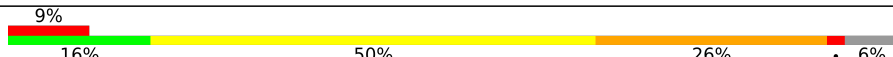
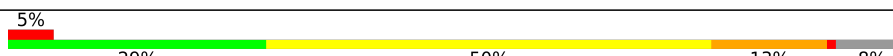
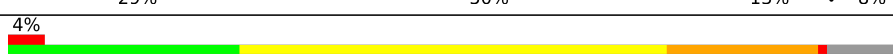
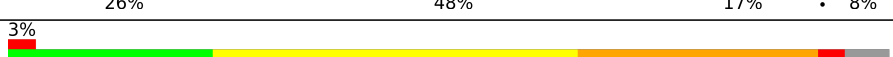
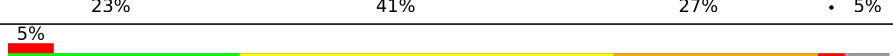
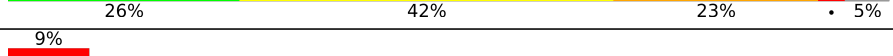
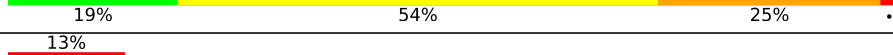
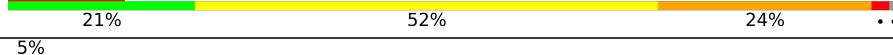
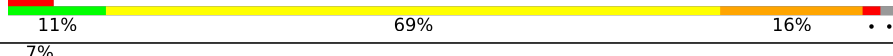
| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| R <sub>free</sub>     | 180053                      | 1025 (3.56-3.48)                                      |
| Clashscore            | 190562                      | 1079 (3.56-3.48)                                      |
| Ramachandran outliers | 187476                      | 1052 (3.56-3.48)                                      |
| Sidechain outliers    | 187428                      | 1053 (3.56-3.48)                                      |
| RSRZ outliers         | 180081                      | 1024 (3.56-3.48)                                      |
| RNA backbone          | 3983                        | 1018 (4.00-3.04)                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain                                                                                                  |
|-----|-------|--------|-------------------------------------------------------------------------------------------------------------------|
| 1   | AA    | 1522   | <div><div>5%</div><div><div></div><div>49%</div><div>35%</div><div>15%</div><div>.</div></div></div>              |
| 1   | CA    | 1522   | <div><div>5%</div><div><div></div><div>49%</div><div>34%</div><div>16%</div><div>.</div></div></div>              |
| 2   | AB    | 256    | <div><div>2%</div><div><div></div><div>20%</div><div>50%</div><div>20%</div><div>8%</div><div>.</div></div></div> |
| 2   | CB    | 256    | <div><div>2%</div><div><div></div><div>16%</div><div>50%</div><div>23%</div><div>8%</div><div>.</div></div></div> |

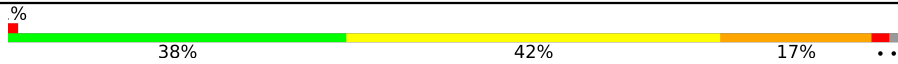
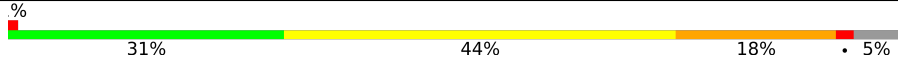
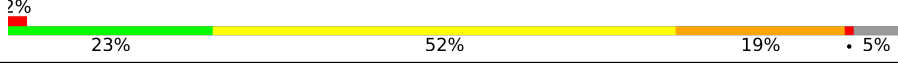
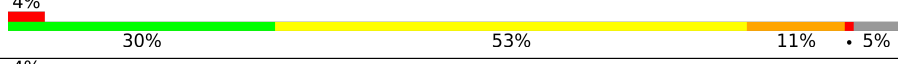
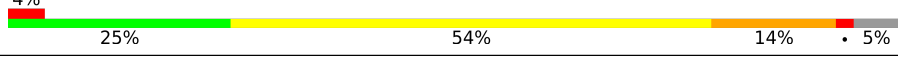
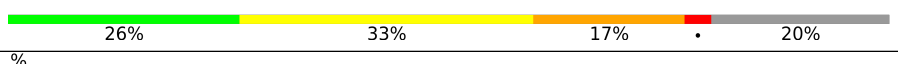
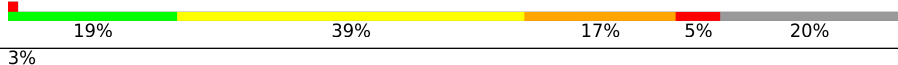
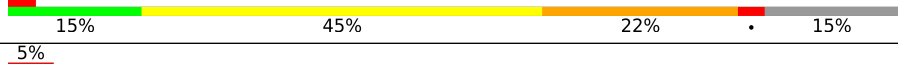
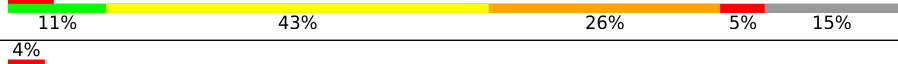
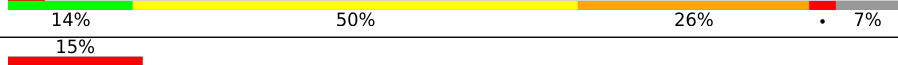
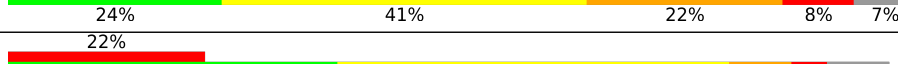
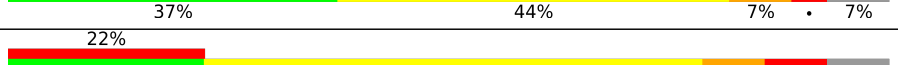
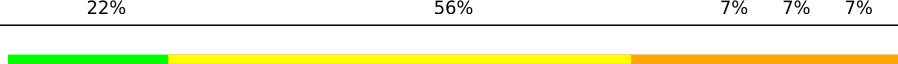
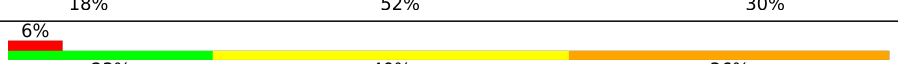
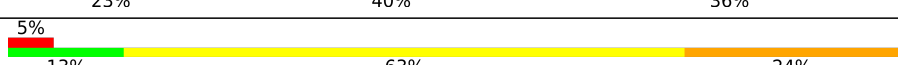
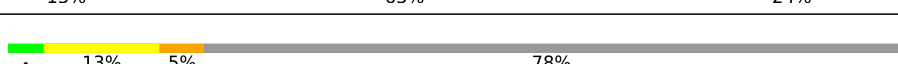
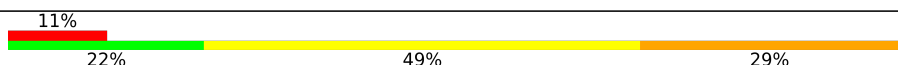
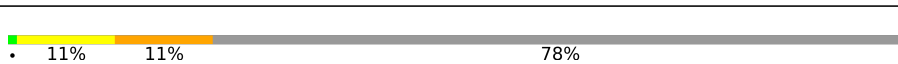
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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 3   | AC    | 239    |    |
| 3   | CC    | 239    |    |
| 4   | AD    | 209    |    |
| 4   | CD    | 209    |    |
| 5   | AE    | 162    |    |
| 5   | CE    | 162    |    |
| 6   | AF    | 101    |    |
| 6   | CF    | 101    |    |
| 7   | AG    | 156    |    |
| 7   | CG    | 156    |    |
| 8   | AH    | 138    |    |
| 8   | CH    | 138    |    |
| 9   | AI    | 128    |   |
| 9   | CI    | 128    |  |
| 10  | AJ    | 105    |  |
| 10  | CJ    | 105    |  |
| 11  | AK    | 129    |  |
| 11  | CK    | 129    |  |
| 12  | AL    | 132    |  |
| 12  | CL    | 132    |  |
| 13  | AM    | 126    |  |
| 13  | CM    | 126    |  |
| 14  | AN    | 61     |  |
| 14  | CN    | 61     |  |
| 15  | AO    | 89     |  |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 15  | CO    | 89     |    |
| 16  | AP    | 88     |    |
| 16  | CP    | 88     |    |
| 17  | AQ    | 105    |    |
| 17  | CQ    | 105    |    |
| 18  | AR    | 88     |    |
| 18  | CR    | 88     |    |
| 19  | AS    | 93     |    |
| 19  | CS    | 93     |    |
| 20  | AT    | 106    |    |
| 20  | CT    | 106    |    |
| 21  | AU    | 27     |   |
| 21  | CU    | 27     |  |
| 22  | AV    | 77     |  |
| 22  | CV    | 77     |  |
| 23  | AW    | 76     |  |
| 23  | AY    | 76     |  |
| 23  | CW    | 76     |  |
| 23  | CY    | 76     |  |
| 24  | AX    | 24     |  |
| 24  | CX    | 24     |  |
| 25  | BA    | 2915   |  |
| 25  | DA    | 2915   |  |
| 26  | BB    | 122    |  |
| 26  | DB    | 122    |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 27  | BC    | 229    |                  |
| 27  | DC    | 229    |                  |
| 28  | BD    | 276    |                  |
| 28  | DD    | 276    |                  |
| 29  | BE    | 206    |                  |
| 29  | DE    | 206    |                  |
| 30  | BF    | 210    |                  |
| 30  | DF    | 210    |                  |
| 31  | BG    | 182    |                  |
| 31  | DG    | 182    |                  |
| 32  | BH    | 180    |                  |
| 32  | DH    | 180    |                  |
| 33  | BI    | 148    |                  |
| 33  | DI    | 148    |                  |
| 34  | BN    | 140    |                  |
| 34  | DN    | 140    |                  |
| 35  | BO    | 122    |                  |
| 35  | DO    | 122    |                  |
| 36  | BP    | 150    |                  |
| 36  | DP    | 150    |                  |
| 37  | BQ    | 141    |                  |
| 37  | DQ    | 141    |                  |
| 38  | BR    | 118    |                  |
| 38  | DR    | 118    |                  |
| 39  | BS    | 112    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 39  | DS    | 112    |                  |
| 40  | BT    | 146    |                  |
| 40  | DT    | 146    |                  |
| 41  | BU    | 118    |                  |
| 41  | DU    | 118    |                  |
| 42  | BV    | 101    |                  |
| 42  | DV    | 101    |                  |
| 43  | BW    | 113    |                  |
| 43  | DW    | 113    |                  |
| 44  | BX    | 96     |                  |
| 44  | DX    | 96     |                  |
| 45  | BY    | 110    |                  |
| 45  | DY    | 110    |                  |
| 46  | BZ    | 206    |                  |
| 46  | DZ    | 206    |                  |
| 47  | B0    | 85     |                  |
| 47  | D0    | 85     |                  |
| 48  | B1    | 98     |                  |
| 48  | D1    | 98     |                  |
| 49  | B2    | 72     |                  |
| 49  | D2    | 72     |                  |
| 50  | B3    | 60     |                  |
| 50  | D3    | 60     |                  |
| 51  | B4    | 71     |                  |
| 51  | D4    | 71     |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 52  | B5    | 60     |                  |
| 52  | D5    | 60     |                  |
| 53  | B6    | 54     |                  |
| 53  | D6    | 54     |                  |
| 54  | B7    | 49     |                  |
| 54  | D7    | 49     |                  |
| 55  | B8    | 65     |                  |
| 55  | D8    | 65     |                  |
| 56  | B9    | 37     |                  |
| 56  | D9    | 37     |                  |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 57  | MG   | AA    | 7008 | -         | -        | -       | X                |
| 57  | MG   | AA    | 7090 | -         | -        | -       | X                |
| 57  | MG   | BA    | 3101 | -         | -        | -       | X                |
| 57  | MG   | DA    | 9358 | -         | -        | -       | X                |
| 57  | MG   | DA    | 9399 | -         | -        | -       | X                |
| 57  | MG   | DB    | 204  | -         | -        | -       | X                |
| 59  | ZN   | CN    | 101  | -         | -        | X       | -                |

## 2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 293977 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 RNA chain called 16S rRNA.

| Mol | Chain | Residues | Atoms |       |      |       |      | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|---------|-------|
| 1   | AA    | 1504     | Total | C     | N    | O     | P    | 0       | 0       | 0     |
|     |       |          | 32328 | 14390 | 5992 | 10443 | 1503 |         |         |       |
| 1   | CA    | 1504     | Total | C     | N    | O     | P    | 0       | 0       | 0     |
|     |       |          | 32328 | 14390 | 5992 | 10443 | 1503 |         |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment             | Reference     |
|-------|---------|----------|--------|---------------------|---------------|
| AA    | 299     | A        | G      | engineered mutation | GB AP008226.1 |
| CA    | 299     | A        | G      | engineered mutation | GB AP008226.1 |

- Molecule 2 is a protein called 30S ribosomal protein S2.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 2   | AB    | 235      | Total | C    | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 1901  | 1213 | 342 | 341 | 5 |         |         |       |
| 2   | CB    | 235      | Total | C    | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 1901  | 1213 | 342 | 341 | 5 |         |         |       |

- Molecule 3 is a protein called 30S ribosomal protein S3.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 3   | AC    | 207      | Total | C    | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 1613  | 1016 | 315 | 281 | 1 |         |         |       |
| 3   | CC    | 207      | Total | C    | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 1613  | 1016 | 315 | 281 | 1 |         |         |       |

- Molecule 4 is a protein called 30S ribosomal protein S4.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 4   | AD    | 208      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1703  | 1066 | 339 | 291 | 7 |         |         |       |

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| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 4   | CD    | 208      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1703  | 1066 | 339 | 291 | 7 |         |         |       |

- Molecule 5 is a protein called 30S ribosomal protein S5.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 5   | AE    | 151      | Total | C   | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 1147  | 724 | 218 | 201 | 4 |         |         |       |
| 5   | CE    | 151      | Total | C   | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 1147  | 724 | 218 | 201 | 4 |         |         |       |

- Molecule 6 is a protein called 30S ribosomal protein S6.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 6   | AF    | 101      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 843   | 531 | 155 | 154 | 3 |         |         |       |
| 6   | CF    | 101      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 843   | 531 | 155 | 154 | 3 |         |         |       |

- Molecule 7 is a protein called 30S ribosomal protein S7.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 7   | AG    | 155      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1257  | 781 | 252 | 218 | 6 |         |         |       |
| 7   | CG    | 155      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1257  | 781 | 252 | 218 | 6 |         |         |       |

- Molecule 8 is a protein called 30S ribosomal protein S8.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 8   | AH    | 138      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1116  | 705 | 215 | 193 | 3 |         |         |       |
| 8   | CH    | 138      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1116  | 705 | 215 | 193 | 3 |         |         |       |

- Molecule 9 is a protein called 30S ribosomal protein S9.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 9   | AI    | 127      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1010  | 639 | 197 | 174 |         |         |       |
| 9   | CI    | 127      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1010  | 639 | 197 | 174 |         |         |       |

- Molecule 10 is a protein called 30S ribosomal protein S10.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10  | AJ    | 99       | Total | C   | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 795   | 499 | 157 | 138 | 1 |         |         |       |
| 10  | CJ    | 99       | Total | C   | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 795   | 499 | 157 | 138 | 1 |         |         |       |

- Molecule 11 is a protein called 30S ribosomal protein S11.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 11  | AK    | 119      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 885   | 549 | 168 | 165 | 3 |         |         |       |
| 11  | CK    | 119      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 885   | 549 | 168 | 165 | 3 |         |         |       |

- Molecule 12 is a protein called 30S ribosomal protein S12.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 12  | AL    | 125      | Total | C   | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 971   | 611 | 196 | 163 | 1 |         |         |       |
| 12  | CL    | 125      | Total | C   | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 971   | 611 | 196 | 163 | 1 |         |         |       |

- Molecule 13 is a protein called 30S ribosomal protein S13.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 13  | AM    | 125      | Total | C   | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 988   | 611 | 206 | 169 | 2 |         |         |       |
| 13  | CM    | 125      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 997   | 617 | 207 | 171 | 2 |         |         |       |

- Molecule 14 is a protein called 30S ribosomal protein S14 type Z.

| Mol | Chain | Residues | Atoms |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 14  | AN    | 60       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 492   | 312 | 104 | 72 | 4 |         |         |       |
| 14  | CN    | 60       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 492   | 312 | 104 | 72 | 4 |         |         |       |

- Molecule 15 is a protein called 30S ribosomal protein S15.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 15  | AO    | 88       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 734   | 459 | 147 | 126 | 2 |         |         |       |
| 15  | CO    | 88       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 734   | 459 | 147 | 126 | 2 |         |         |       |

- Molecule 16 is a protein called 30S ribosomal protein S16.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 16  | AP    | 84       | Total | C   | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 701   | 443 | 140 | 117 | 1 |         |         |       |
| 16  | CP    | 84       | Total | C   | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 701   | 443 | 140 | 117 | 1 |         |         |       |

- Molecule 17 is a protein called 30S ribosomal protein S17.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 17  | AQ    | 100      | Total | C   | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 824   | 528 | 152 | 142 | 2 |         |         |       |
| 17  | CQ    | 100      | Total | C   | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 824   | 528 | 152 | 142 | 2 |         |         |       |

- Molecule 18 is a protein called 30S ribosomal protein S18.

| Mol | Chain | Residues | Atoms |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---------|---------|-------|
| 18  | AR    | 70       | Total | C   | N   | O  | 0       | 0       | 0     |
|     |       |          | 574   | 367 | 112 | 95 |         |         |       |
| 18  | CR    | 70       | Total | C   | N   | O  | 0       | 0       | 0     |
|     |       |          | 574   | 367 | 112 | 95 |         |         |       |

- Molecule 19 is a protein called 30S ribosomal protein S19.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 19  | AS    | 79       | Total | C   | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 630   | 403 | 115 | 110 | 2 |         |         |       |
| 19  | CS    | 79       | Total | C   | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 630   | 403 | 115 | 110 | 2 |         |         |       |

- Molecule 20 is a protein called 30S ribosomal protein S20.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 20  | AT    | 99       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 763   | 470 | 162 | 129 | 2 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 20  | CT    | 99       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 763   | 470 | 162 | 129 | 2 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 21  | AU    | 25       | Total | C   | N  | O  | 0       | 0       | 1     |
|     |       |          | 209   | 128 | 51 | 30 |         |         |       |
| 21  | CU    | 25       | Total | C   | N  | O  | 0       | 0       | 1     |
|     |       |          | 209   | 128 | 51 | 30 |         |         |       |

- Molecule 22 is a RNA chain called P-SITE tRNA fMet.

| Mol | Chain | Residues | Atoms |     |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 22  | AV    | 77       | Total | C   | N   | O   | P  | 0       | 0       | 0     |
|     |       |          | 1644  | 732 | 297 | 538 | 77 |         |         |       |
| 22  | CV    | 77       | Total | C   | N   | O   | P  | 0       | 0       | 0     |
|     |       |          | 1643  | 732 | 297 | 537 | 77 |         |         |       |

- Molecule 23 is a RNA chain called E-SITE TRNA PHE OR A-SITE tRNA Phe.

| Mol | Chain | Residues | Atoms |     |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 23  | AW    | 76       | Total | C   | N   | O   | P  | 0       | 0       | 0     |
|     |       |          | 1619  | 723 | 290 | 531 | 75 |         |         |       |
| 23  | AY    | 17       | Total | C   | N   | O   | P  | 0       | 0       | 0     |
|     |       |          | 365   | 163 | 68  | 117 | 17 |         |         |       |
| 23  | CW    | 76       | Total | C   | N   | O   | P  | 0       | 0       | 0     |
|     |       |          | 1619  | 723 | 290 | 531 | 75 |         |         |       |
| 23  | CY    | 17       | Total | C   | N   | O   | P  | 0       | 0       | 0     |
|     |       |          | 365   | 163 | 68  | 117 | 17 |         |         |       |

- Molecule 24 is a RNA chain called mRNA.

| Mol | Chain | Residues | Atoms |     |    |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|----|---------|---------|-------|
| 24  | AX    | 12       | Total | C   | N  | O  | P  | 0       | 0       | 0     |
|     |       |          | 255   | 115 | 46 | 82 | 12 |         |         |       |
| 24  | CX    | 10       | Total | C   | N  | O  | P  | 0       | 0       | 0     |
|     |       |          | 210   | 96  | 39 | 66 | 9  |         |         |       |

- Molecule 25 is a RNA chain called 23S rRNA.

| Mol | Chain | Residues | Atoms |       |       |       |      | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|---------|-------|
| 25  | BA    | 2810     | Total | C     | N     | O     | P    | 0       | 0       | 0     |
|     |       |          | 60527 | 26937 | 11326 | 19455 | 2809 |         |         |       |
| 25  | DA    | 2824     | Total | C     | N     | O     | P    | 0       | 0       | 0     |
|     |       |          | 60827 | 27071 | 11381 | 19552 | 2823 |         |         |       |

- Molecule 26 is a RNA chain called 5S rRNA.

| Mol | Chain | Residues | Atoms |      |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|---------|-------|
| 26  | BB    | 119      | Total | C    | N   | O   | P   | 0       | 0       | 0     |
|     |       |          | 2551  | 1136 | 471 | 826 | 118 |         |         |       |
| 26  | DB    | 119      | Total | C    | N   | O   | P   | 0       | 0       | 0     |
|     |       |          | 2551  | 1136 | 471 | 826 | 118 |         |         |       |

- Molecule 27 is a protein called 50S RIBOSOMAL PROTEIN L1.

| Mol | Chain | Residues | Atoms |     |     |     |  | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 27  | BC    | 191      | Total | C   | N   | O   |  | 0       | 0       | 1     |
|     |       |          | 1142  | 691 | 221 | 230 |  |         |         |       |
| 27  | DC    | 191      | Total | C   | N   | O   |  | 0       | 0       | 1     |
|     |       |          | 1142  | 691 | 221 | 230 |  |         |         |       |

- Molecule 28 is a protein called 50S RIBOSOMAL PROTEIN L2.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 28  | BD    | 272      | Total | C    | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 2105  | 1329 | 417 | 356 | 3 |         |         |       |
| 28  | DD    | 272      | Total | C    | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 2105  | 1329 | 417 | 356 | 3 |         |         |       |

- Molecule 29 is a protein called 50S RIBOSOMAL PROTEIN L3.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 29  | BE    | 205      | Total | C   | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 1564  | 988 | 300 | 270 | 6 |         |         |       |
| 29  | DE    | 205      | Total | C   | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 1564  | 988 | 300 | 270 | 6 |         |         |       |

- Molecule 30 is a protein called 50S RIBOSOMAL PROTEIN L4.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 30  | BF    | 208      | Total | C    | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 1624  | 1035 | 304 | 282 | 3 |         |         |       |

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| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 30  | DF    | 202      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1585  | 1011 | 297 | 275 | 2 |         |         |       |

- Molecule 31 is a protein called 50S RIBOSOMAL PROTEIN L5.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 31  | BG    | 181      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1474  | 942 | 268 | 260 | 4 |         |         |       |
| 31  | DG    | 181      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1474  | 942 | 268 | 260 | 4 |         |         |       |

- Molecule 32 is a protein called 50S RIBOSOMAL PROTEIN L6.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 32  | BH    | 160      | Total | C   | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 1223  | 773 | 229 | 220 | 1 |         |         |       |
| 32  | DH    | 168      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1290  | 820 | 240 | 229 | 1 |         |         |       |

- Molecule 33 is a protein called 50S RIBOSOMAL PROTEIN L9.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 33  | BI    | 145      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1131  | 723 | 200 | 207 | 1 |         |         |       |
| 33  | DI    | 146      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1136  | 726 | 201 | 208 | 1 |         |         |       |

- Molecule 34 is a protein called 50S RIBOSOMAL PROTEIN L13.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 34  | BN    | 139      | Total | C   | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 1105  | 712 | 207 | 182 | 4 |         |         |       |
| 34  | DN    | 139      | Total | C   | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 1105  | 712 | 207 | 182 | 4 |         |         |       |

- Molecule 35 is a protein called 50S RIBOSOMAL PROTEIN L14.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 35  | BO    | 122      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 933   | 588 | 171 | 170 | 4 |         |         |       |
| 35  | DO    | 122      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 933   | 588 | 171 | 170 | 4 |         |         |       |

- Molecule 36 is a protein called 50S RIBOSOMAL PROTEIN L15.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 36  | BP    | 150      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1145  | 712 | 232 | 198 | 3 |         |         |       |
| 36  | DP    | 150      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1145  | 712 | 232 | 198 | 3 |         |         |       |

- Molecule 37 is a protein called 50S RIBOSOMAL PROTEIN L16.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 37  | BQ    | 141      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1122  | 715 | 212 | 188 | 7 |         |         |       |
| 37  | DQ    | 141      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1122  | 715 | 212 | 188 | 7 |         |         |       |

- Molecule 38 is a protein called 50S RIBOSOMAL PROTEIN L17.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 38  | BR    | 117      | Total | C   | N   | O   |   | 0       | 0       | 0     |
|     |       |          | 960   | 599 | 202 | 159 |   |         |         |       |
| 38  | DR    | 118      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 968   | 604 | 203 | 160 | 1 |         |         |       |

- Molecule 39 is a protein called 50S RIBOSOMAL PROTEIN L18.

| Mol | Chain | Residues | Atoms |     |     |     |  | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 39  | BS    | 99       | Total | C   | N   | O   |  | 0       | 0       | 1     |
|     |       |          | 771   | 486 | 155 | 130 |  |         |         |       |
| 39  | DS    | 111      | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 882   | 556 | 176 | 150 |  |         |         |       |

- Molecule 40 is a protein called 50S RIBOSOMAL PROTEIN L19.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 40  | BT    | 138      | Total | C   | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 1142  | 710 | 235 | 196 | 1 |         |         |       |
| 40  | DT    | 138      | Total | C   | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 1142  | 710 | 235 | 196 | 1 |         |         |       |

- Molecule 41 is a protein called 50S RIBOSOMAL PROTEIN L20.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 41  | BU    | 117      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 964   | 610 | 202 | 151 | 1 |         |         |       |
| 41  | DU    | 117      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 958   | 604 | 202 | 151 | 1 |         |         |       |

- Molecule 42 is a protein called 50S RIBOSOMAL PROTEIN L21.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 42  | BV    | 101      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 779   | 501 | 142 | 135 | 1 |         |         |       |
| 42  | DV    | 101      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 779   | 501 | 142 | 135 | 1 |         |         |       |

- Molecule 43 is a protein called 50S RIBOSOMAL PROTEIN L22.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 43  | BW    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 896   | 563 | 176 | 155 | 2 |         |         |       |
| 43  | DW    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 896   | 563 | 176 | 155 | 2 |         |         |       |

- Molecule 44 is a protein called 50S RIBOSOMAL PROTEIN L23.

| Mol | Chain | Residues | Atoms |     |     |     |  | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 44  | BX    | 93       | Total | C   | N   | O   |  | 0       | 0       | 1     |
|     |       |          | 726   | 471 | 132 | 123 |  |         |         |       |
| 44  | DX    | 93       | Total | C   | N   | O   |  | 0       | 0       | 1     |
|     |       |          | 726   | 471 | 132 | 123 |  |         |         |       |

- Molecule 45 is a protein called 50S RIBOSOMAL PROTEIN L24.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 45  | BY    | 101      | Total | C   | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 776   | 500 | 149 | 123 | 4 |         |         |       |
| 45  | DY    | 102      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 785   | 505 | 150 | 125 | 5 |         |         |       |

- Molecule 46 is a protein called 50S RIBOSOMAL PROTEIN L25.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 46  | BZ    | 177      | Total | C   | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 1404  | 897 | 253 | 252 | 2 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 46  | DZ    | 177      | Total | C   | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 1404  | 897 | 253 | 252 | 2 |         |         |       |

- Molecule 47 is a protein called 50S RIBOSOMAL PROTEIN L27.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 47  | B0    | 84       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 662   | 410 | 140 | 111 | 1 |         |         |       |
| 47  | D0    | 84       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 662   | 410 | 140 | 111 | 1 |         |         |       |

- Molecule 48 is a protein called 50S RIBOSOMAL PROTEIN L28.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 48  | B1    | 94       | Total | C   | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 732   | 460 | 146 | 125 | 1 |         |         |       |
| 48  | D1    | 94       | Total | C   | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 732   | 460 | 146 | 125 | 1 |         |         |       |

- Molecule 49 is a protein called 50S RIBOSOMAL PROTEIN L29.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 49  | B2    | 71       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 598   | 370 | 121 | 106 | 1 |         |         |       |
| 49  | D2    | 71       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 598   | 370 | 121 | 106 | 1 |         |         |       |

- Molecule 50 is a protein called 50S RIBOSOMAL PROTEIN L30.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 50  | B3    | 60       | Total | C   | N  | O  | S | 0       | 0       | 1     |
|     |       |          | 468   | 298 | 91 | 78 | 1 |         |         |       |
| 50  | D3    | 60       | Total | C   | N  | O  | S | 0       | 0       | 1     |
|     |       |          | 468   | 298 | 91 | 78 | 1 |         |         |       |

- Molecule 51 is a protein called 50S RIBOSOMAL PROTEIN L31.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 51  | B4    | 31       | Total | C   | N  | O  | S | 0       | 0       | 1     |
|     |       |          | 226   | 142 | 37 | 43 | 4 |         |         |       |
| 51  | D4    | 40       | Total | C   | N  | O  | S | 0       | 0       | 1     |
|     |       |          | 298   | 189 | 50 | 54 | 5 |         |         |       |

- Molecule 52 is a protein called 50S RIBOSOMAL PROTEIN L32.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 52  | B5    | 59       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 459   | 288 | 90 | 76 | 5 |         |         |       |
| 52  | D5    | 59       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 459   | 288 | 90 | 76 | 5 |         |         |       |

- Molecule 53 is a protein called 50S RIBOSOMAL PROTEIN L33.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 53  | B6    | 45       | Total | C   | N  | O  | S | 0       | 0       | 1     |
|     |       |          | 381   | 235 | 78 | 64 | 4 |         |         |       |
| 53  | D6    | 45       | Total | C   | N  | O  | S | 0       | 0       | 1     |
|     |       |          | 381   | 235 | 78 | 64 | 4 |         |         |       |

- Molecule 54 is a protein called 50S RIBOSOMAL PROTEIN L34.

| Mol | Chain | Residues | Atoms |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 54  | B7    | 49       | Total | C   | N   | O  | S | 0       | 0       | 1     |
|     |       |          | 419   | 257 | 105 | 55 | 2 |         |         |       |
| 54  | D7    | 49       | Total | C   | N   | O  | S | 0       | 0       | 1     |
|     |       |          | 419   | 257 | 105 | 55 | 2 |         |         |       |

- Molecule 55 is a protein called 50S RIBOSOMAL PROTEIN L35.

| Mol | Chain | Residues | Atoms |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 55  | B8    | 64       | Total | C   | N   | O  | S | 0       | 0       | 1     |
|     |       |          | 508   | 326 | 102 | 78 | 2 |         |         |       |
| 55  | D8    | 64       | Total | C   | N   | O  | S | 0       | 0       | 1     |
|     |       |          | 508   | 326 | 102 | 78 | 2 |         |         |       |

- Molecule 56 is a protein called 50S RIBOSOMAL PROTEIN L36.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 56  | B9    | 36       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 299   | 183 | 67 | 46 | 3 |         |         |       |
| 56  | D9    | 36       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 299   | 183 | 67 | 46 | 3 |         |         |       |

- Molecule 57 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

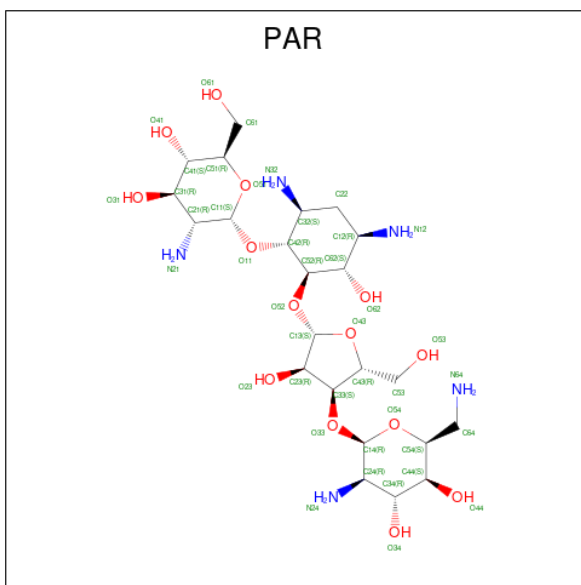
| Mol | Chain | Residues | Atoms               | ZeroOcc | AltConf |
|-----|-------|----------|---------------------|---------|---------|
| 57  | AA    | 110      | Total Mg<br>110 110 | 0       | 0       |
| 57  | AE    | 1        | Total Mg<br>1 1     | 0       | 0       |
| 57  | AV    | 5        | Total Mg<br>5 5     | 0       | 0       |
| 57  | AX    | 1        | Total Mg<br>1 1     | 0       | 0       |
| 57  | BA    | 323      | Total Mg<br>323 323 | 0       | 0       |
| 57  | BB    | 5        | Total Mg<br>5 5     | 0       | 0       |
| 57  | BD    | 2        | Total Mg<br>2 2     | 0       | 0       |
| 57  | BE    | 3        | Total Mg<br>3 3     | 0       | 0       |
| 57  | BF    | 1        | Total Mg<br>1 1     | 0       | 0       |
| 57  | BN    | 1        | Total Mg<br>1 1     | 0       | 0       |
| 57  | BO    | 1        | Total Mg<br>1 1     | 0       | 0       |
| 57  | BP    | 1        | Total Mg<br>1 1     | 0       | 0       |
| 57  | BU    | 1        | Total Mg<br>1 1     | 0       | 0       |
| 57  | B5    | 1        | Total Mg<br>1 1     | 0       | 0       |
| 57  | B7    | 1        | Total Mg<br>1 1     | 0       | 0       |
| 57  | CA    | 141      | Total Mg<br>141 141 | 0       | 0       |
| 57  | CE    | 2        | Total Mg<br>2 2     | 0       | 0       |
| 57  | CV    | 5        | Total Mg<br>5 5     | 0       | 0       |
| 57  | CW    | 1        | Total Mg<br>1 1     | 0       | 0       |
| 57  | CX    | 1        | Total Mg<br>1 1     | 0       | 0       |
| 57  | CY    | 1        | Total Mg<br>1 1     | 0       | 0       |
| 57  | DA    | 397      | Total Mg<br>397 397 | 0       | 0       |

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| Mol | Chain | Residues | Atoms      |         | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 57  | DB    | 5        | Total<br>5 | Mg<br>5 | 0       | 0       |
| 57  | DD    | 3        | Total<br>3 | Mg<br>3 | 0       | 0       |
| 57  | DE    | 2        | Total<br>2 | Mg<br>2 | 0       | 0       |
| 57  | DF    | 1        | Total<br>1 | Mg<br>1 | 0       | 0       |
| 57  | DP    | 3        | Total<br>3 | Mg<br>3 | 0       | 0       |
| 57  | DQ    | 1        | Total<br>1 | Mg<br>1 | 0       | 0       |
| 57  | DU    | 3        | Total<br>3 | Mg<br>3 | 0       | 0       |
| 57  | DW    | 1        | Total<br>1 | Mg<br>1 | 0       | 0       |
| 57  | DX    | 1        | Total<br>1 | Mg<br>1 | 0       | 0       |
| 57  | D0    | 2        | Total<br>2 | Mg<br>2 | 0       | 0       |
| 57  | D1    | 2        | Total<br>2 | Mg<br>2 | 0       | 0       |
| 57  | D2    | 1        | Total<br>1 | Mg<br>1 | 0       | 0       |
| 57  | D5    | 2        | Total<br>2 | Mg<br>2 | 0       | 0       |
| 57  | D8    | 1        | Total<br>1 | Mg<br>1 | 0       | 0       |

- Molecule 58 is PAROMOMYCIN (CCD ID: PAR) (formula:  $C_{23}H_{45}N_5O_{14}$ ).

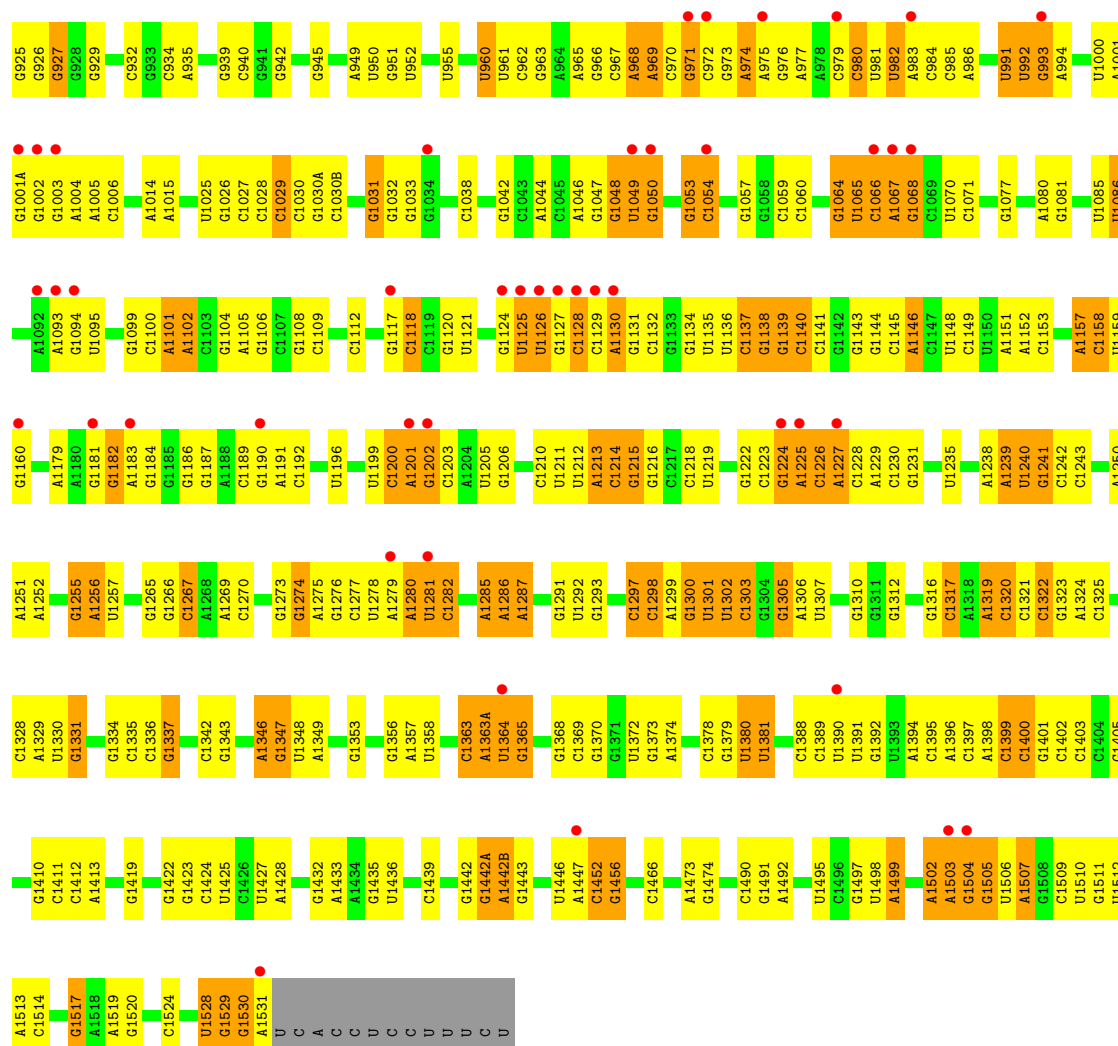


| Mol | Chain | Residues | Atoms       |         |        |         | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|--------|---------|---------|---------|
| 58  | AA    | 1        | Total<br>42 | C<br>23 | N<br>5 | O<br>14 | 0       | 0       |
| 58  | CA    | 1        | Total<br>42 | C<br>23 | N<br>5 | O<br>14 | 0       | 0       |

- Molecule 59 is ZINC ION (CCD ID: ZN) (formula: Zn).

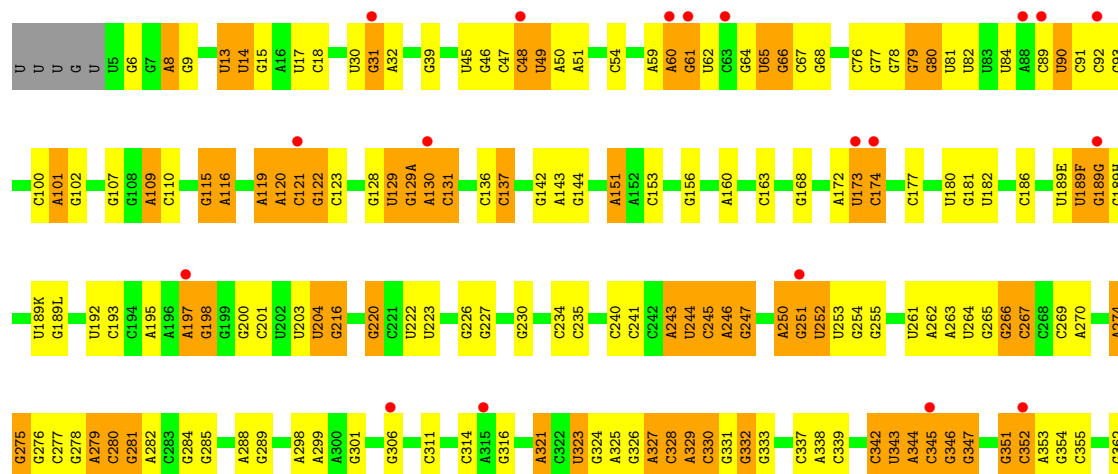
| Mol | Chain | Residues | Atoms           | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 59  | AD    | 1        | Total Zn<br>1 1 | 0       | 0       |
| 59  | AN    | 1        | Total Zn<br>1 1 | 0       | 0       |
| 59  | CD    | 1        | Total Zn<br>1 1 | 0       | 0       |
| 59  | CN    | 1        | Total Zn<br>1 1 | 0       | 0       |





• Molecule 1: 16S rRNA

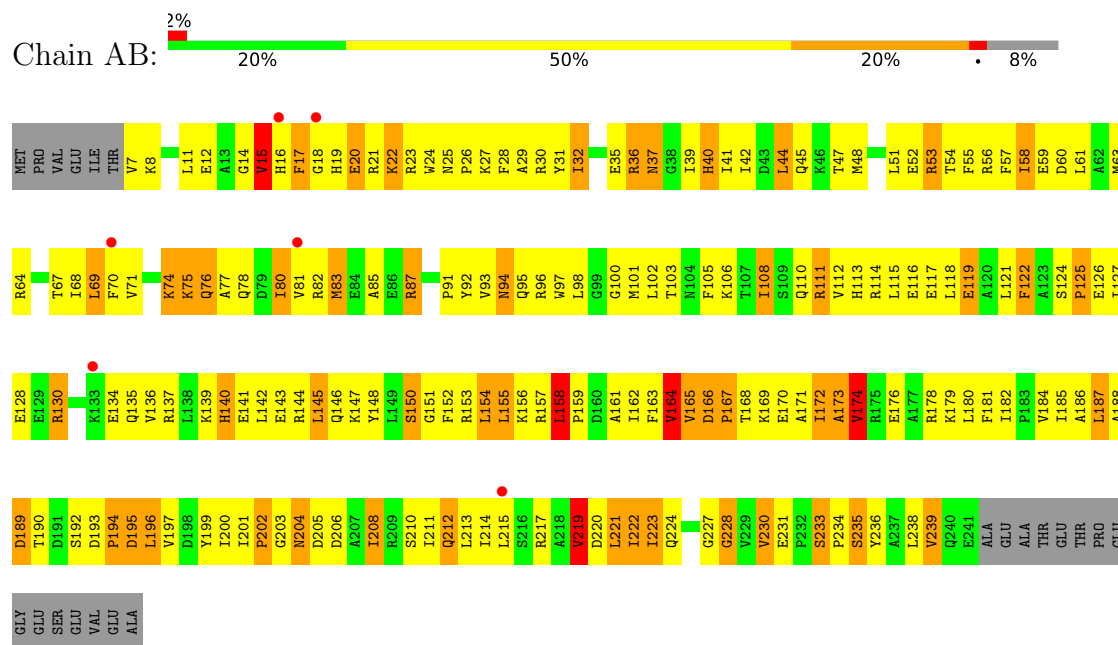
Chain CA: 5% 49% 34% 16%



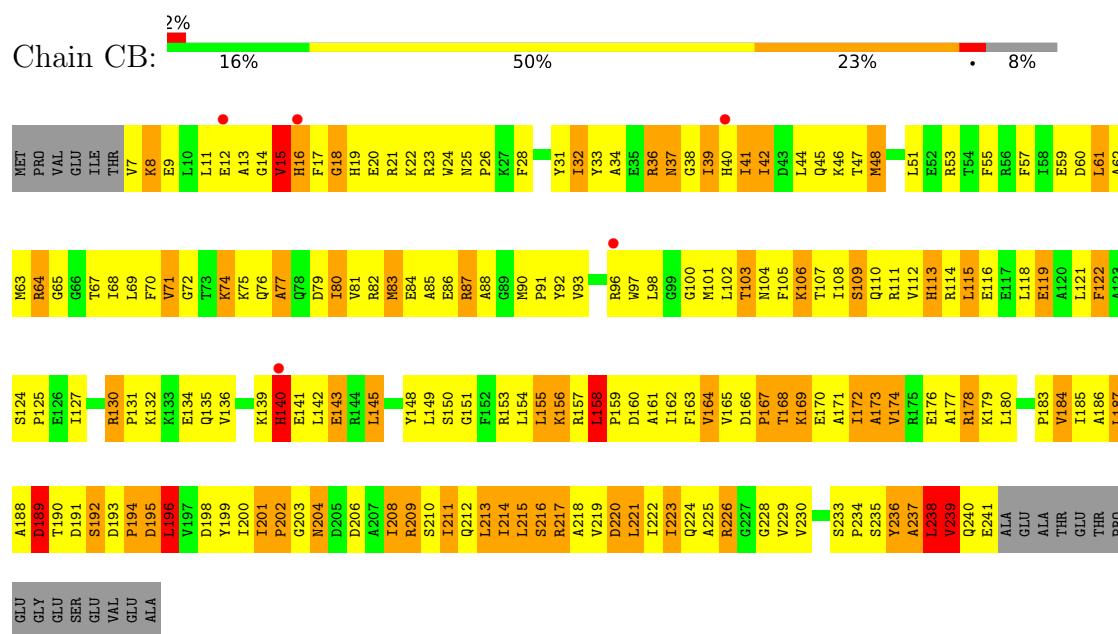
|       |        |        |       |       |       |       |        |      |      |      |      |      |      |
|-------|--------|--------|-------|-------|-------|-------|--------|------|------|------|------|------|------|
| U1522 | A1433  | C1359  | A1288 | U2111 | A1130 | A1046 | A985   | G858 | C747 | G657 | G538 | C442 | A383 |
| U1528 | A1434  | A1360  | G1290 | U1212 | G1131 | G1047 | G966   | A859 | C748 | G662 | G542 | C443 | A364 |
| G1529 | G1435  | C1363  | G1291 | A1213 | G1132 | U1048 | C957   | A860 | C749 | A663 | G546 | C444 | U365 |
| G1530 | U1436  | U1292  | G1292 | C1214 | G1133 | U1049 | A968   | G861 | C750 | A664 | G547 | C445 | U367 |
|       | C1439  | A1363A | G1293 | G1215 | G1134 | G1050 | A969   | G869 | U751 | A665 | G548 | C446 |      |
|       | G1440  | G1294  | G1295 | U1052 | U1135 | U1052 | G971   | U870 | G752 | G666 |      |      | G371 |
| U     | G1441  | G1365  | G1296 | G1217 | U1136 | G1053 | G972   | A871 | C753 | G667 |      |      | C372 |
| C     | G1442  | C1366  | C1297 | U1218 | C1137 | C1054 | G973   | A872 | G754 | G668 | A559 | A452 | C373 |
| A     | G1442A | C1367  | C1298 | U1219 | G1138 | A1055 | A974   | A873 | C755 | G669 | U560 | A453 | A374 |
| C     | G1442B |        | C1299 | G1139 | C1140 | U1056 | A975   | G874 | U756 | U672 | C458 |      | U375 |
| U     | G1443  |        | G1300 | G1141 | G1142 | G1057 | G976   | C877 | C757 | G673 | U561 | C460 | G376 |
| C     | G1444  |        | U1301 | G1143 | G1144 | G1058 | A977   | G878 | U758 | G674 | C562 | C470 | G377 |
| C     | G1445  |        | U1302 | G1143 | G1144 | C1059 | A978   |      |      | G675 | C563 | C471 | G378 |
| U     | G1446  |        | G1303 | G1144 | C1145 | U1060 | C979   | G881 | C764 | A676 | C564 | C472 | C379 |
| U     | A1447  |        | G1304 | C1145 | C1146 | G1061 | C980   | G882 | G765 | U677 | U565 | C473 | G380 |
| U     | A1477  |        | G1305 | C1146 | C1147 | U1062 | U981   | G883 | G766 | C767 | C567 | C474 | C381 |
| C     | G1452  |        | G1306 | C1147 | U1148 | G1063 | U982   | G885 | A777 | U686 |      |      | A382 |
| U     | G1456  |        | U1307 | G1230 | C1149 | U1065 | A983   | G886 |      | A887 | A572 |      | A383 |
| C     | G1457  |        | U1308 | G1231 | C1150 | U1066 | G984   | G887 | G786 | U688 | A573 | U480 | G384 |
| U     | G1458  |        | G1309 | U1232 | U1151 | C1067 | A986   | A889 | A790 | C688 | A574 | C481 | U387 |
|       | G1459  |        |       | U1236 | A1152 | A1067 |        | G890 | G791 | C689 | C575 | C482 | G388 |
|       | A1460  |        |       | C1237 | A1153 | G1068 | U991   | A901 | U792 | G691 | C577 | C483 | A389 |
|       | A1468  |        |       | A1238 | C1153 | C1069 | U992   | G902 | A793 | C701 | C578 | C484 | G390 |
|       | G1469  |        |       | U1239 |       |       | G993   |      | A794 | A702 | C579 | U486 | G391 |
|       |        |        |       | U1240 | A1157 | G1074 | C994   | G906 | C797 | G703 | U580 | A487 | G396 |
|       |        |        |       | G1241 | C1158 | G1077 | C995   |      |      | G704 | C581 | C490 | A397 |
|       |        |        |       | C1244 | U1159 |       |        |      |      | U705 |      | C491 | C398 |
|       |        |        |       | A1245 | G1160 | A1080 | U1000  | A913 | C812 | A706 | G595 |      | C401 |
|       |        |        |       | C1246 | C1161 | G1081 | G1001  | A914 | U813 | C707 | C596 |      | C402 |
|       |        |        |       | U1247 | C1162 |       | G1001A | A915 | A814 | C708 |      |      | U405 |
|       |        |        |       | U1248 | C1163 | G1084 | G1002  |      | A815 | C709 |      |      | G406 |
|       |        |        |       | C1249 | G1171 | U1085 | G1003  | U921 | C817 | U498 |      |      | G407 |
|       |        |        |       | U1250 | C1172 | U1086 | A1004  | G922 | G818 | A499 |      |      |      |
|       |        |        |       | A1251 | G1178 | G1094 | A1005  | A923 | A819 | G500 |      |      |      |
|       |        |        |       | U1252 |       | U1095 |        | G924 | U820 |      |      |      |      |
|       |        |        |       |       | G1181 | C1096 | A1014  | G925 | C821 | C508 |      |      |      |
|       |        |        |       | G1255 | G1182 | C1097 | A1015  | G926 | G822 | A509 |      |      |      |
|       |        |        |       | U1257 | A1183 | U1025 |        | G927 | G823 | A510 |      |      |      |
|       |        |        |       | C1259 | G1184 | G1026 | U1026  |      | C824 | C511 |      |      |      |
|       |        |        |       |       |       | A1101 | G1027  | C934 | G825 | U512 |      |      |      |
|       |        |        |       |       |       | A1102 | C1028  | A935 | C826 |      |      |      |      |
|       |        |        |       | G1266 | C1189 | G1108 | C1029  | G945 | U827 | G517 |      |      |      |
|       |        |        |       | C1267 | G1190 | C1109 | C1030  | A946 | A828 | C518 |      |      |      |
|       |        |        |       | U1268 | C1192 | U1120 | G1030A | G947 | C726 | C519 |      |      |      |
|       |        |        |       | A1269 | G1193 | C1112 | C1030B | C948 | G834 | C522 |      |      |      |
|       |        |        |       | C1270 |       | C1118 | G1030C | A949 |      | C523 |      |      |      |
|       |        |        |       |       | U1196 | C1119 | A1030D | U950 | G837 | C524 |      |      |      |
|       |        |        |       | U1278 | G1197 | G1125 | G1031  | G951 | C838 | G517 |      |      |      |
|       |        |        |       | A1279 | U1198 | U1126 | C1032  | U952 | U839 | C518 |      |      |      |
|       |        |        |       | U1280 | U1199 | G1127 | G1033  | G953 | C840 | C519 |      |      |      |
|       |        |        |       | U1281 | C1200 | U1128 | G1033  | G954 | U841 | C522 |      |      |      |
|       |        |        |       | C1282 | A1201 | U1129 | C1037  | U960 | C848 | C543 |      |      |      |
|       |        |        |       |       | C1203 | U1129 | G1038  | U961 | C849 | C543 |      |      |      |
|       |        |        |       | A1285 | U1204 | U1129 | C1039  | G962 | G854 | A532 |      |      |      |
|       |        |        |       | U1286 | U1205 | U1129 | G1044  | G963 | G855 | A533 |      |      |      |
|       |        |        |       | A1287 | U1206 | U1129 | A1044  |      |      | U534 |      |      |      |
|       |        |        |       | U1288 |       | U1129 | C1045  | A964 |      | A653 |      |      |      |
|       |        |        |       |       |       |       |        |      |      | C556 |      |      |      |



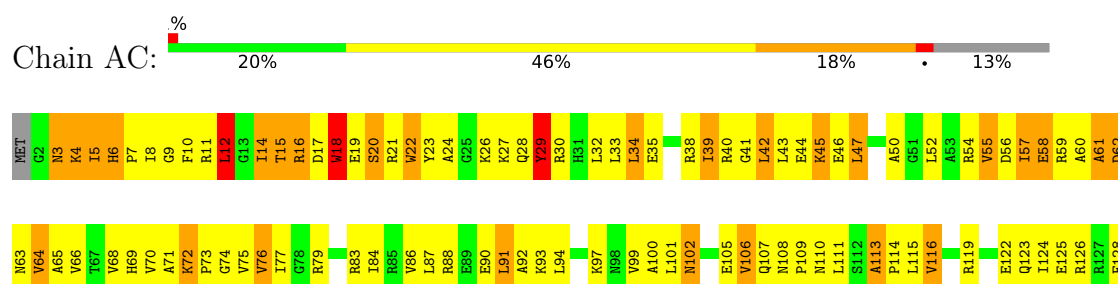
• Molecule 2: 30S ribosomal protein S2

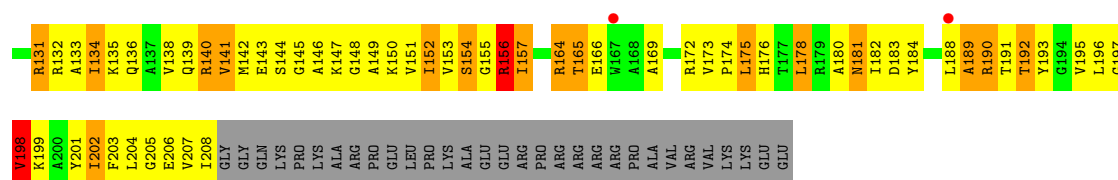


• Molecule 2: 30S ribosomal protein S2

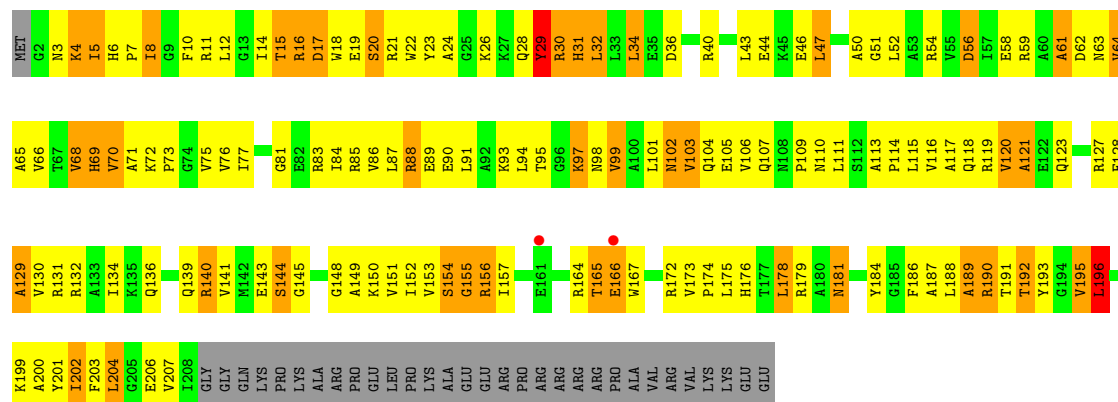


• Molecule 3: 30S ribosomal protein S3

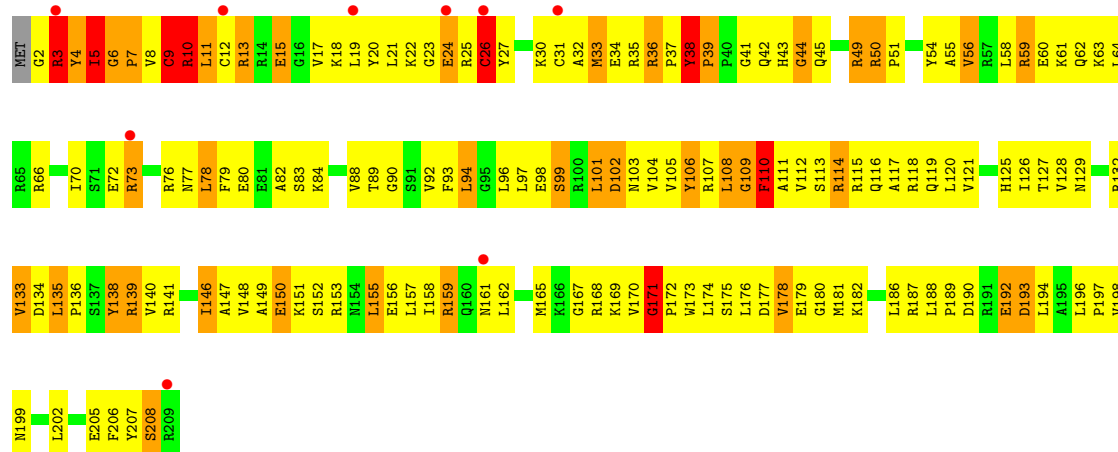




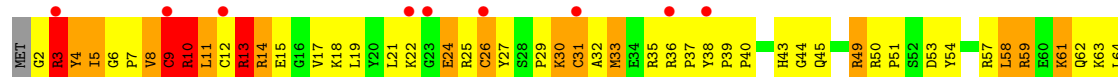
• Molecule 3: 30S ribosomal protein S3

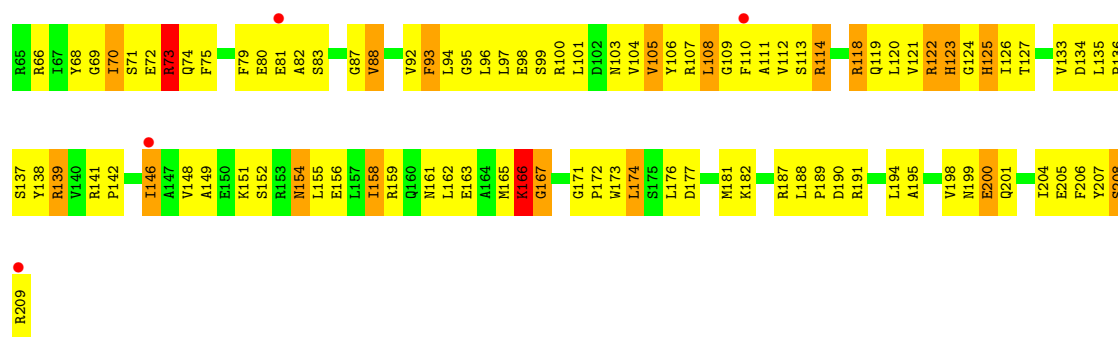


• Molecule 4: 30S ribosomal protein S4

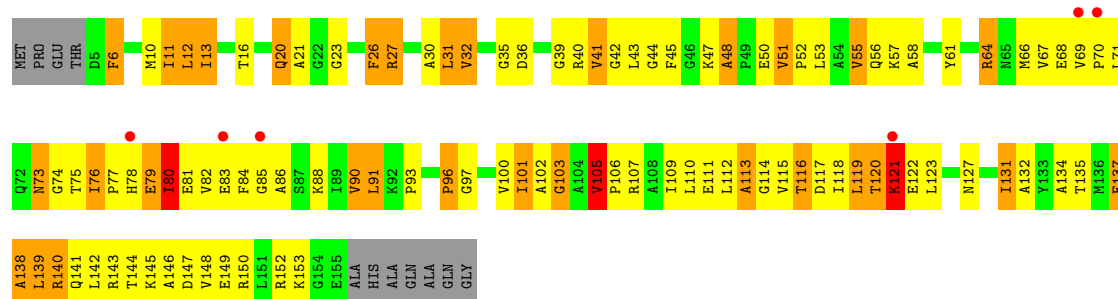


• Molecule 4: 30S ribosomal protein S4

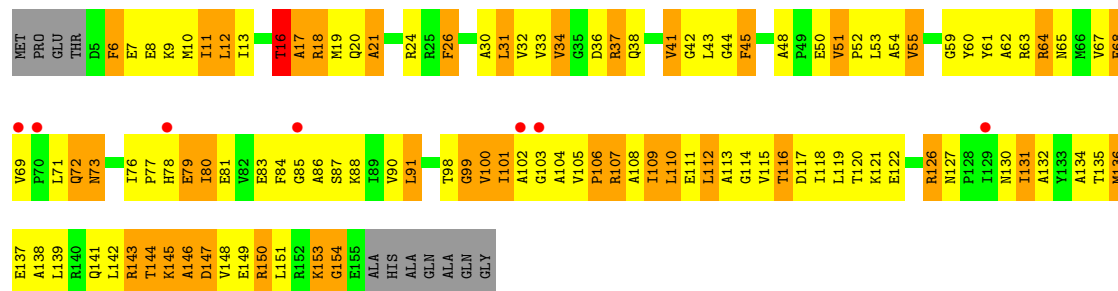




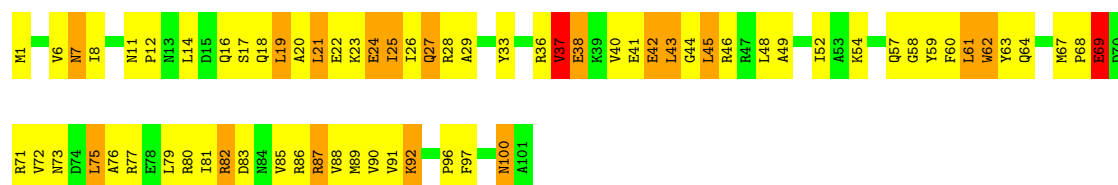
• Molecule 5: 30S ribosomal protein S5



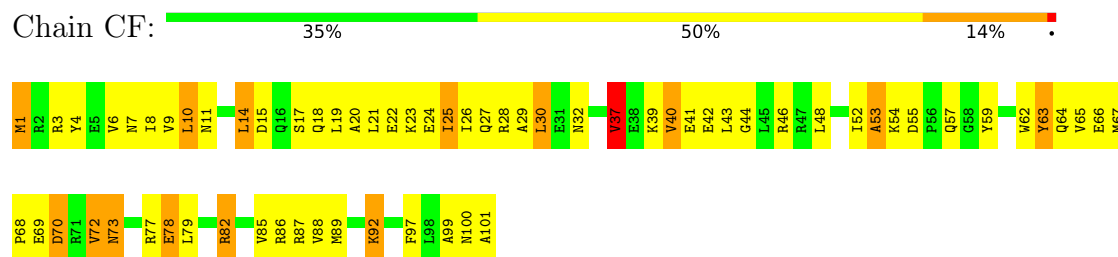
• Molecule 5: 30S ribosomal protein S5



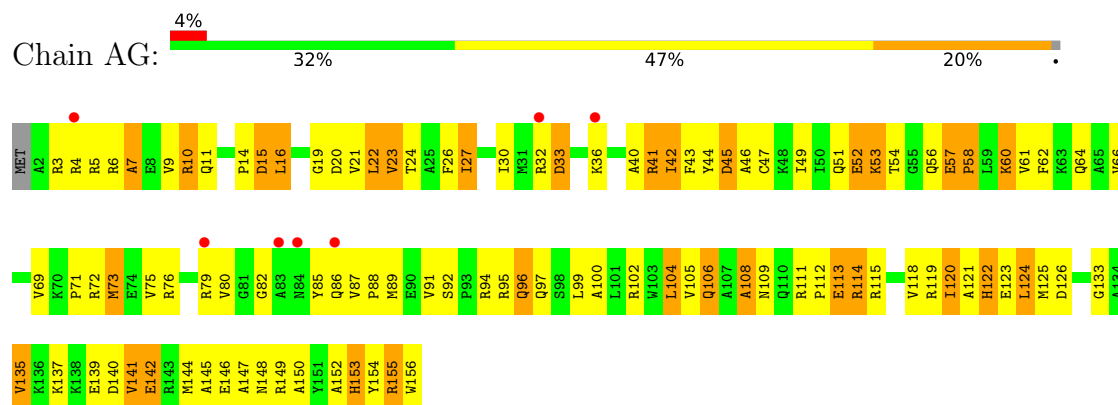
• Molecule 6: 30S ribosomal protein S6



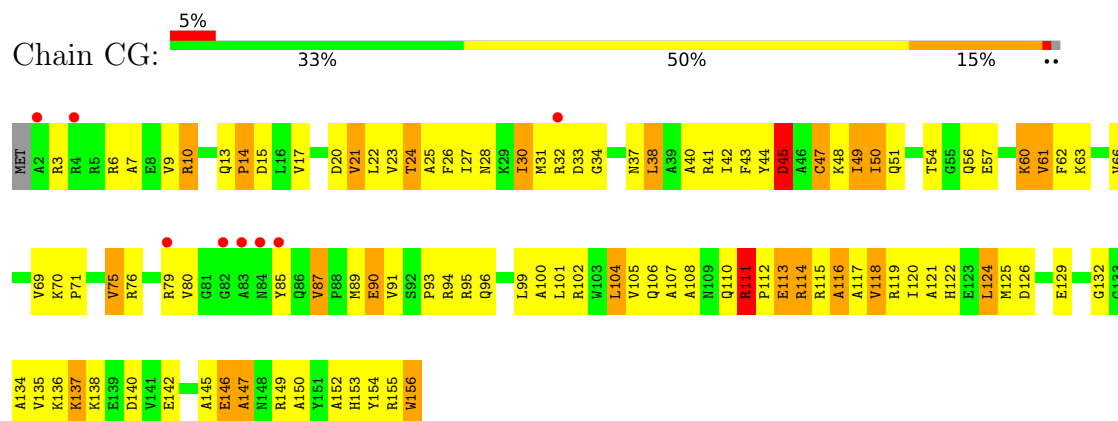
• Molecule 6: 30S ribosomal protein S6



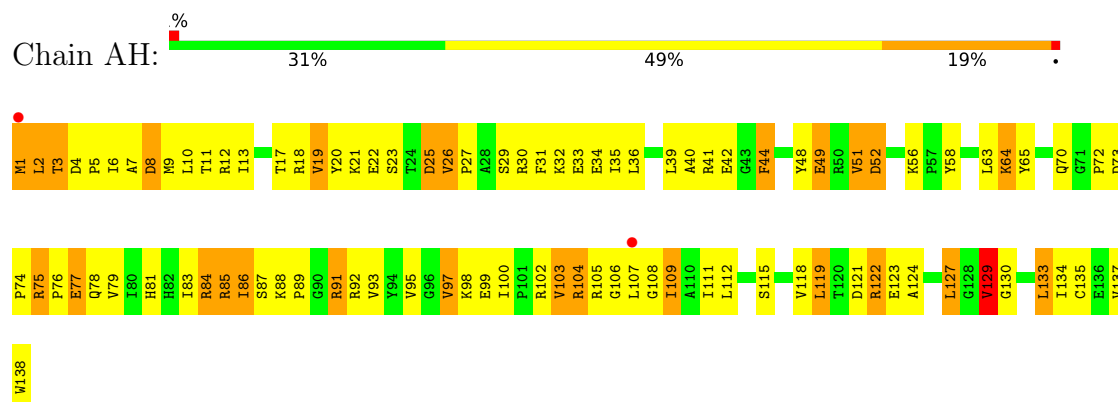
• Molecule 7: 30S ribosomal protein S7



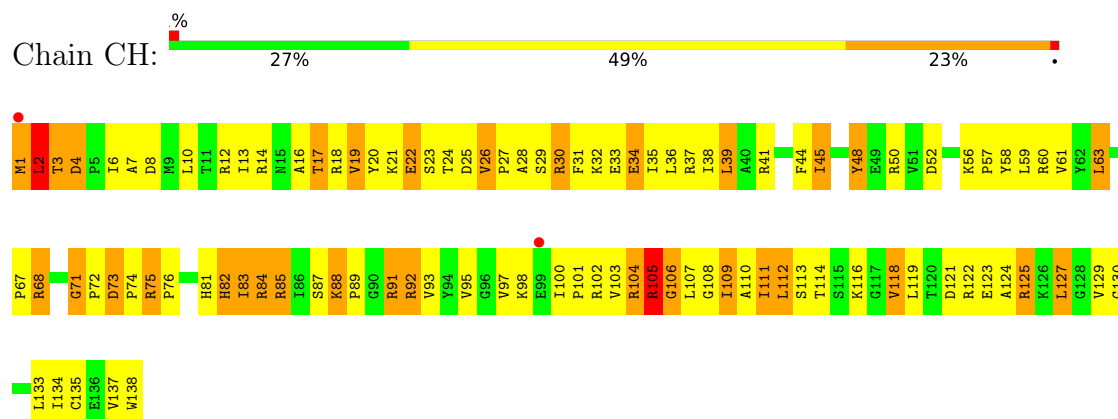
• Molecule 7: 30S ribosomal protein S7



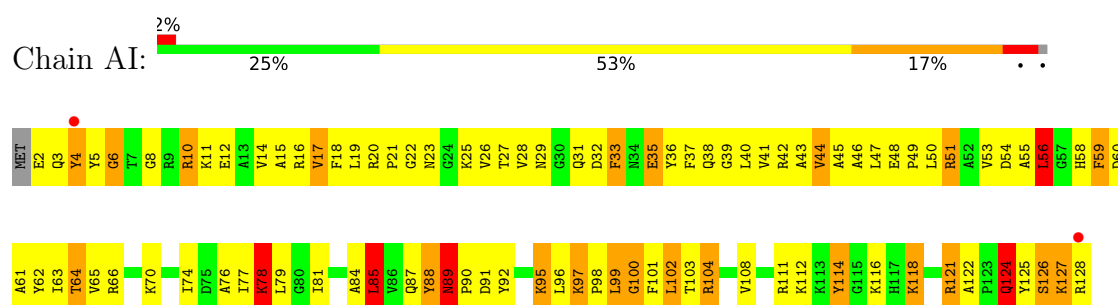
• Molecule 8: 30S ribosomal protein S8



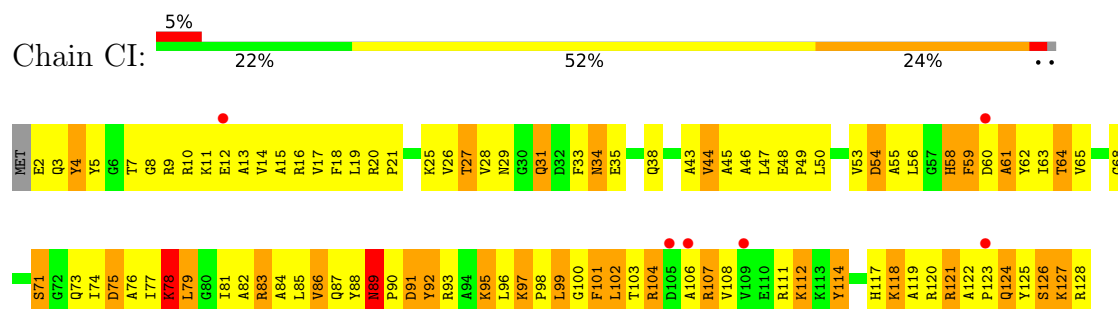
- Molecule 8: 30S ribosomal protein S8



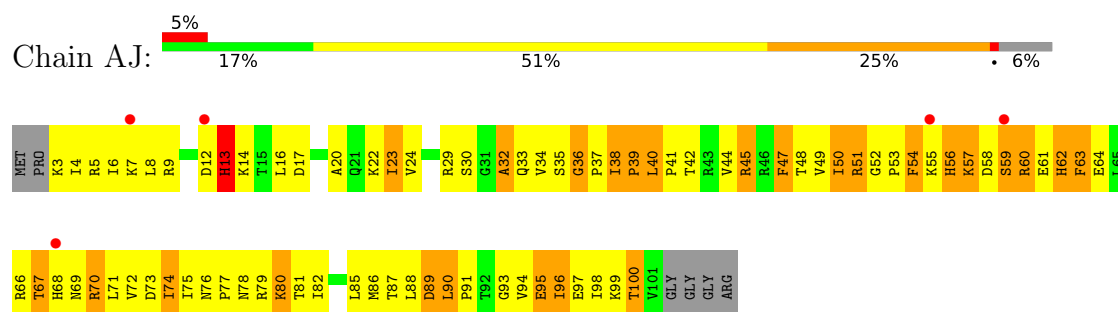
- Molecule 9: 30S ribosomal protein S9



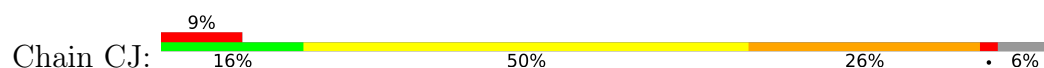
- Molecule 9: 30S ribosomal protein S9

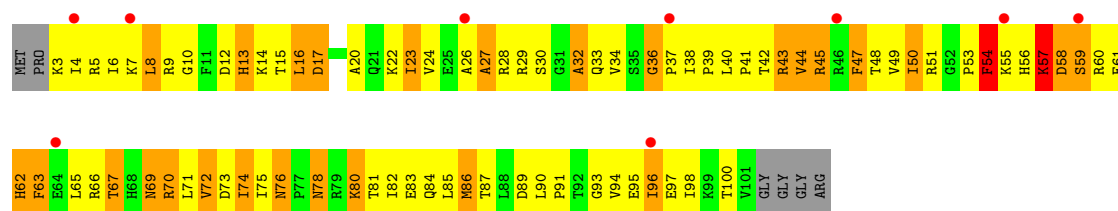


- Molecule 10: 30S ribosomal protein S10

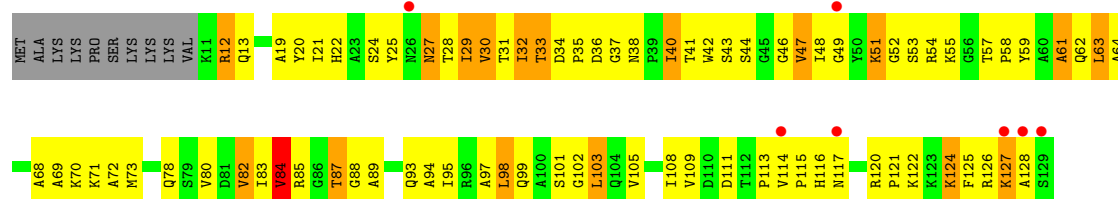


- Molecule 10: 30S ribosomal protein S10

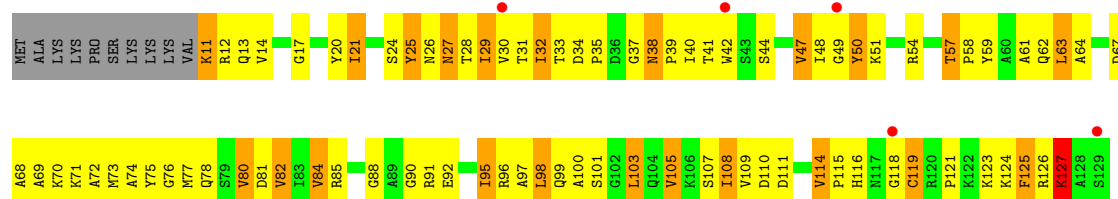




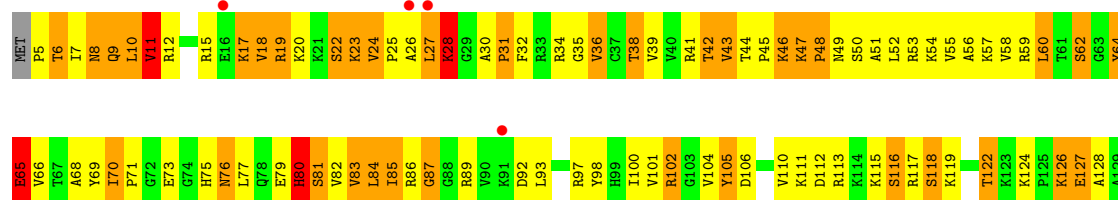
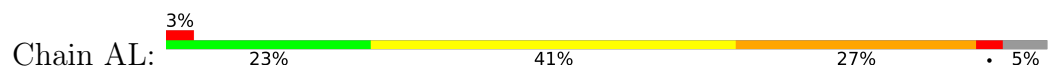
• Molecule 11: 30S ribosomal protein S11



• Molecule 11: 30S ribosomal protein S11



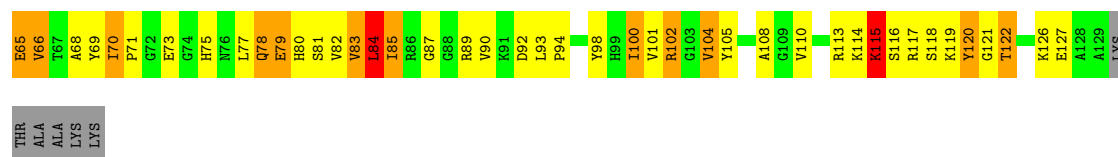
• Molecule 12: 30S ribosomal protein S12



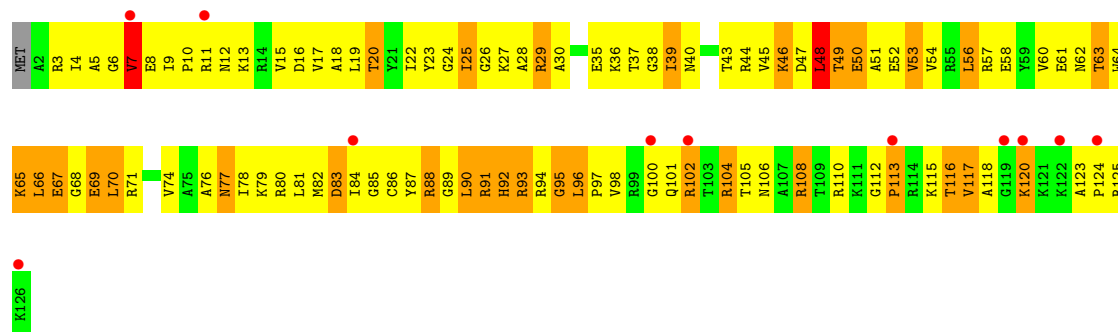
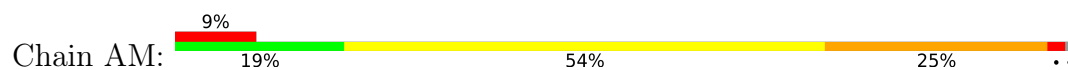
LYS  
THR  
ALA  
ALA  
LYS  
LYS

• Molecule 12: 30S ribosomal protein S12

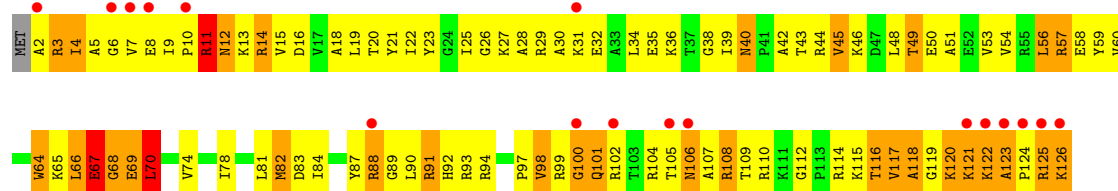




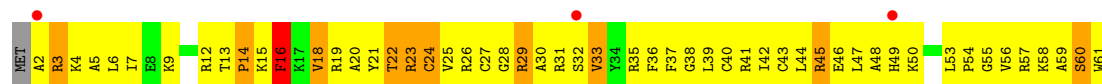
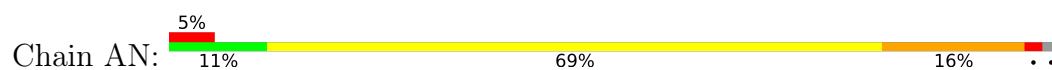
- Molecule 13: 30S ribosomal protein S13



- Molecule 13: 30S ribosomal protein S13



- Molecule 14: 30S ribosomal protein S14 type Z

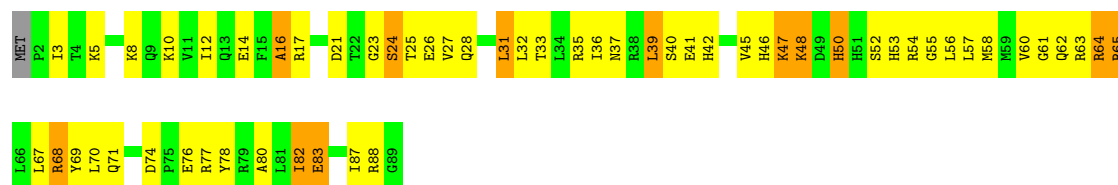


- Molecule 14: 30S ribosomal protein S14 type Z

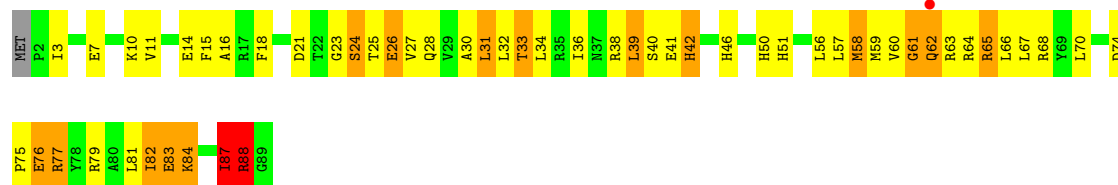
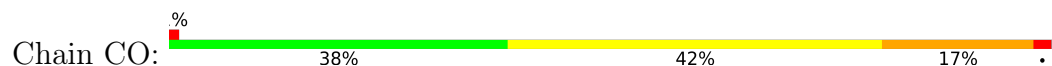


- Molecule 15: 30S ribosomal protein S15

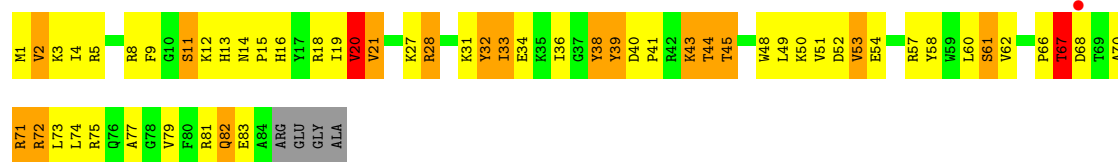




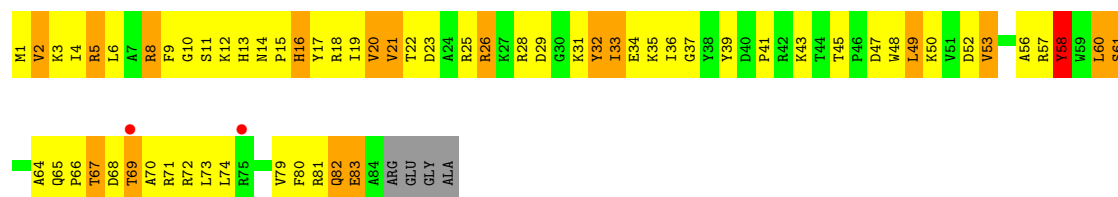
• Molecule 15: 30S ribosomal protein S15



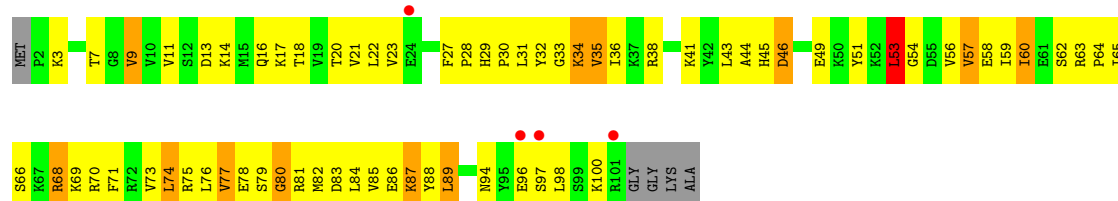
• Molecule 16: 30S ribosomal protein S16



• Molecule 16: 30S ribosomal protein S16

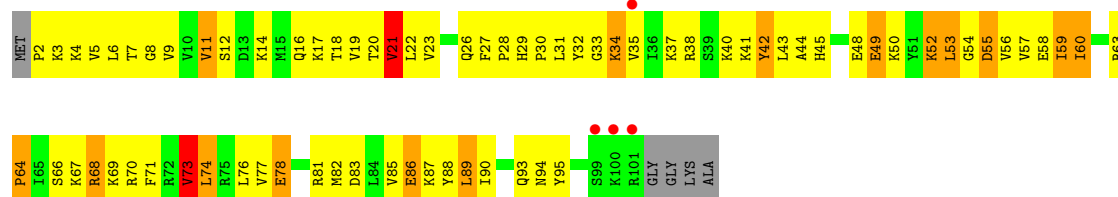
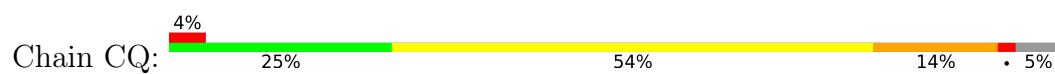


• Molecule 17: 30S ribosomal protein S17

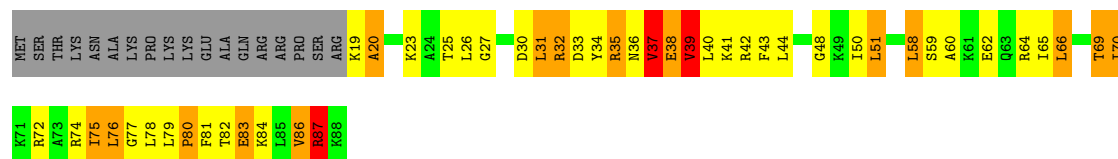
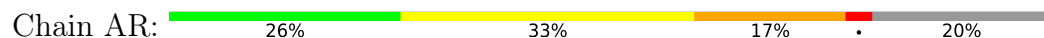


• Molecule 17: 30S ribosomal protein S17

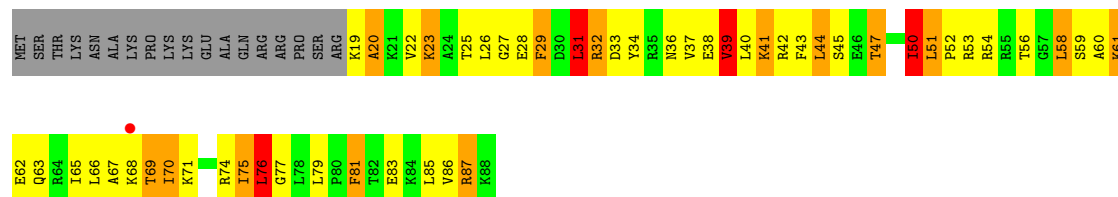
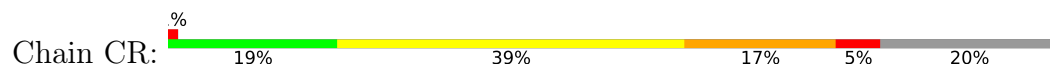




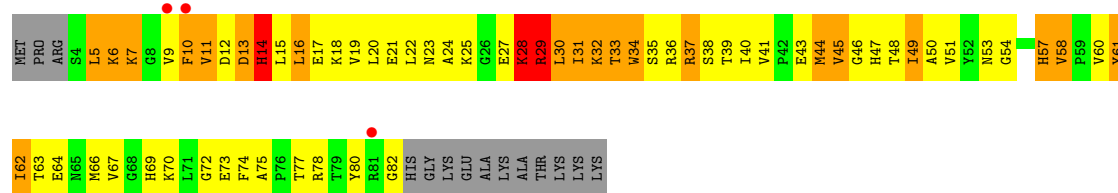
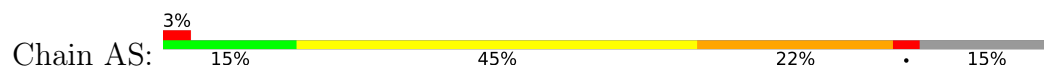
- Molecule 18: 30S ribosomal protein S18



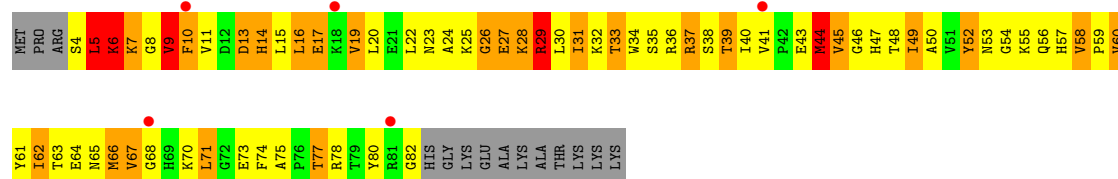
- Molecule 18: 30S ribosomal protein S18



- Molecule 19: 30S ribosomal protein S19

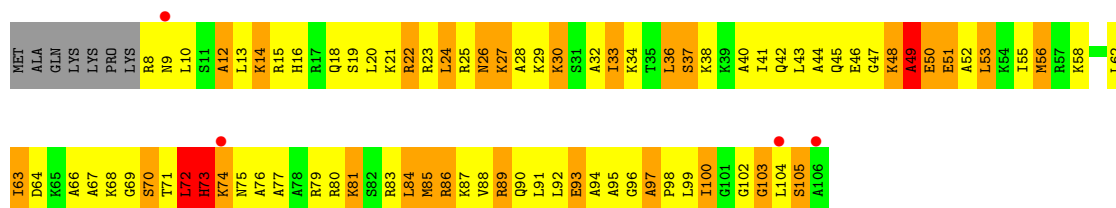


- Molecule 19: 30S ribosomal protein S19



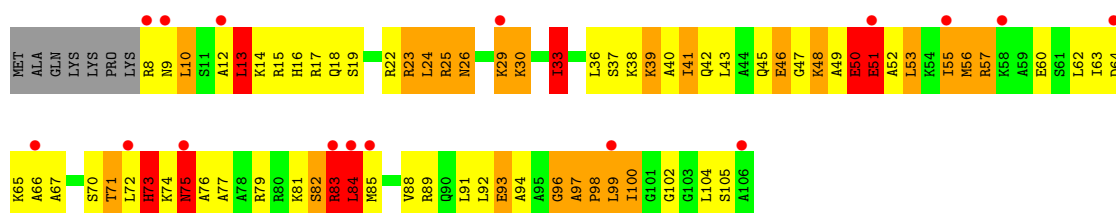
- Molecule 20: 30S ribosomal protein S20

Chain AT: 



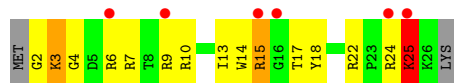
- Molecule 20: 30S ribosomal protein S20

Chain CT: 

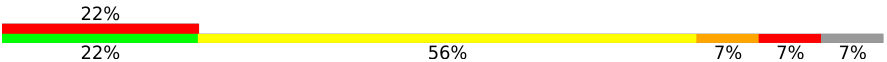


- Molecule 21: 30S ribosomal protein Thx

Chain AU: 

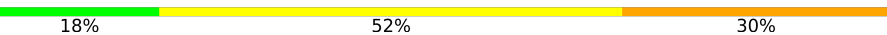


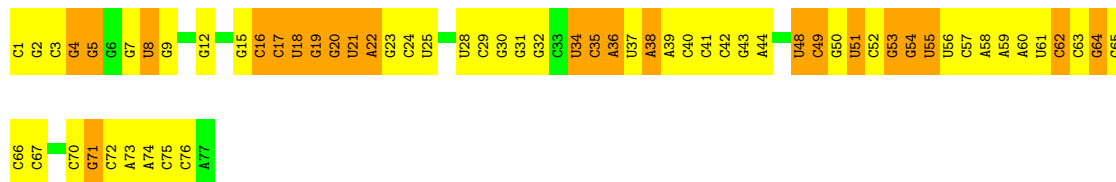
- Molecule 21: 30S ribosomal protein Thx

Chain CU: 



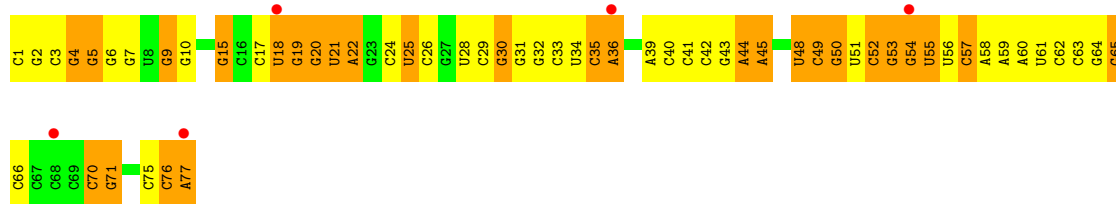
- Molecule 22: P-SITE tRNA fMet

Chain AV: 

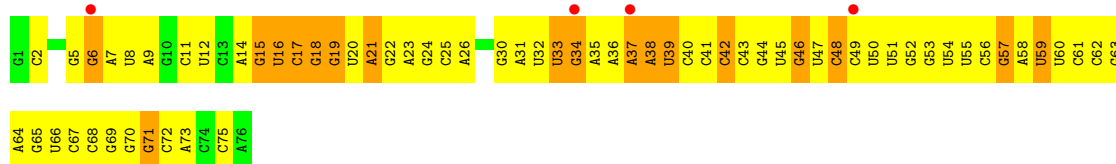
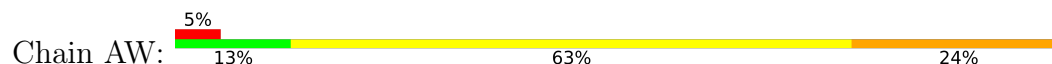


- Molecule 22: P-SITE tRNA fMet

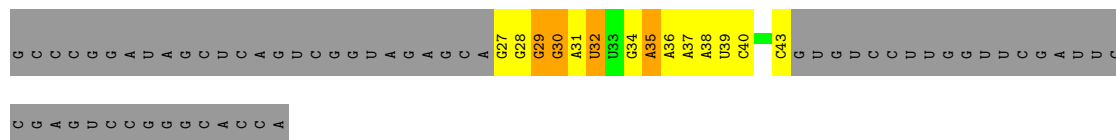
Chain CV: 



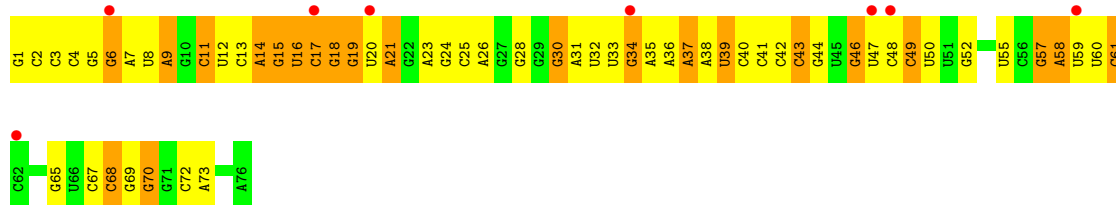
- Molecule 23: E-SITE TRNA PHE OR A-SITE tRNA Phe



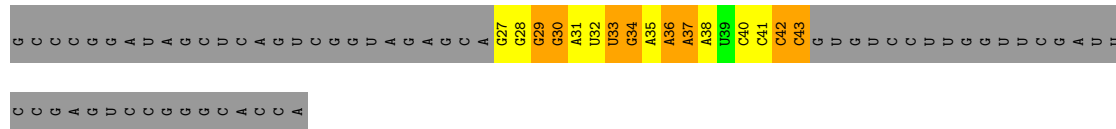
- Molecule 23: E-SITE TRNA PHE OR A-SITE tRNA Phe



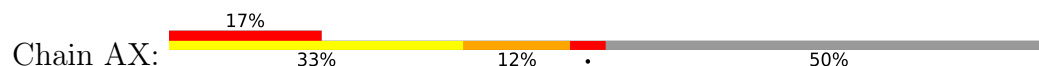
- Molecule 23: E-SITE TRNA PHE OR A-SITE tRNA Phe

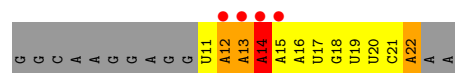


- Molecule 23: E-SITE TRNA PHE OR A-SITE tRNA Phe

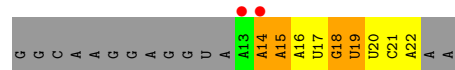


- Molecule 24: mRNA

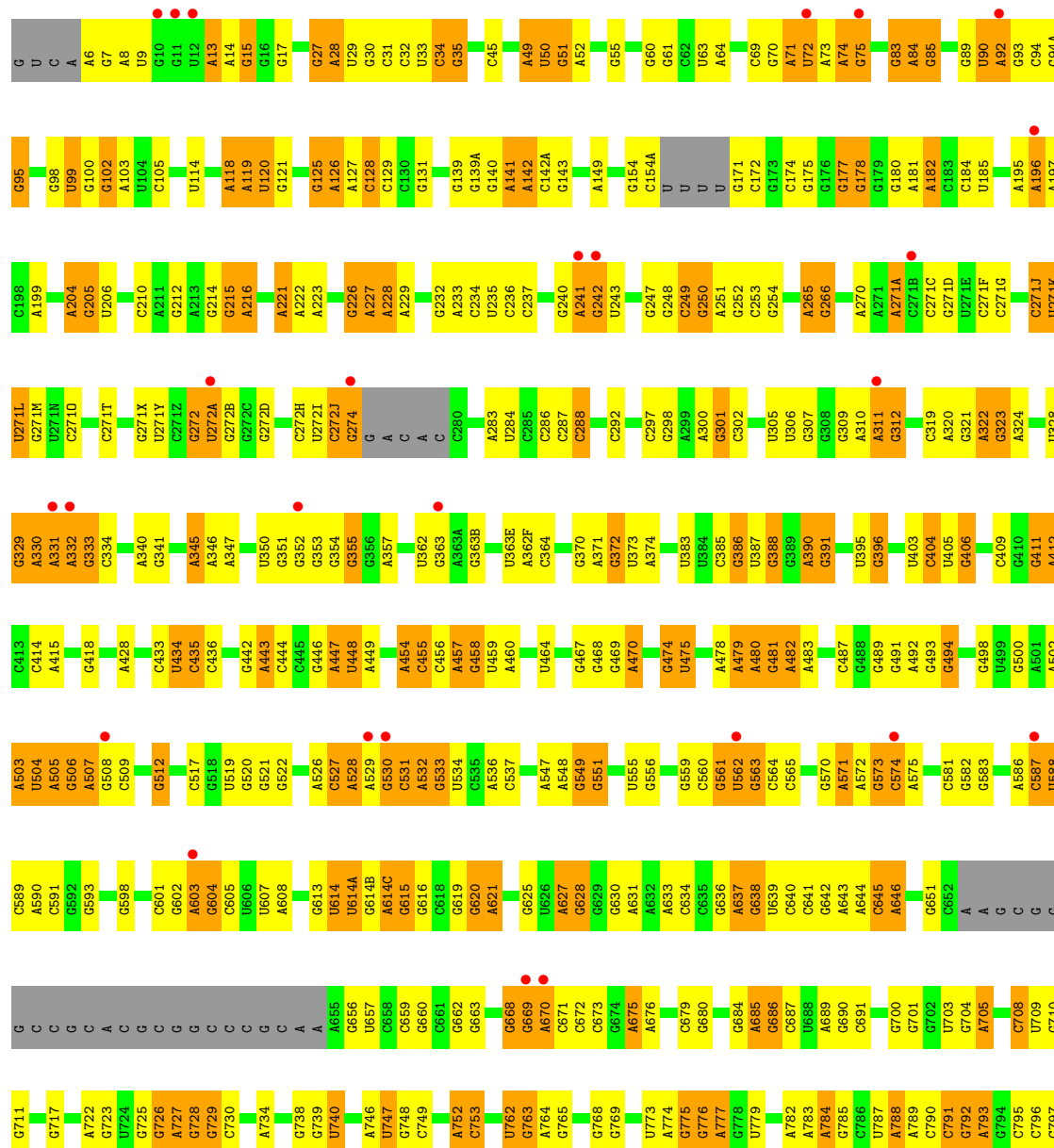




• Molecule 24: mRNA

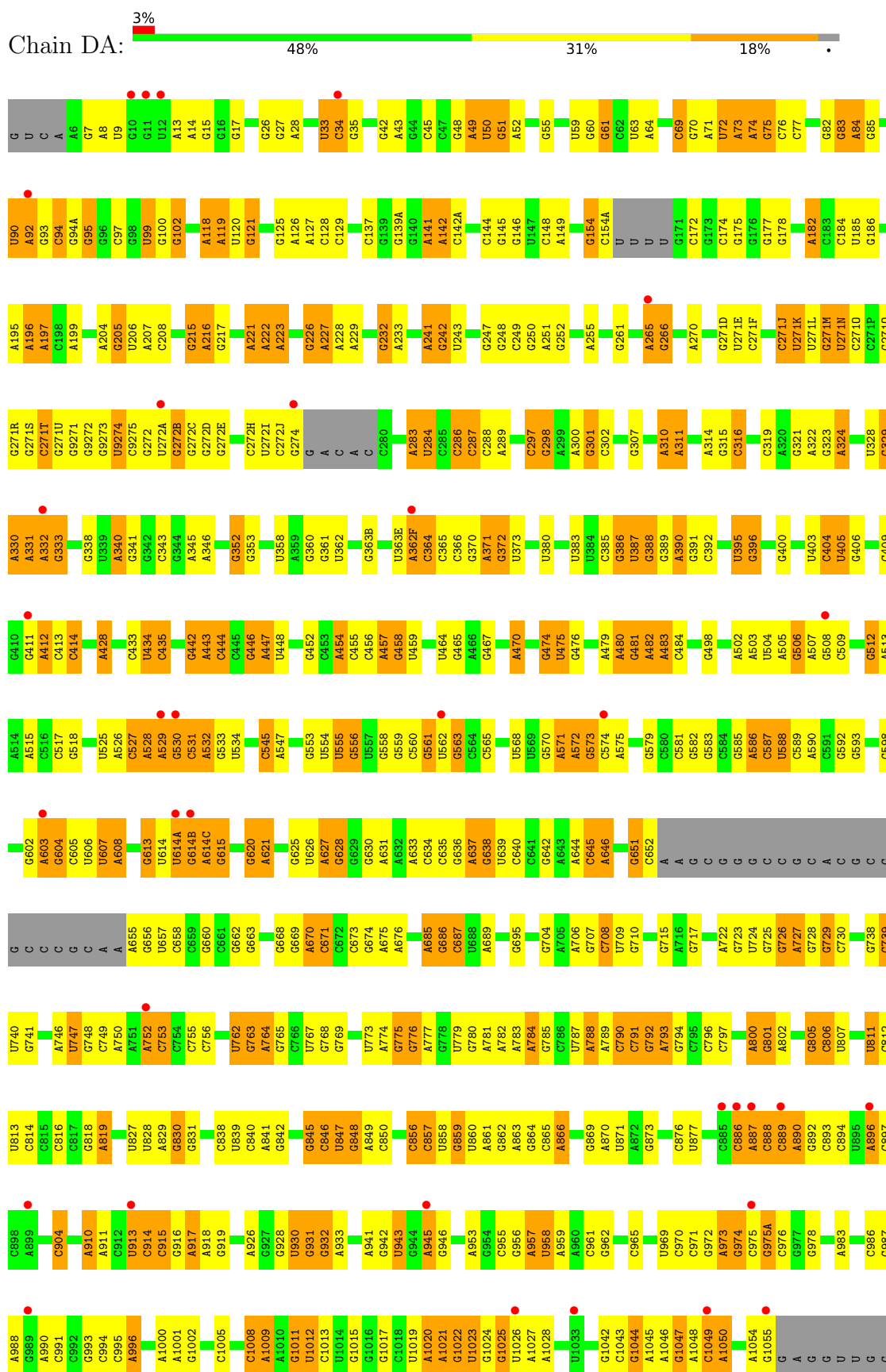


• Molecule 25: 23S rRNA



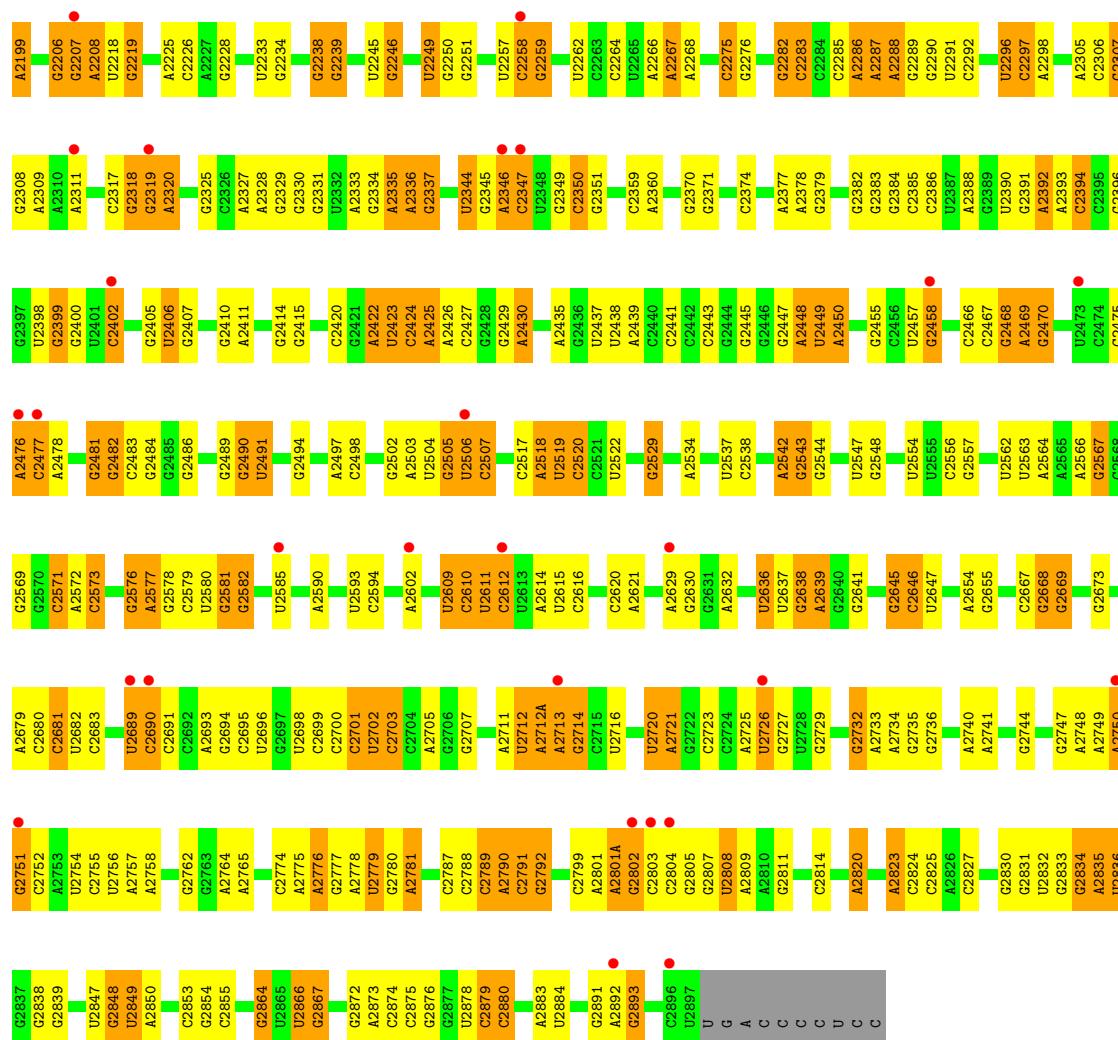
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|-------|--------|-------|-------|--------|-------|-------|-------|--------|-------|-------|------|------|
| G1792 | C1694  | A1603 | G1520 | A1445  | A1360 | G1283 | G1185 | G      | G1047 | G975A | G892 | G800 |
| G1795 | G1695  | C1607 | U1523 | C1445A | C1363 | A1284 | G1186 | U1108  | A1048 | C976  | C893 | G801 |
| U1796 | G1696  | A1608 | G1524 | G1446  | G1364 | A1285 | G1187 | C1109  | C1049 | A890  | A896 | A802 |
| A1797 | A1698  | A1609 | G1525 | G1447  | A1365 | A1286 | U1188 | G1110  | A1050 | G897  | C897 | U803 |
| G1798 | G1699  | A1610 | G1526 | A1448  | G1368 | U1287 | G1189 | A1111  | G1051 | A893  | U804 | G805 |
| G1799 | A1700  | C1611 | G1527 | G1450  | G1368 | U1288 | G1195 | G1112  | C1052 | A900  | G805 | C806 |
| C1800 | A1701  |       | A1528 | C1450A |       | C1289 | G1203 | U1113  | C1053 | A901  |      |      |
| A1801 | G1706  | C1615 | C1532 | C1451  | A1378 | G1290 | A1204 | G1114  | A     | G987  |      |      |
| A1802 | U1707  | A1616 | U     | A1452  | G1379 | C1291 | U1205 | G1115  | G     | A988  |      |      |
| A1803 | G1707  | U1453 | C     | U1453  | G1380 | U1292 | G1206 | C1116  | A     | G989  |      |      |
| A1809 | G1718  | G1455 | A     | G1455  | A1384 | U1299 | G1209 | C1118  | G     | C991  |      |      |
| G1812 | G1719  | A1457 |       | A1457  | G1385 | U1300 | A1210 | G1122  | U     | A910  |      |      |
| G1813 | U1720  | C1458 | G1537 | C1458  | G1387 | A1301 | U1211 | G1125  | U     | A911  |      |      |
| G1814 | G1721  | G1459 |       | G1459  | C1387 | A1302 | G1212 | A1126  | G     | A996  |      |      |
| A1815 | U1722  | A1460 |       | A1460  | U1390 | C1303 | A1213 | A1127  | U     | G997  |      |      |
| G1816 | U1739  | G1461 |       | G1461  | U1391 | C1305 | A1214 | A1128  | C     | C914  |      |      |
| G1817 | G1740  | C1464 |       | C1464  | U1392 | C1306 | A1220 | U1129  | U     | A1000 |      |      |
| G1818 | A1741  | G1465 |       | G1465  | A1393 | G1310 | C1224 | U1130  | A     | A917  |      |      |
| U1819 | G1742  | G1466 |       | G1466  | U1394 | G1311 | C1224 | A1131  | G     | A918  |      |      |
| U1820 | C1743  | C1467 |       | C1467  | A1395 | U1312 | U1236 | A1132  | A     | G919  |      |      |
| A1821 | C1744  | C1468 |       | C1468  | U1396 | U1313 | A1237 | U1133  | A     | G920  |      |      |
|       |        | A1469 |       | A1469  | U1397 | C1314 | G1238 | G1135  | G     | G921  |      |      |
|       | G1747A | G1470 |       | G1470  |       |       |       | G1136  | C     | U922  |      |      |
| G1824 | G1748  | A1471 |       | A1471  | C1403 | G1319 | A1241 | G1139  | A     | A926  |      |      |
| A1825 | A1749  | A1472 |       | A1472  |       | C1320 |       | U1130  | G     | U833  |      |      |
| G1826 | G1750  | G1473 |       | G1473  | U1406 | A1321 | A1241 | C1140  | A     | U834  |      |      |
| G1827 |        |       |       |        | C1407 | A1322 | G1244 | U1141  | C     | U930  |      |      |
| G1828 | C1754  | A1558 |       |        | U1408 | U1323 | G1245 | U1142  | C     | G932  |      |      |
| A1829 | U1755  | G1559 |       |        | C1409 | G1324 | A1246 | A1142A | U     | A933  |      |      |
|       | G1756  | G1560 |       |        | G1410 | G1325 | A1247 | A1143  | C     |       |      |      |
| G1835 | U1757  | A1566 |       |        | C1411 | U1326 | U1248 | G1144  | C     | A941  |      |      |
| G1836 | G1758  | G1567 |       |        | A1412 | U1327 | U1249 | U1145  | C     | G942  |      |      |
| C1837 | A1759  | G1568 |       |        | G1413 | G1328 | G1250 | G1149  | U     | U943  |      |      |
| G1838 |        | A1569 |       |        | G1414 | U1329 | C1251 | C1150  | U     | G944  |      |      |
| G1839 | A1762  | A1570 |       |        | U1415 | C1330 | G1252 | A1020  | A     | A945  |      |      |
|       | G1763  | A1571 |       |        | G1416 | A1331 | A1253 | A1021  | A     | G946  |      |      |
| G1846 | G1764  | A1572 |       |        | C1417 | G1332 |       | G1022  | A     |       |      |      |
| A1847 |        | U1572 |       |        | A1418 | C1333 | G1256 | G1153  | A     | G855  |      |      |
| A1848 | G1769  | U1578 |       |        | G1419 | A1336 | A1265 | G1154  | G     | C856  |      |      |
| A1854 | A1773  | A1579 |       |        | U1420 | G1337 | G1266 | A1155  | A     | C857  |      |      |
| G1855 |        | G1580 |       |        | G1421 | G1339 | U1267 | G1157  | G     | U858  |      |      |
|       | G1776  | G1581 |       |        | G1422 | U1340 | G1270 | C1161  | U     | G859  |      |      |
| G1858 | U1777  | C1584 |       |        | G1426 | U1341 | G1271 | G1162  | C     | A861  |      |      |
| A1859 | U1778  | A1586 |       |        | A1427 | A1342 | A1272 | G1170  | U     | A959  |      |      |
| U1864 | A1779  | A1587 |       |        | C1428 | A1343 | U1273 | G1171  | A     | A960  |      |      |
| G1865 | U1780  | A1588 |       |        | G1429 | G1344 | A1274 | G1173  | U     | C961  |      |      |
| C1866 | C1781  | C1588 |       |        |       | C1345 | A1275 | U1175  | A     | G962  |      |      |
|       | G1782  | U1593 |       |        | C1432 | C1346 | A1276 | A1176  | G     | U963  |      |      |
| A1876 | A1783  | G1594 |       |        | U1433 | G1348 | A1277 | G1177  | A     | G869  |      |      |
| A1877 | U1784  | C1595 |       |        | A1434 | A1349 | G1277 | A1178  | A     | A870  |      |      |
| G1878 | A1785  | G1599 |       |        | C1437 | U1352 | A1278 | C1179  | U     | G873  |      |      |
|       | U1786  | C1600 |       |        |       | A1353 | G1281 | C1180  | C     | C886  |      |      |
| C1881 | A1787  | U1602 |       |        |       | U1354 | U1282 | G1183  | A     | A887  |      |      |
| C1882 | C1788  |       |       |        |       | A1359 |       | G1184  | C     | C888  |      |      |
| G1883 | U1789  | G1601 |       |        |       |       |       |        | U     | A1045 |      |      |
| A1884 | C1790  |       |       |        |       |       |       |        | C     | G974  |      |      |
|       | A1791  |       |       |        |       |       |       |        | G     | C975  |      |      |

|       |       |       |       |       |       |         |       |       |       |       |       |       |
|-------|-------|-------|-------|-------|-------|---------|-------|-------|-------|-------|-------|-------|
| C2879 | C2803 | A2711 | U2611 | U2506 | A2435 | A2366   | A2288 | A2198 | G2125 | C2055 | U1976 | G1888 |
| A2892 | C2804 | U2712 | C2612 | C2517 | G2436 | G2367   | G2289 | A2199 | A2126 | G2056 | C1979 | A1889 |
| G2893 | G2805 | A2713 | U2613 | A2518 | U2437 | C2368   | G2290 | G2206 | G2127 | G2057 | G1980 | A1890 |
| G2894 | G2806 | G2714 | U2615 | U2519 | A2438 | A2369   | U2291 | C2207 | C2128 | A2058 | C1981 | G1896 |
| U2895 | U2809 | C2715 | C2619 | C2520 | C2440 | G2370   | C2292 | A2208 | G2131 | A2059 | C1982 | G1897 |
| U2896 | A2810 | U2716 | C2620 | G2524 | C2441 | C2374   | U2296 | U2218 | U2132 | A2060 | U1988 | U1898 |
| U2897 | G2811 | G2717 | C2621 | G2525 | C2442 | G2375   | C2297 | G2219 | G2133 | G2061 | G1989 | G1899 |
| U     | G2812 | G2718 | G2629 | G2526 | A2443 | A2376   | G2300 | G2222 | A2134 | A2062 | C1990 | A1900 |
| G     | A2813 | G2719 | G2630 | C2527 | G2444 | A2377   | G2301 | G2225 | G2135 | C2063 | U1991 | A1901 |
| A     | C2814 | A2720 | A2632 | U2528 | G2445 | A2378   | G2302 | G2226 | G2136 | C2064 | C1992 | C1902 |
| C     | C2815 | C2721 | U2636 | G2529 | G2446 | G2379   | G2303 | A2227 | C2140 | C2065 | G1906 | G1906 |
| C     | G2816 | U2722 | U2637 | G2530 | G2447 | G2380   | G2304 | A2228 | G2141 | G2067 | C1996 | A1912 |
| C     | G2817 | A2723 | U2638 | G2531 | A2448 | G2381   | A2305 | G2229 | C2142 | U2068 | G1997 | A1913 |
| C     | A2820 | G2724 | A2639 | A2542 | A2449 | C2382   | G2306 | G2230 | C2143 | G2069 | A1918 | C1914 |
| C     | G2821 | U2725 | C2646 | G2543 | A2450 | G2383   | G2307 | G2231 | G2144 | A2070 | G2001 | A1919 |
| C     | A2822 | A2726 | U2647 | G2544 | A2451 | G2384   | G2308 | U2232 | G2145 | G2072 | G2002 | C1920 |
| C     | G2823 | G2727 | U2648 | U2554 | U2457 | U2389   | A2311 | U2233 | C2146 | G2073 | G2003 | U1917 |
| C     | A2824 | U2728 | U2649 | U2555 | G2458 | U2390   | U2312 | U2234 | G2147 | U2074 | G2004 | A1918 |
| C     | G2825 | A2729 | U2650 | U2556 | A2459 | A2391   | U2313 | G2235 | G2148 | U2075 | G2005 | A1919 |
| C     | G2826 | G2730 | U2651 | U2557 | U2460 | A2392   | G2314 | G2236 | G2149 | G2076 | G2006 | C1920 |
| C     | U2831 | U2731 | U2652 | U2558 | U2461 | C2393   | C2315 | G2237 | G2150 | A2077 | G2009 | U1923 |
| C     | G2832 | A2732 | U2653 | C2559 | U2462 | C2394   | C2316 | G2238 | G2151 | G2078 | U2011 | G1929 |
| C     | U2833 | A2733 | U2654 | C2560 | U2463 | U2395   | C2317 | G2239 | G2152 | A2079 | G2012 | G1930 |
| C     | G2834 | U2734 | U2655 | C2561 | U2464 | U2396   | C2318 | U2240 | G2153 | U2080 | A2013 | U1931 |
| C     | A2835 | G2735 | U2656 | U2562 | C2465 | U2397   | G2319 | U2241 | G2154 | U2081 | A2014 | A1936 |
| C     | U2836 | U2736 | U2657 | U2563 | U2466 | U2400   | G2320 | U2242 | G2155 | G2082 | A2015 | A1937 |
| C     | G2837 | A2737 | U2658 | U2564 | U2467 | C2401   | G2321 | U2243 | G2156 | C2083 | U2016 | A1938 |
| C     | U2838 | U2738 | U2659 | U2565 | U2468 | C2402   | G2322 | U2244 | G2157 | U2084 | U2017 | A1939 |
| C     | G2839 | A2739 | U2660 | U2566 | U2469 | U2403   | G2323 | U2245 | G2158 | C1941 | G2023 | U1940 |
| C     | U2840 | U2740 | U2661 | U2567 | U2470 | U2404   | G2324 | U2246 | G2159 | C1942 | U1943 | G1942 |
| C     | G2841 | G2741 | U2662 | U2568 | U2471 | U2405   | U2325 | G2258 | G2160 | U2088 | U1944 | U1945 |
| C     | U2842 | A2742 | U2663 | U2569 | U2472 | U2406   | G2326 | G2259 | G2161 | U2089 | G2027 | A1952 |
| C     | A2843 | U2743 | U2664 | U2570 | U2473 | U2407   | G2327 | U2260 | G2162 | C2103 | A2030 | A1953 |
| C     | G2844 | G2744 | U2665 | U2571 | U2474 | U2408   | U2328 | U2261 | G2163 | G2104 | A2031 | G1954 |
| C     | U2845 | A2745 | U2666 | U2572 | U2475 | U2409   | G2329 | U2262 | G2164 | U2034 | U2032 | U1955 |
| C     | G2846 | U2746 | U2667 | U2573 | U2476 | U2410   | G2330 | U2263 | G2165 | G2035 | C2036 | U1956 |
| C     | U2847 | A2747 | U2668 | U2574 | U2477 | U2411   | U2331 | U2264 | G2166 | G2110 | C2037 | C1957 |
| C     | G2848 | U2748 | U2669 | U2575 | U2478 | U2412   | U2332 | U2265 | G2167 | C2111 | G2038 | U1958 |
| C     | U2849 | G2749 | U2670 | U2576 | U2479 | U2413   | G2333 | U2266 | G2168 | G2112 | C2039 | G1962 |
| C     | A2850 | A2750 | U2671 | U2577 | U2480 | U2414   | G2334 | U2267 | G2169 | C2113 | U2040 | U1963 |
| C     | G2851 | U2751 | U2672 | U2578 | U2481 | U2415   | G2335 | U2268 | G2170 | G2114 | U2041 | G1964 |
| C     | U2852 | A2752 | U2673 | U2579 | U2482 | U2416   | G2336 | U2269 | G2171 | G2115 | A2042 | C1965 |
| C     | G2853 | G2753 | U2674 | U2580 | U2483 | U2417   | G2337 | U2270 | G2172 | A2117 | C2043 | C1967 |
| C     | U2854 | U2754 | U2675 | U2581 | U2484 | U2418   | G2338 | U2271 | G2173 | G2118 | G2046 | A1968 |
| C     | G2855 | A2755 | U2676 | U2582 | U2485 | U2419   | U2339 | U2272 | G2174 | A2119 | G2120 | A1969 |
| C     | U2856 | U2756 | U2677 | U2583 | U2486 | U2420   | G2340 | U2273 | G2175 | G2121 | G2049 | A1970 |
| C     | G2857 | A2757 | U2678 | U2584 | U2487 | U2421   | U2341 | U2274 | G2176 | G2122 | C2050 | A1971 |
| C     | U2858 | U2758 | U2679 | U2585 | U2488 | U2422   | U2342 | U2275 | G2177 | U2123 | A2051 | G1972 |
| C     | A2859 | G2759 | U2680 | U2586 | U2489 | U2423   | U2343 | U2276 | G2178 | G2124 | G2052 |       |
| C     | G2860 | U2760 | U2681 | U2587 | U2490 | U2424   | U2344 | U2277 | G2179 |       |       |       |
| C     | U2861 | A2761 | U2682 | U2588 | U2491 | U2425   | U2345 | U2278 | G2180 |       |       |       |
| C     | G2862 | G2762 | U2683 | U2589 | U2492 | U2426   | U2346 | U2279 | G2181 |       |       |       |
| C     | U2863 | A2763 | U2684 | U2590 | U2493 | U2427   | U2347 | U2280 | G2182 |       |       |       |
| C     | G2864 | U2764 | U2685 | U2591 | U2494 | U2428   | U2348 | U2281 | G2183 |       |       |       |
| C     | U2865 | A2765 | U2686 | U2592 | U2495 | U2429   | U2349 | U2282 | G2184 |       |       |       |
| C     | G2866 | G2766 | U2687 | U2593 | U2496 | U2430   | U2350 | U2283 | G2185 |       |       |       |
| C     | U2867 | U2767 | U2688 | U2594 | U2497 | U2431   | U2351 | U2284 | G2186 |       |       |       |
| C     | G2868 | A2768 | U2689 | U2595 | U2498 | U2432   | U2352 | U2285 | G2187 |       |       |       |
| C     | U2869 | G2769 | U2690 | U2596 | U2499 | U2433   | U2353 | U2286 | G2188 |       |       |       |
| C     | G2870 | U2770 | U2691 | U2597 | U2500 | U2434   | U2354 | U2287 | G2189 |       |       |       |
| C     | U2871 | A2771 | U2692 | U2598 | U2501 | U2435   | U2355 | U2288 | G2190 |       |       |       |
| C     | G2872 | G2772 | U2693 | U2599 | U2502 | U2436   | U2356 | U2289 | G2191 |       |       |       |
| C     | U2873 | U2773 | U2694 | U2600 | U2503 | U2437   | U2357 | U2290 | G2192 |       |       |       |
| C     | G2874 | A2774 | U2695 | U2601 | U2504 | U2438   | U2358 | U2291 | G2193 |       |       |       |
| C     | U2875 | G2775 | U2696 | U2602 | U2505 | U2439   | U2359 | U2292 | G2194 |       |       |       |
| C     | G2876 | U2776 | U2697 | U2603 | U2506 | U2440   | U2360 | U2293 | G2195 |       |       |       |
| C     | U2877 | A2777 | U2698 | U2604 | U2507 | U2441   | U2361 | U2294 | G2196 |       |       |       |
| C     | G2878 | G2778 | U2699 | U2605 | U2508 | U2442   | U2362 | U2295 | G2197 |       |       |       |
| C     | U2879 | U2779 | U2700 | U2606 | U2509 | U2443   | U2363 | U2296 | G2198 |       |       |       |
| C     | A2880 | A2780 | U2701 | U2607 | U2510 | U2444   | U2364 | U2297 | G2199 |       |       |       |
| C     | G2881 | G2781 | U2702 | U2608 | U2511 | U2445   | U2365 | U2298 | G2200 |       |       |       |
| C     | U2882 | U2782 | U2703 | U2609 | U2512 | U2446   | U2366 | U2299 | G2201 |       |       |       |
| C     | G2883 | A2783 | U2704 | U2610 | U2513 | U2447   | U2367 | U2300 | G2202 |       |       |       |
| C     | U2884 | G2784 | U2705 | U2611 | U2514 | U2448   | U2368 | U2301 | G2203 |       |       |       |
| C     | G2885 | U2785 | U2706 | U2612 | U2515 | U2449   | U2369 | U2302 | G2204 |       |       |       |
| C     | U2886 | A2786 | U2707 | U2613 | U2516 | U2450   | U2370 | U2303 | G2205 |       |       |       |
| C     | G2887 | G2787 | U2708 | U2614 | U2517 | U2451   | U2371 | U2304 | G2206 |       |       |       |
| C     | U2888 | U2788 | U2709 | U2615 | U2518 | U2452   | U2372 | U2305 | G2207 |       |       |       |
| C     | G2889 | A2789 | U2710 | U2616 | U2519 | U2453   | U2373 | U2306 | G2208 |       |       |       |
| C     | U2890 | G2790 | U2711 | U2617 | U2520 | U2454   | U2374 | U2307 | G2209 |       |       |       |
| C     | G2891 | U2791 | U2712 | U2618 | U2521 | U2455   | U2375 | U2308 | G2210 |       |       |       |
| C     | U2892 | A2792 | U2713 | U2619 | U2522 | U2456   | U2376 | U2309 | G2211 |       |       |       |
| C     | G2893 | G2793 | U2714 | U2620 | U2523 | U2457   | U2377 | U2310 | G2212 |       |       |       |
| C     | U2894 | U2794 | U2715 | U2621 | U2524 | U2458   | U2378 | U2311 | G2213 |       |       |       |
| C     | G2895 | A2795 | U2716 | U2622 | U2525 | U2459   | U2379 | U2312 | G2214 |       |       |       |
| C     | U2896 | G2796 | U2717 | U2623 | U2526 | U2460   | U2380 | U2313 | G2215 |       |       |       |
| C     | G2897 | U2797 | U2718 | U2624 | U2527 | U2461   | U2381 | U2314 | G2216 |       |       |       |
| C     | U2898 | A2798 | U2719 | U2625 | U2528 | U2462   | U2382 | U2315 | G2217 |       |       |       |
| C     | G2899 | G2799 | U2720 | U2626 | U2529 | U2463   | U2383 | U2316 | G2218 |       |       |       |
| C     | U2900 | U2800 | U2721 | U2627 | U2530 | U2464   | U2384 | U2317 | G2219 |       |       |       |
| C     | G2901 | A2801 | U2722 | U2628 | U2531 | U2465   | U2385 | U2318 | G2220 |       |       |       |
| C     | U2902 | G2802 | U2723 | U2629 | U2532 | U2466   | U2386 | U2319 | G2221 |       |       |       |
| C     | G2903 | U2803 | U2724 | U2630 | U2533 | U2467   | U2387 | U2320 | G2222 |       |       |       |
| C     | U2904 | A2804 | U2725 | U2631 | U2534 | U2468   | U2388 | U2321 | G2223 |       |       |       |
| C     | G2905 | G2805 | U2726 | U2632 | U2535 | U2469   | U2389 | U2322 | G2224 |       |       |       |
| C     | U2906 | U2806 | U2727 | U2633 | U2536 | U2470   | U2390 | U2323 | G2225 |       |       |       |
| C     | G2907 | A2807 | U2728 | U2634 | U2537 | U2471   | U2391 | U2324 | G2226 |       |       |       |
| C     | U2908 | G2808 | U2729 | U2635 | U2538 | U2472   | U2392 | U2325 | G2227 |       |       |       |
| C     | G2909 | U2809 | U2730 | U2636 | U2539 | U2473   | U2393 | U2326 | G2228 |       |       |       |
| C     | U2910 | A2810 | U2731 | U2637 | U2540 | U2474   | U2394 | U2327 | G2229 |       |       |       |
| C     | G2911 | G2811 | U2732 | U2638 | U2541 | U2475   | U2395 | U2328 | G2230 |       |       |       |
| C     | U2912 | U2812 | A2733 | U2639 | U2542 | U2476   | U2396 | U2329 | G2231 |       |       |       |
| C     | G2913 | A2813 | U2734 | U2640 | U2543 | U2477   | U2397 | U2330 | G2232 |       |       |       |
| C     | U2914 | G2814 | G2735 | U2641 | U2544 | U2478   | U2398 | U2331 | G2233 |       |       |       |
| C     | G2915 | U2815 | U2736 | U2642 | U2545 | U2479</ |       |       |       |       |       |       |



|       |       |       |       |       |       |       |        |        |       |       |        |       |
|-------|-------|-------|-------|-------|-------|-------|--------|--------|-------|-------|--------|-------|
| U2118 | A2033 | G1945 | C1838 | C1752 | C1648 | A1558 | U1481  | A1395  | U1312 | A1220 | U1130  | C     |
| A2119 | U2034 | A1952 | G1839 | C1753 | G1651 | A1559 | G1482  | A1396  | C1314 | C1221 | G1131  | U     |
| G2120 | G2035 | A1953 | G1840 | G1754 | G1652 | G1560 | G1484  | U1397  | C1314 | G1223 | A1132  | A     |
| U2122 | C2036 | A1954 | G1846 | G1755 | G1653 | C1565 | A1486  | G1403  | G1319 | G1224 | G1133  | G     |
| G2123 | U2041 | U1955 | A1847 | U1757 | A1654 | C1566 | G1487  | C1403  | C1320 | G1227 | G1136  | A     |
| A2042 | A2042 | U1956 | A1848 | G1758 | A1654 | A1566 | G1488  | C1404  | A1321 | G1227 | G1139  | A     |
| G2125 | C2043 | C1957 | A1853 | A1759 | A1664 | A1567 | U1489  | U1405  | G1324 | C1230 | G1140  | G     |
| A2126 | G2046 | C1958 | A1854 | G1763 | G1666 | A1569 | G1490  | U1406  | G1325 | G1231 | U1141  | A     |
| G2127 | G2046 | C1958 | A1854 | G1763 | G1667 | A1570 | G1492  | C1408  | G1325 | G1232 | U1142  | G     |
| C2128 | G2050 | C1962 | G1858 | G1764 | A1668 | C1577 | C1493  | C1409  | U1329 | G1236 | A1142A | C     |
| U2129 | U1963 | U1963 | U1854 | A1764 | A1669 | U1578 | A1494  | A1412  | C1330 | A1237 | A1143  | C     |
| A2051 | G1964 | G1964 | U1854 | A1769 | G1674 | A1579 | A1495  | G1413  | A1331 | G1238 | G1144  | A     |
| G2131 | C1965 | C1965 | G1865 | A1773 | G1675 | A1579 | A1496  | G1413  | G1332 | G1239 | G1149  | C     |
| C2055 | G2056 | C1967 | C1866 | A1773 | A1676 | A1583 | U1497  | G1416  | C1333 | U1240 | C1150  | C     |
| A2056 | G2056 | G1968 | A1876 | U1778 | A1677 | C1584 | C1499  | G1417  | A1336 | U1240 | G1151  | U     |
| C2059 | A2059 | A1969 | A1877 | U1779 | G1678 | A1586 | G1500  | G1418  | G1337 | A1247 | C1152  | U     |
| A2060 | A2060 | U1970 | G1878 | U1779 | G1678 | A1587 | C1501  | A1419  | G1338 | A1247 | G1153  | U     |
| G2061 | A2061 | A1971 | C1879 | A1780 | G1681 | C1588 | U1502  | U1420  | G1339 | G1248 | G1154  | A     |
| A2062 | A2062 | A1972 | C1880 | C1781 | G1681 | C1589 | G1503  | G1421  | U1340 | U1249 | A1155  | A     |
| C2133 | G2062 | C1882 | C1881 | G1782 | G1682 | C1589 | U1503  | G1421  | U1341 | G1250 | A1156  | A     |
| A2134 | G1980 | G1980 | C1882 | A1783 | U1688 | G1594 | C1504  | A1427  | A1342 | G1251 | G1157  | G     |
| A2135 | A1981 | A1981 | G1883 | A1784 | A1688 | G1594 | C1504  | A1427  | A1342 | G1251 | G1157  | G     |
| C2136 | U1981 | U1981 | G1883 | A1785 | A1689 | G1595 | A1508  | C1428  | G1343 | G1252 | A      |       |
| G2145 | U2068 | C1982 | A1884 | A1785 | A1689 | G1595 | C1509  | G1429  | G1344 | A1253 | G1162  | A     |
| C2146 | G2069 | A1987 | A1885 | A1786 | U1693 | C1598 | A1509A | C1430  | C1345 | U1254 | G1162  | G     |
| G2147 | G2070 | G1987 | A1888 | A1787 | U1693 | C1598 | A1509A | U1431  | C1345 | A1254 | G1162  | G     |
| U2148 | A2071 | C1988 | G1888 | C1790 | G1694 | U1602 | C1513  | A1434  | A1349 | G1256 | G1169  | C     |
| C2072 | G1989 | C1989 | A1889 | A1791 | G1695 | A1603 | G1513  | A1434  | A1349 | G1256 | G1170  | C     |
| G2073 | C2072 | C1989 | A1889 | A1791 | G1696 | A1603 | G1513  | A1434  | A1349 | G1256 | G1170  | C     |
| U2075 | U1991 | U1991 | U1898 | C1990 | G1697 | U1602 | C1513  | A1434  | A1349 | G1256 | G1170  | C     |
| C2076 | G1992 | G1992 | G1899 | U1796 | A1697 | C1607 | G1520  | C1437  | U1352 | G1264 | G1171  | U     |
| U2077 | U2075 | U1993 | A1900 | C1797 | G1698 | A1607 | U1523  | C1437  | A1353 | A1265 | A1174  | A     |
| G2086 | U2086 | C1993 | A1901 | U1798 | G1699 | A1608 | G1524  | C1437  | A1354 | G1266 | G1175  | A     |
| C2087 | G2087 | U1995 | C1902 | G1799 | A1700 | A1609 | G1525  | A1445  | G1355 | U1267 | G1176  | U1097 |
| G2090 | G2090 | U1996 | G1903 | C1800 | A1701 | C1611 | G1526  | C1445A | G1356 | A1268 | A1177  | A1098 |
| A2169 | U2091 | C1997 | U1906 | G1801 | U1706 | C1612 | G1527  | A1449  | U1357 | A1269 | C1178  | G1099 |
| U2091 | U2091 | G1997 | G1906 | C1801 | U1706 | C1612 | G1527  | A1449  | U1357 | A1269 | C1178  | G1099 |
| A2170 | U2092 | C1998 | A1912 | A1802 | G1707 | G1613 | A1528A | C1450  | G1358 | C1270 | C1179  | C1100 |
| U2092 | A2170 | U1999 | A1803 | C1708 | C1707 | G1613 | G1529  | G1450A | A1359 | A1271 | C1180  | U1101 |
| G2093 | G2093 | G2000 | C1804 | U1805 | C1711 | A1615 | C1532  | C1451  | A1360 | A1272 | C1102  | C1102 |
| A2173 | A2173 | A2001 | A1913 | U1805 | C1711 | A1616 | C1532  | C1451  | A1360 | A1272 | C1102  | C1102 |
| C2174 | C2097 | G2001 | C1914 | U1915 | C1712 | C1617 | G      | U1453  | G1363 | U1273 | G1187  | A1103 |
| G2175 | U2098 | G2009 | U1915 | G1815 | C1712 | C1617 | U      | U1453  | G1364 | A1275 | U1188  | C1104 |
| A2176 | U2098 | G2010 | U1915 | G1816 | G1718 | A1618 | A      | G1455  | A1365 | A1276 | A1189  | U1105 |
| C2177 | U2099 | G2010 | A1918 | G1817 | G1718 | A1618 | A      | G1456  | C1368 | G1281 | G1191  | G1106 |
| G2178 | C2103 | G2012 | A1919 | U1818 | G1718 | A1618 | A      | C1457  | G1368 | G1281 | G1191  | G1106 |
| C2179 | G2104 | A2013 | A1819 | A1722 | G1721 | G1622 | G1537  | A1457  | G1368 | G1281 | G1191  | G1106 |
| U2182 | C2105 | A2014 | G1929 | U1820 | A1722 | G1622 | G1537  | A1457  | G1368 | G1281 | G1191  | G1106 |
| C2106 | C2107 | A2015 | G1930 | A1821 | U1739 | G1626 | G1540  | A1460  | G1371 | A1286 | G1195  | A1111 |
| G2182 | G2106 | G2018 | G1935 | G1824 | U1739 | G1626 | U1540  | A1460  | U1372 | A1286 | G1195  | A1111 |
| C2183 | C2107 | G2018 | A1825 | G1824 | G1740 | A1634 | G1541  | G1461  | G1374 | A1287 | G1203  | U1113 |
| G2187 | U2109 | A2019 | A1936 | G1826 | A1741 | G1635 | A1542  | G1461  | G1374 | U1288 | A1204  | G1114 |
| C2110 | G2110 | A2020 | A1937 | G1826 | C1744 | C1636 | A1544  | G1465  | G1374 | C1289 | U1205  | G1115 |
| A2190 | C2111 | C2021 | A1938 | C1827 | C1744 | A1637 | A1544  | G1466  | A1378 | C1297 | G1208  | G1117 |
| G2191 | U2112 | U2022 | U1939 | U1827 | G1746 | C1640 | C1547  | C1467  | A1379 | U1300 | G1209  | G1122 |
| C2192 | U2113 | G2023 | A1829 | G1828 | G1747 | A1641 | C1548  | A1471  | G1380 | A1301 | G1209  | G1122 |
| G2193 | A2114 | C1941 | U1940 | A1829 | G1747 | A1641 | C1548  | A1471  | A1384 | A1302 | A1210  | G1125 |
| C2115 | G2115 | A2030 | G1835 | G1835 | G1748 | C1645 | C1550  | G1473  | A1385 | G1303 | G1212  | A1126 |
| A2116 | G2116 | A2031 | C1836 | G1836 | A1749 | G1645 | C1551  | C1474  | C1386 | G1310 | G1218  | A1127 |
| U2197 | A2117 | C2032 | U1943 | C1837 | G1750 | C1646 | A1554  | G1475  | U1391 | G1311 | G1219  | A1128 |
| C2198 | C2117 | C2032 | U1944 | C1838 | C1751 | C1647 | A1554  | G1475  | U1391 | G1311 | G1219  | A1128 |

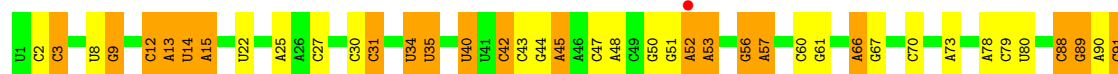




• Molecule 26: 5S rRNA

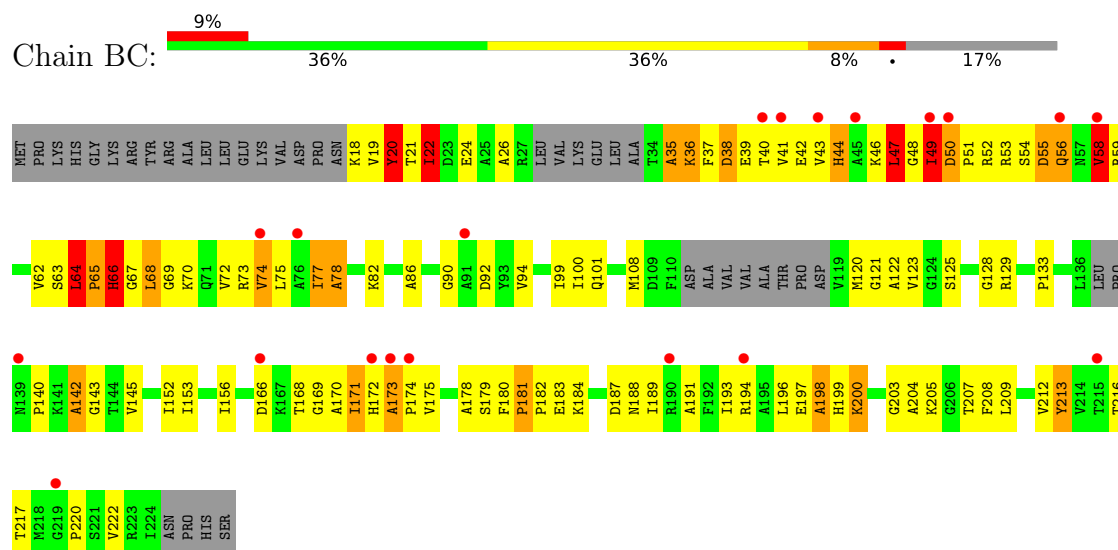


• Molecule 26: 5S rRNA

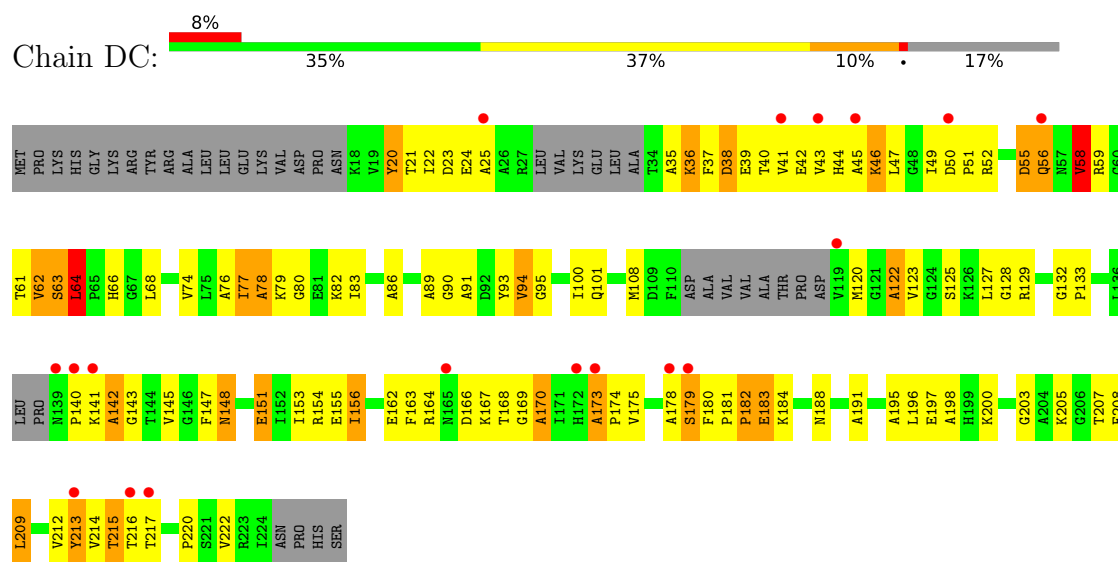




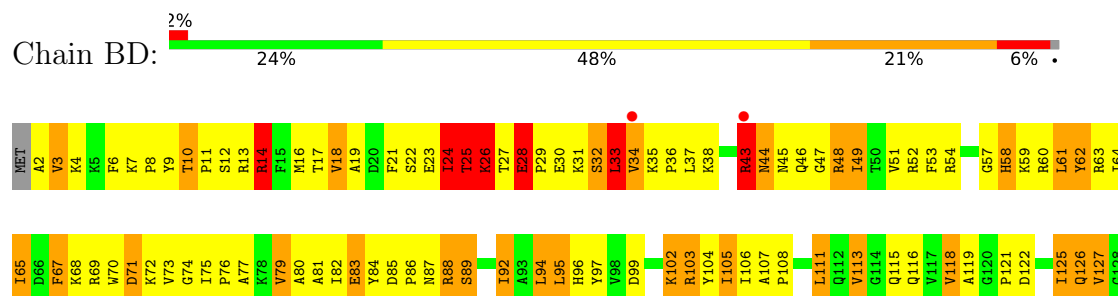
• Molecule 27: 50S RIBOSOMAL PROTEIN L1

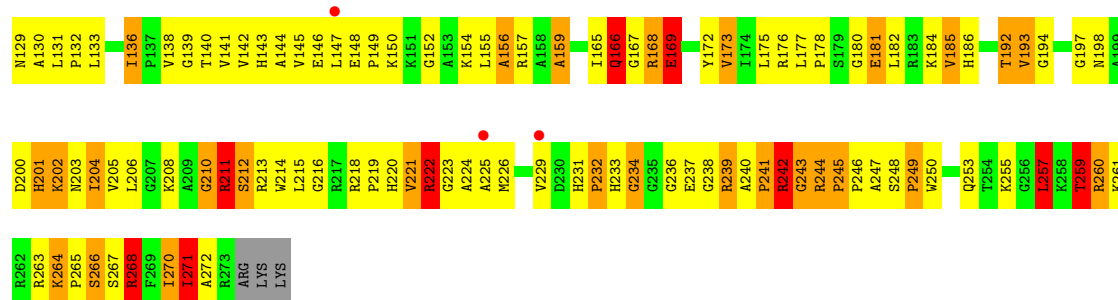


• Molecule 27: 50S RIBOSOMAL PROTEIN L1

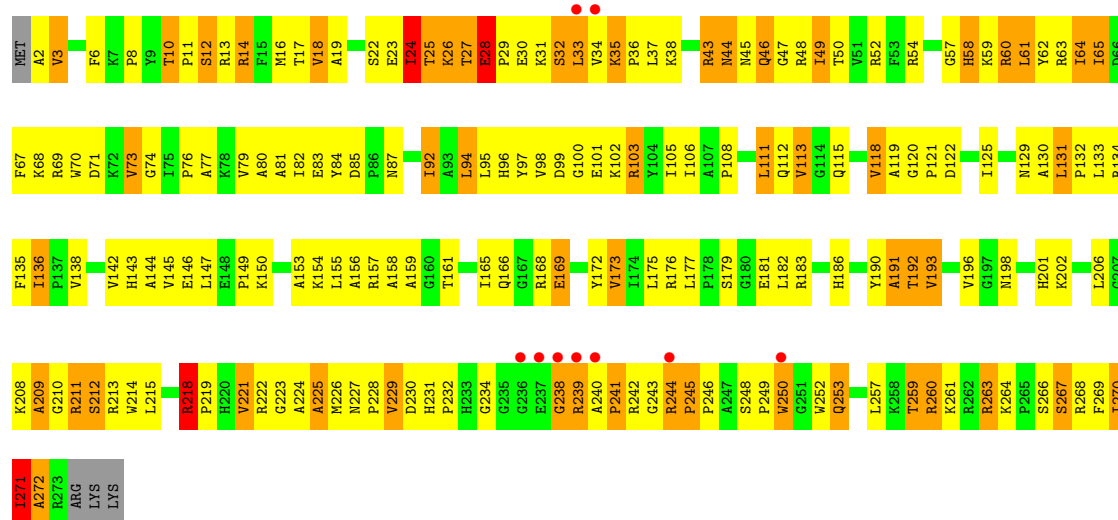


• Molecule 28: 50S RIBOSOMAL PROTEIN L2

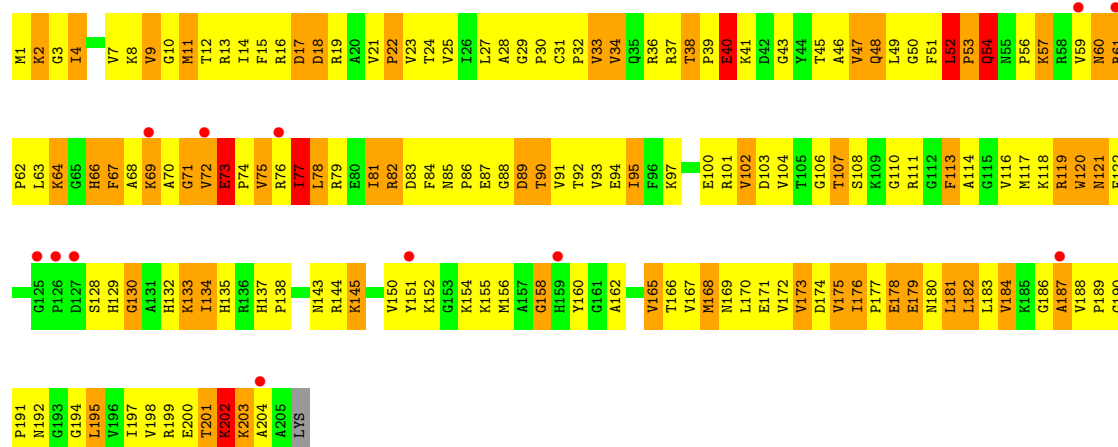




• Molecule 28: 50S RIBOSOMAL PROTEIN L2

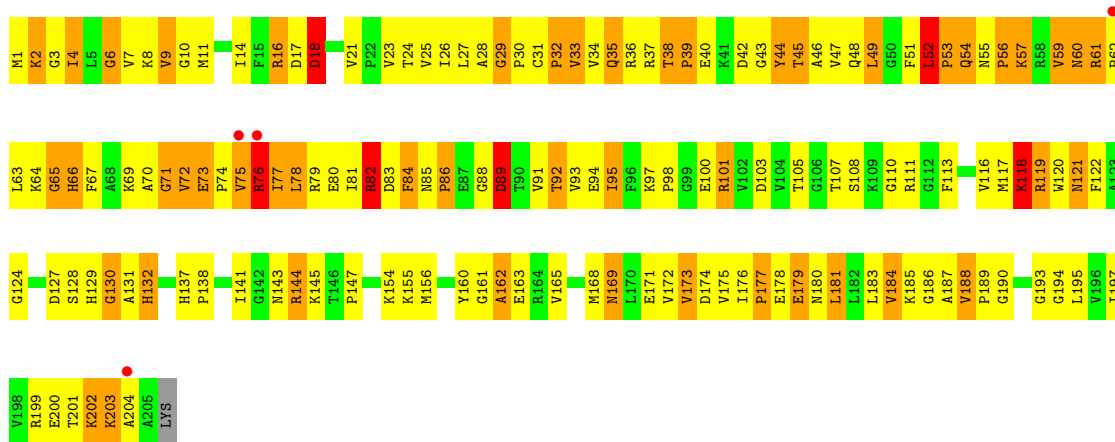


• Molecule 29: 50S RIBOSOMAL PROTEIN L3

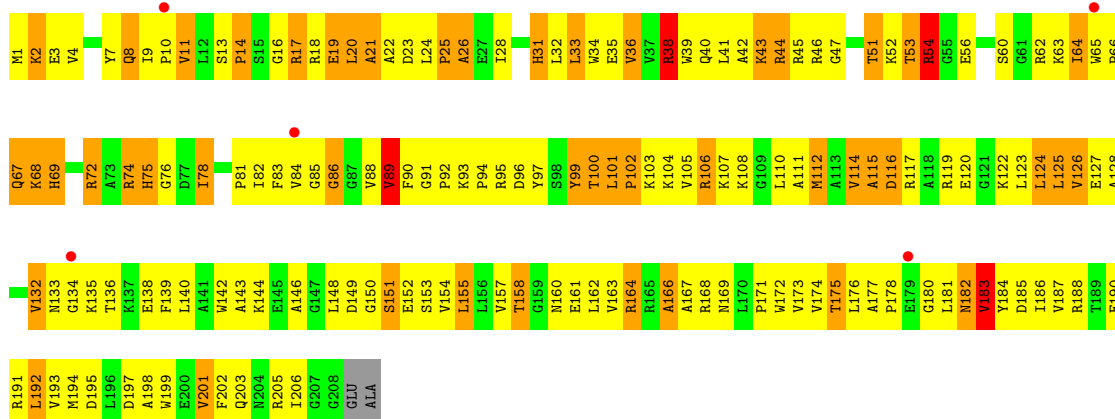


• Molecule 29: 50S RIBOSOMAL PROTEIN L3

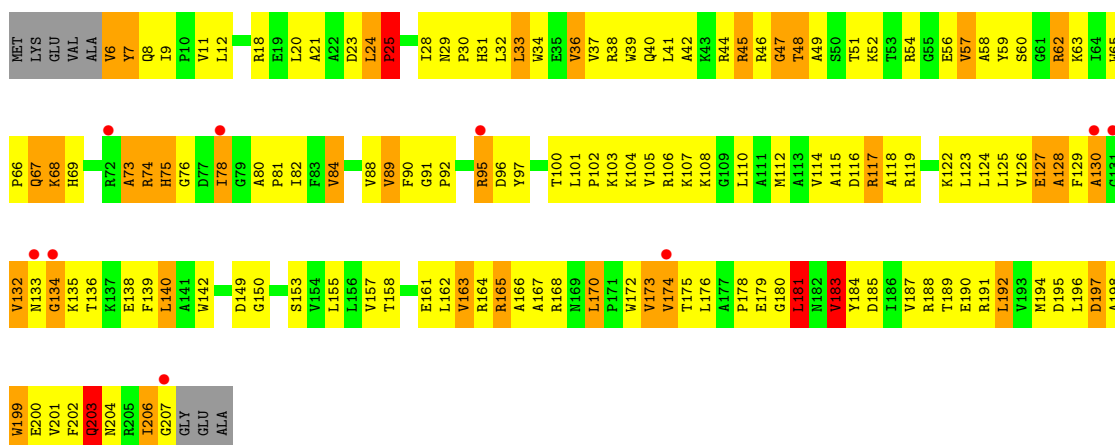




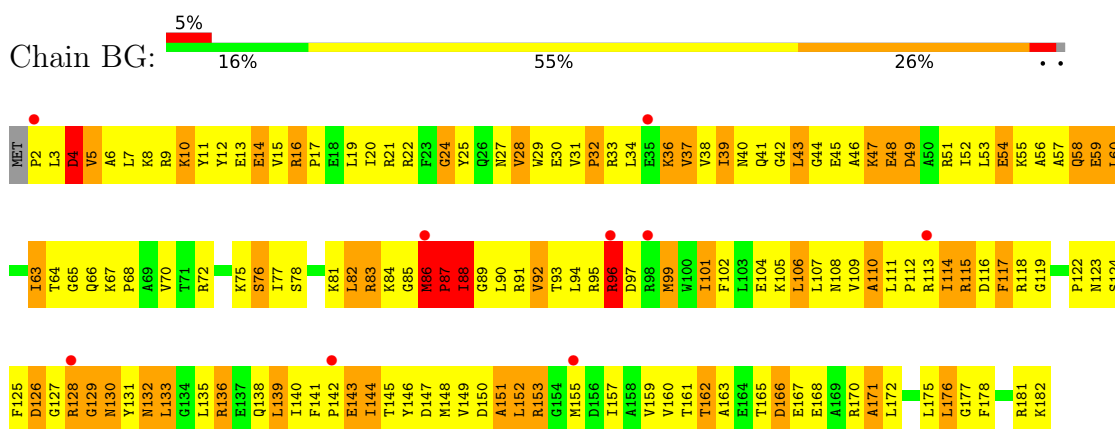
• Molecule 30: 50S RIBOSOMAL PROTEIN L4



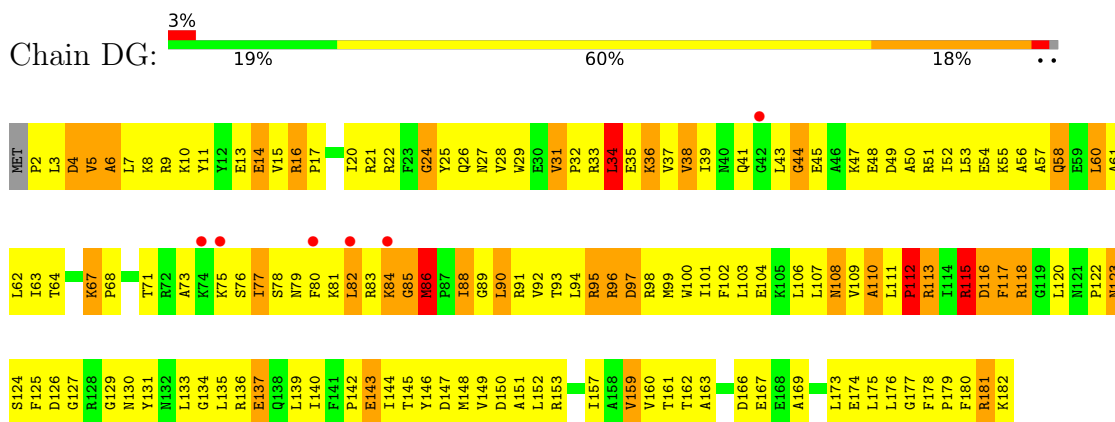
• Molecule 30: 50S RIBOSOMAL PROTEIN L4



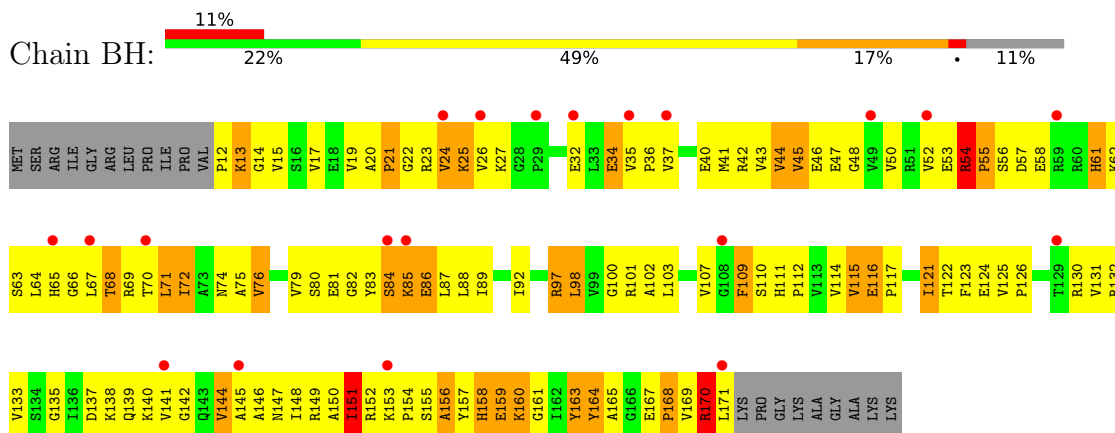
• Molecule 31: 50S RIBOSOMAL PROTEIN L5



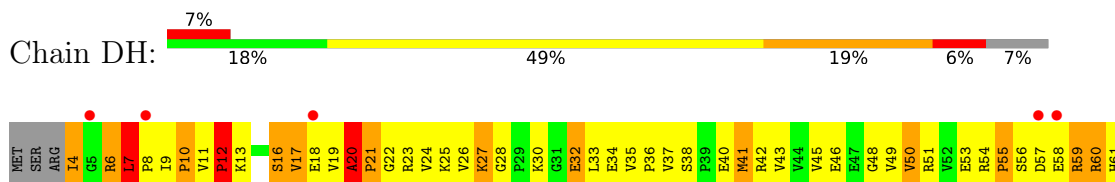
• Molecule 31: 50S RIBOSOMAL PROTEIN L5

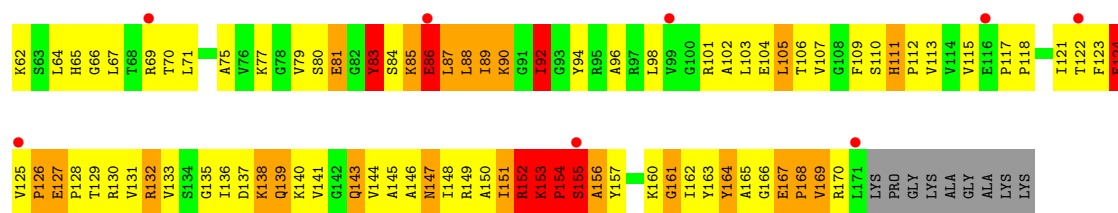


• Molecule 32: 50S RIBOSOMAL PROTEIN L6

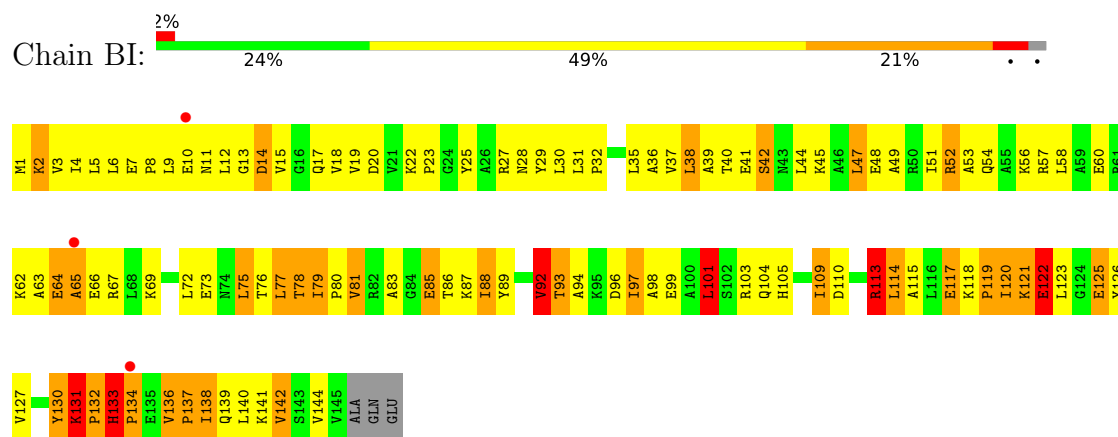


• Molecule 32: 50S RIBOSOMAL PROTEIN L6

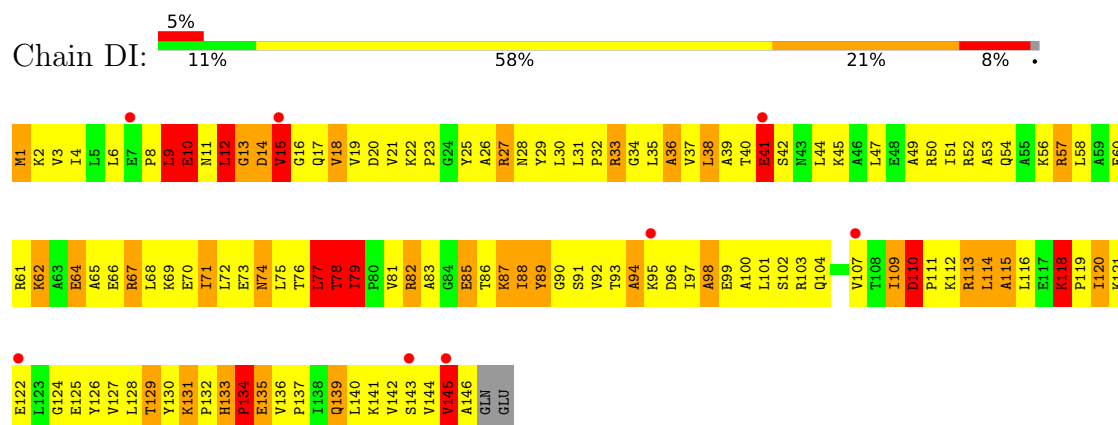




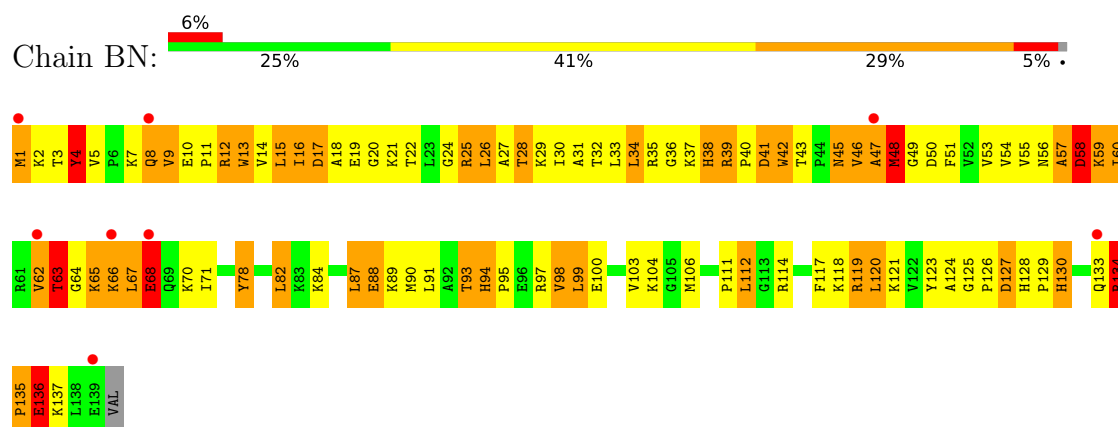
• Molecule 33: 50S RIBOSOMAL PROTEIN L9



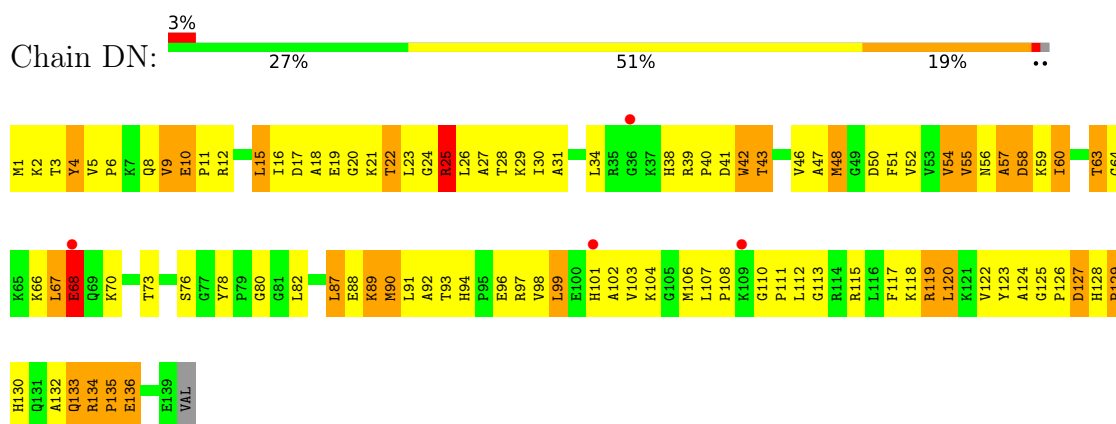
• Molecule 33: 50S RIBOSOMAL PROTEIN L9



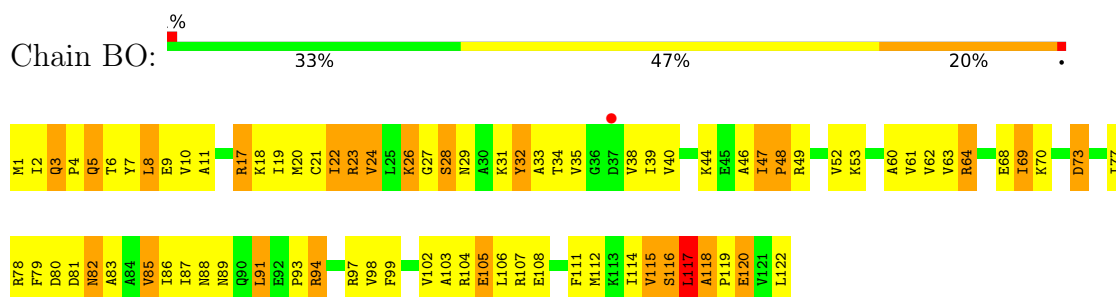
• Molecule 34: 50S RIBOSOMAL PROTEIN L13



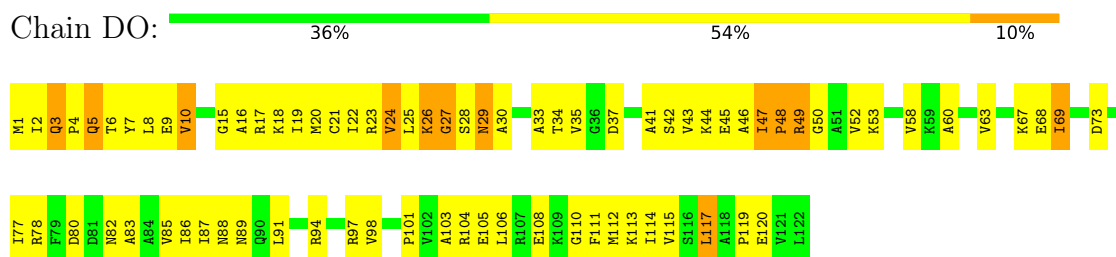
• Molecule 34: 50S RIBOSOMAL PROTEIN L13



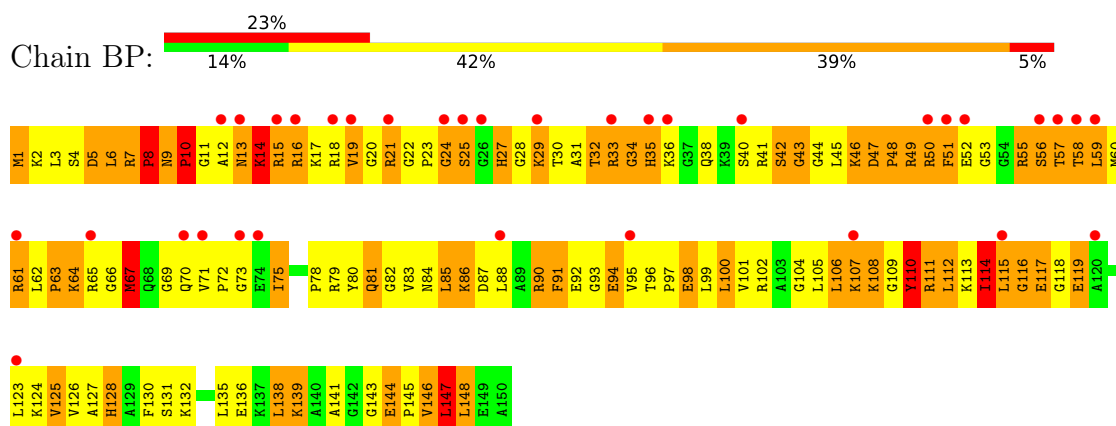
• Molecule 35: 50S RIBOSOMAL PROTEIN L14



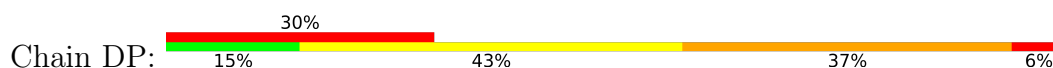
• Molecule 35: 50S RIBOSOMAL PROTEIN L14

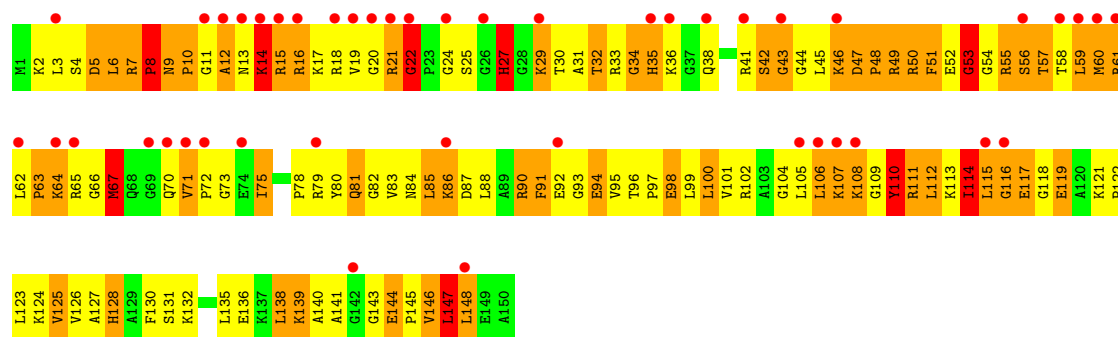


• Molecule 36: 50S RIBOSOMAL PROTEIN L15

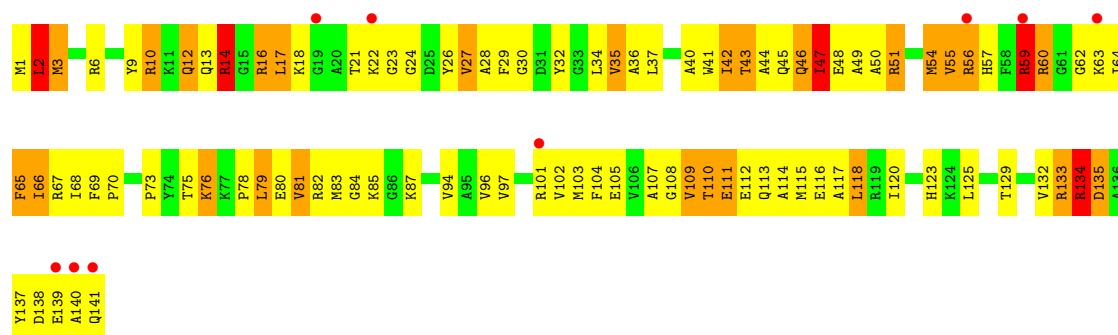


• Molecule 36: 50S RIBOSOMAL PROTEIN L15

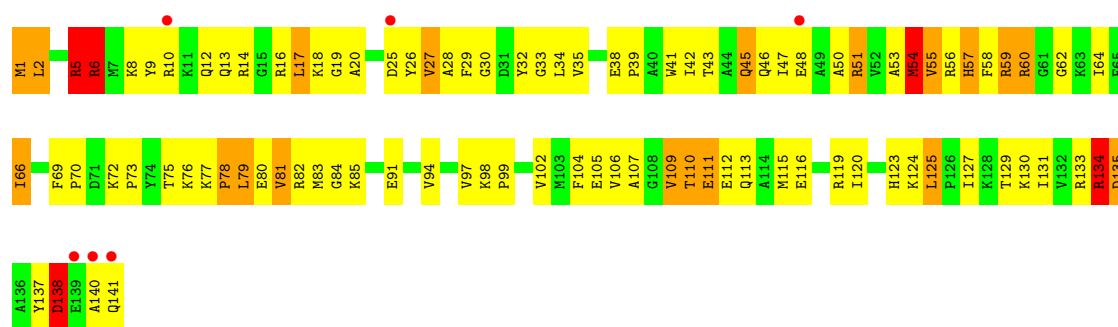




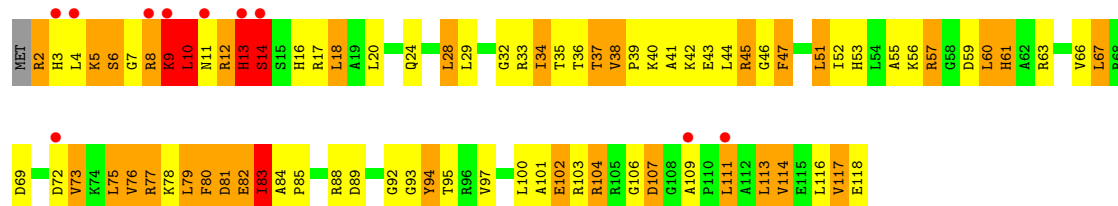
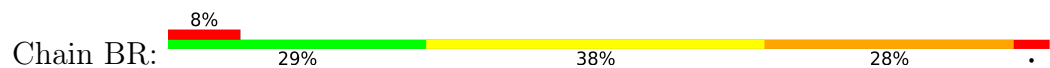
• Molecule 37: 50S RIBOSOMAL PROTEIN L16



• Molecule 37: 50S RIBOSOMAL PROTEIN L16



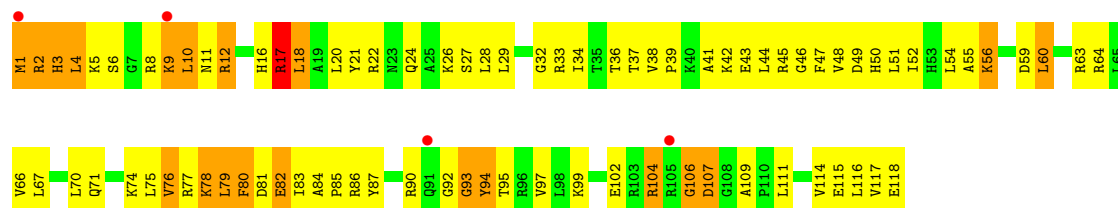
• Molecule 38: 50S RIBOSOMAL PROTEIN L17





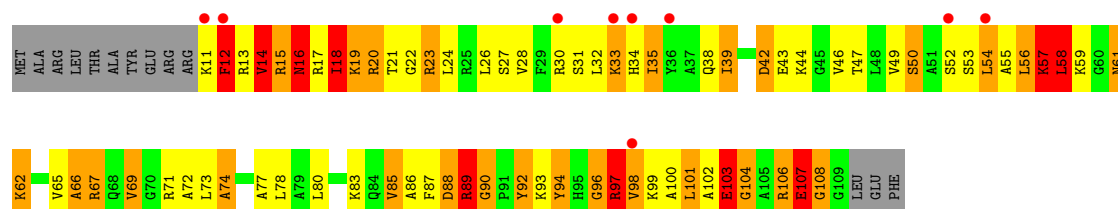
## ● Molecule 38: 50S RIBOSOMAL PROTEIN L17

Chain DR: 

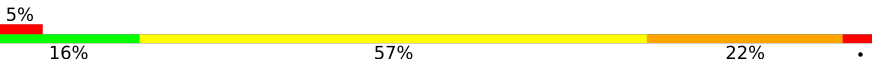


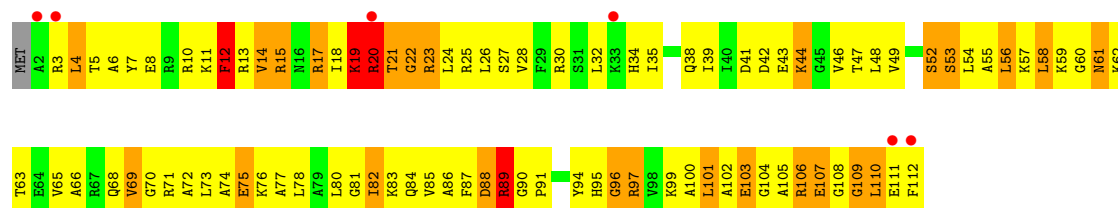
## ● Molecule 39: 50S RIBOSOMAL PROTEIN L18

Chain BS: 



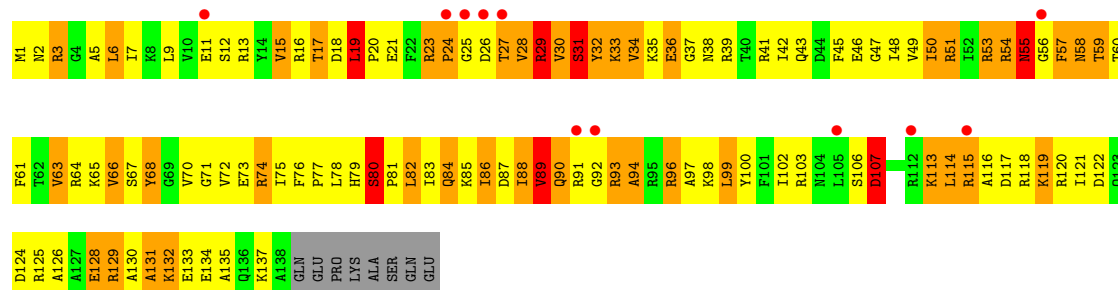
## ● Molecule 39: 50S RIBOSOMAL PROTEIN L18

Chain DS: 



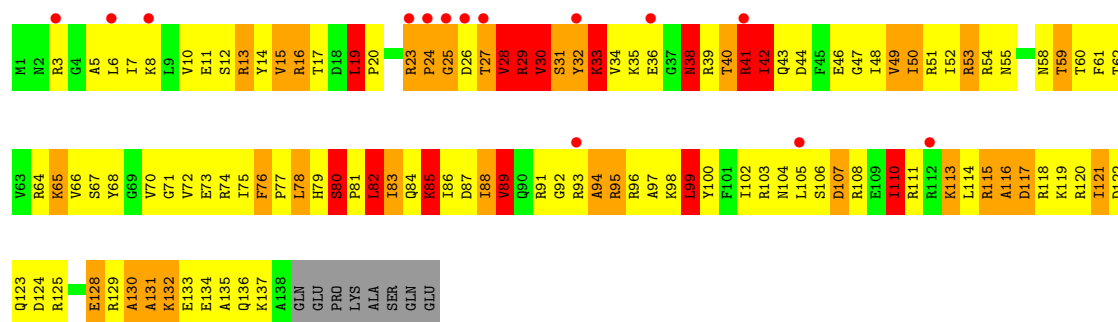
## ● Molecule 40: 50S RIBOSOMAL PROTEIN L19

Chain BT: 

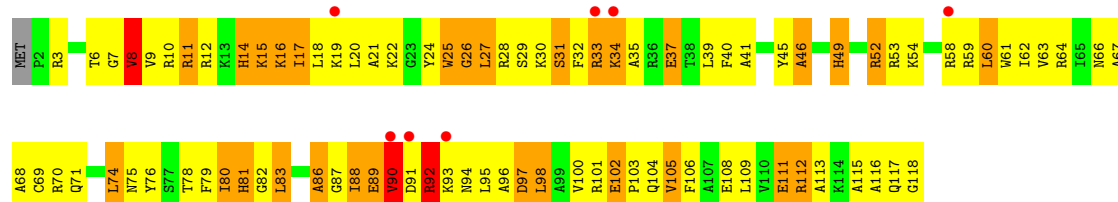


## ● Molecule 40: 50S RIBOSOMAL PROTEIN L19

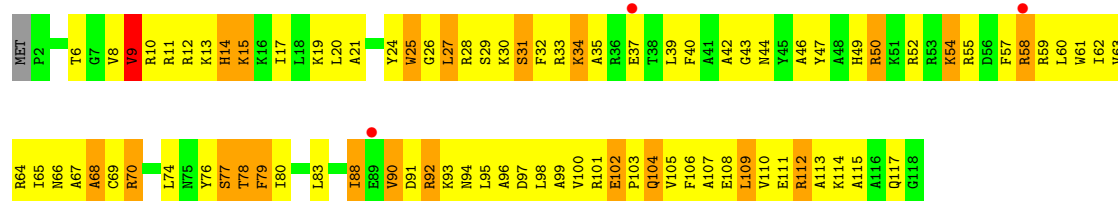
Chain DT: 



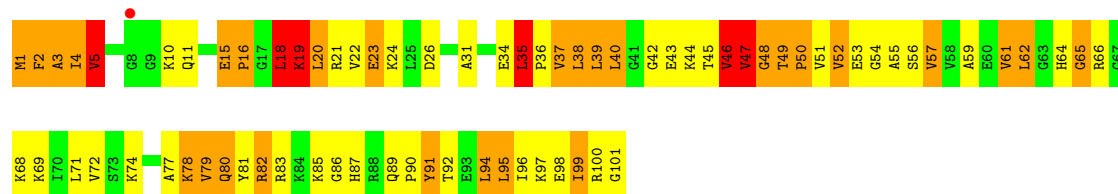
• Molecule 41: 50S RIBOSOMAL PROTEIN L20



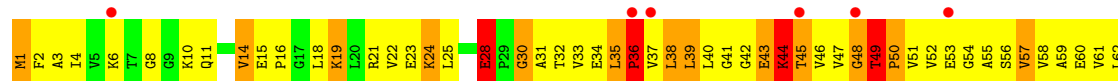
• Molecule 41: 50S RIBOSOMAL PROTEIN L20

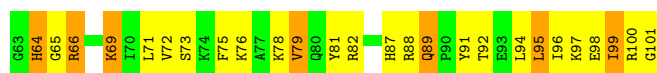


• Molecule 42: 50S RIBOSOMAL PROTEIN L21



• Molecule 42: 50S RIBOSOMAL PROTEIN L21

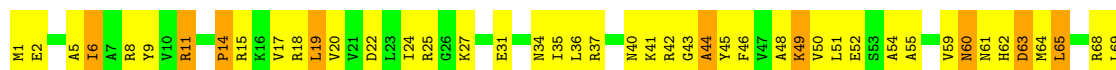




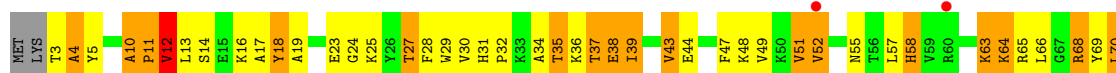
• Molecule 43: 50S RIBOSOMAL PROTEIN L22



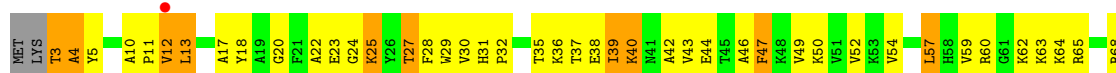
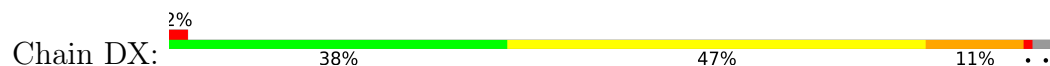
• Molecule 43: 50S RIBOSOMAL PROTEIN L22



• Molecule 44: 50S RIBOSOMAL PROTEIN L23

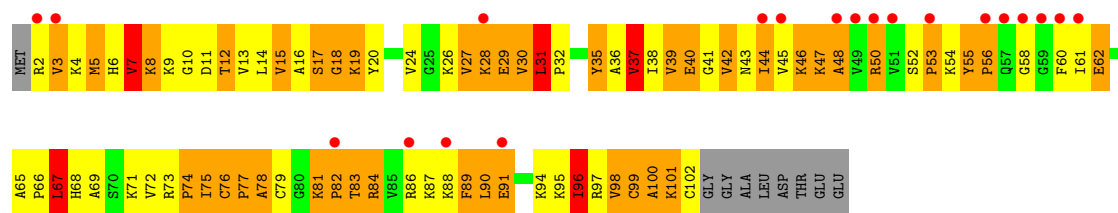


• Molecule 44: 50S RIBOSOMAL PROTEIN L23

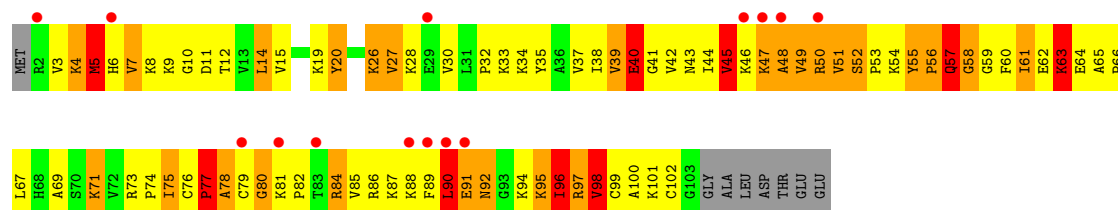
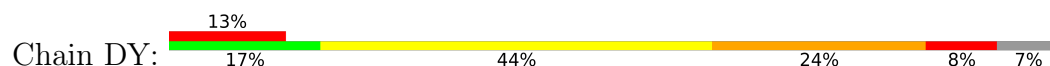


• Molecule 45: 50S RIBOSOMAL PROTEIN L24

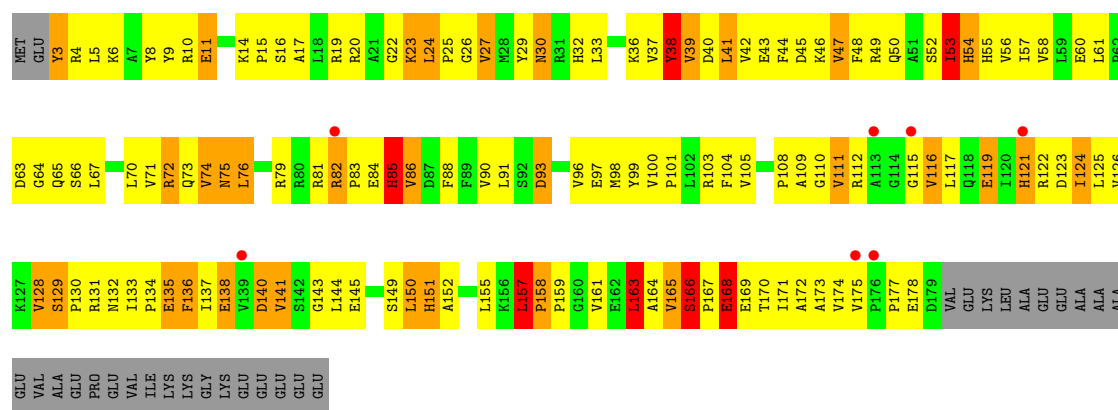
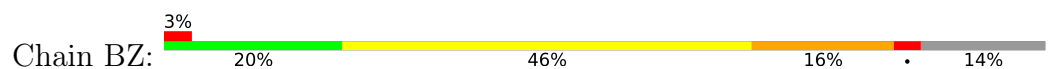




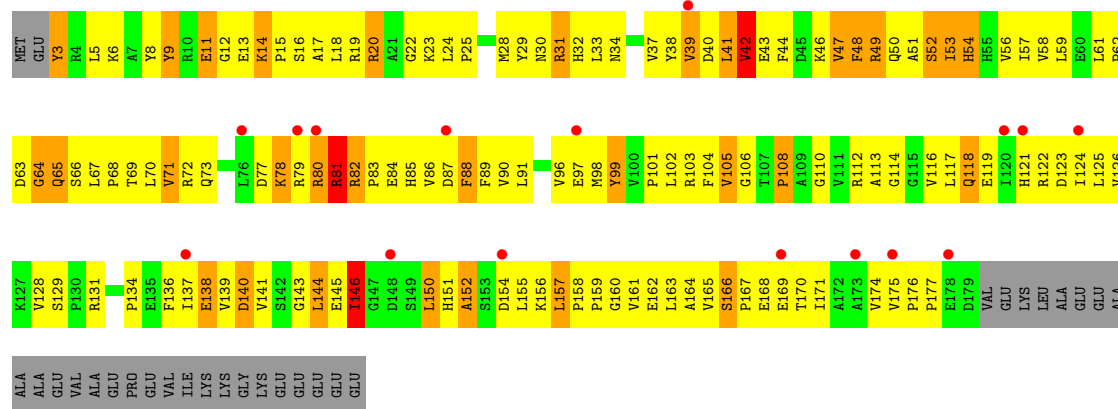
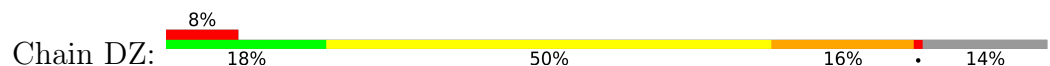
• Molecule 45: 50S RIBOSOMAL PROTEIN L24



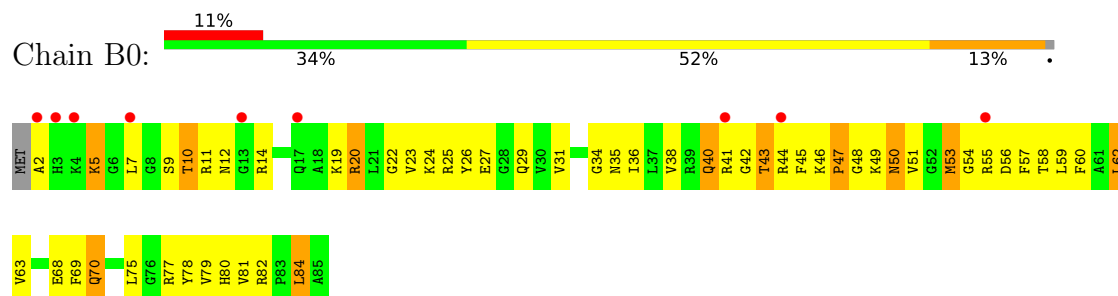
• Molecule 46: 50S RIBOSOMAL PROTEIN L25



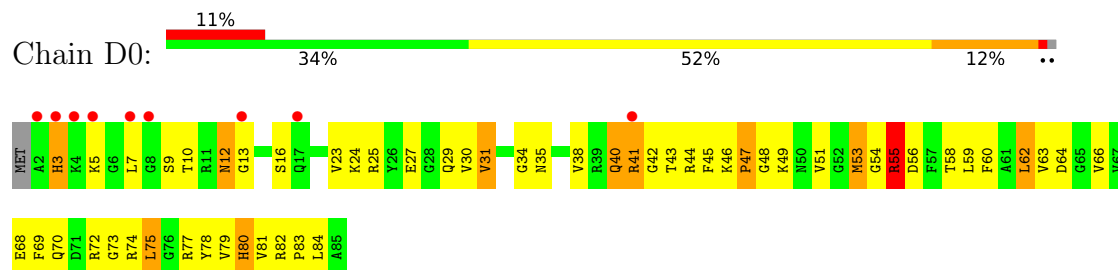
• Molecule 46: 50S RIBOSOMAL PROTEIN L25



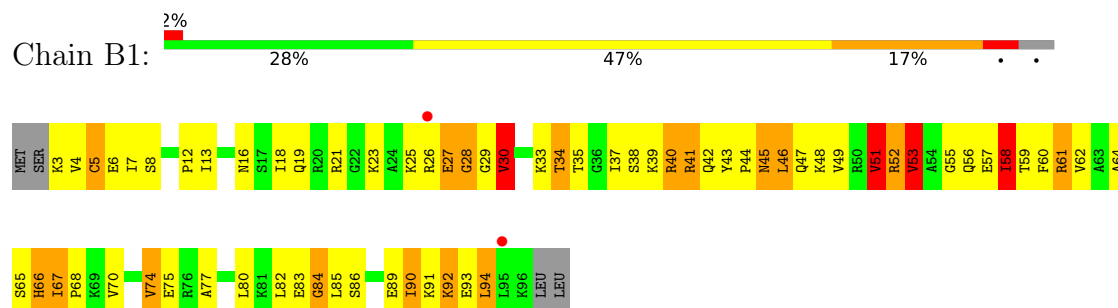
- Molecule 47: 50S RIBOSOMAL PROTEIN L27



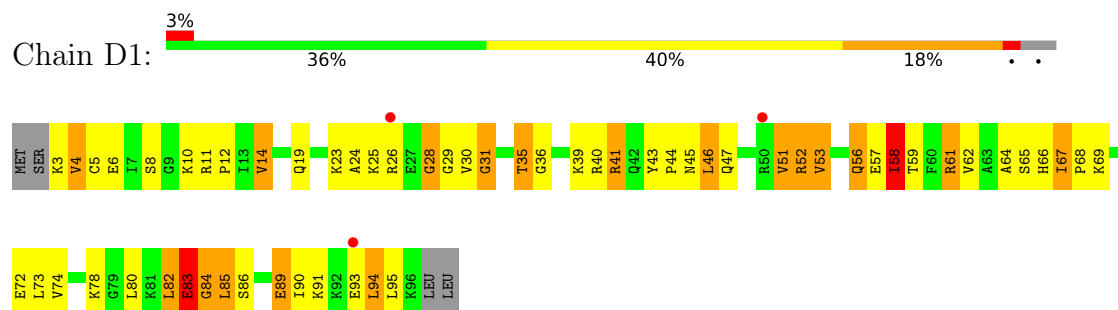
- Molecule 47: 50S RIBOSOMAL PROTEIN L27



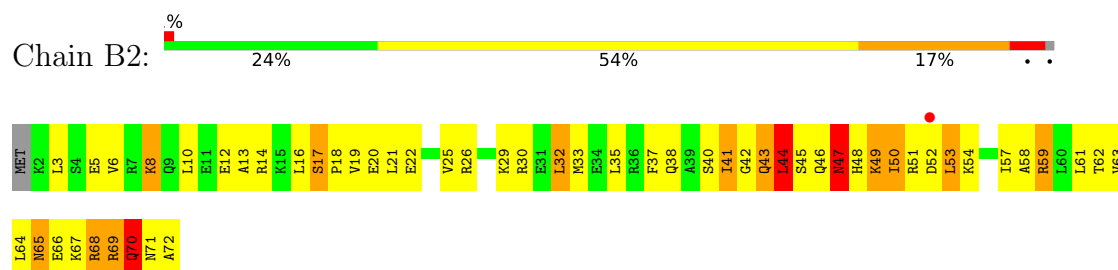
- Molecule 48: 50S RIBOSOMAL PROTEIN L28



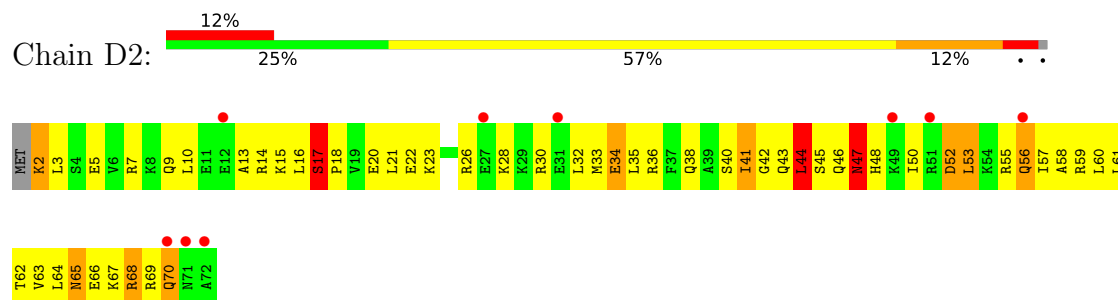
- Molecule 48: 50S RIBOSOMAL PROTEIN L28



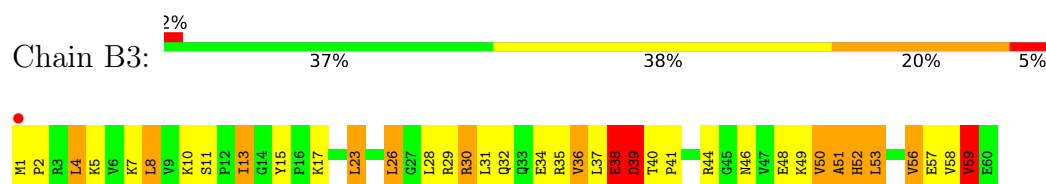
- Molecule 49: 50S RIBOSOMAL PROTEIN L29



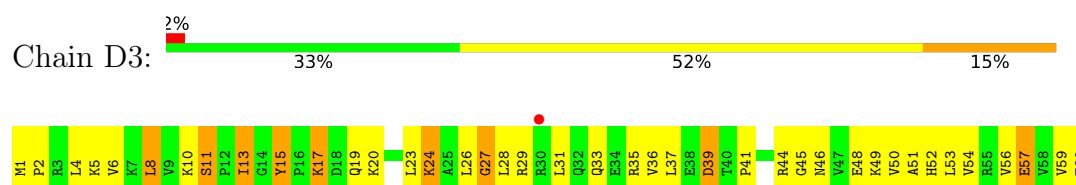
## ● Molecule 49: 50S RIBOSOMAL PROTEIN L29



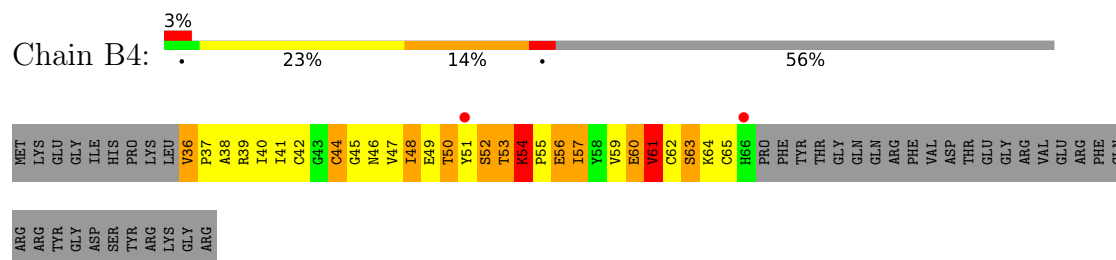
## ● Molecule 50: 50S RIBOSOMAL PROTEIN L30



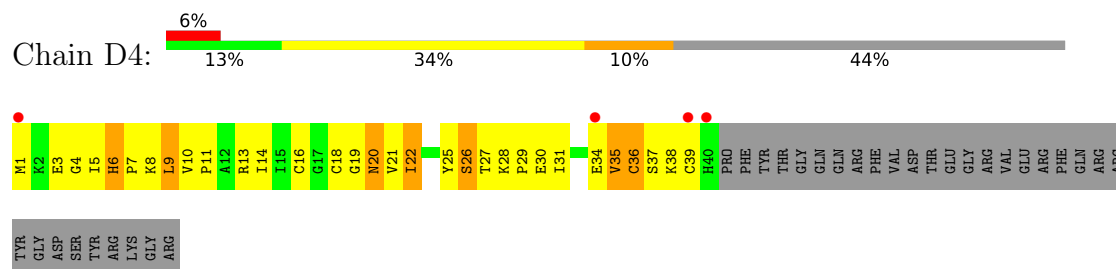
## ● Molecule 50: 50S RIBOSOMAL PROTEIN L30



## ● Molecule 51: 50S RIBOSOMAL PROTEIN L31

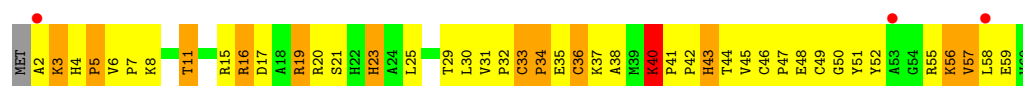


## ● Molecule 51: 50S RIBOSOMAL PROTEIN L31

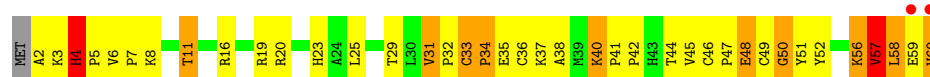


## ● Molecule 52: 50S RIBOSOMAL PROTEIN L32





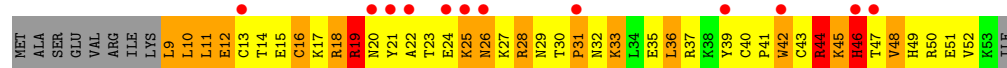
• Molecule 52: 50S RIBOSOMAL PROTEIN L32



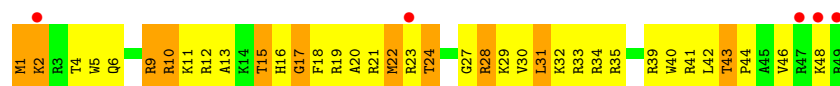
• Molecule 53: 50S RIBOSOMAL PROTEIN L33



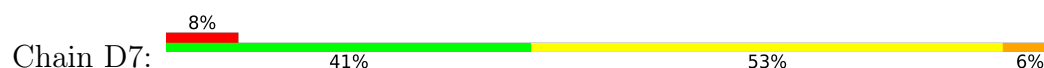
• Molecule 53: 50S RIBOSOMAL PROTEIN L33



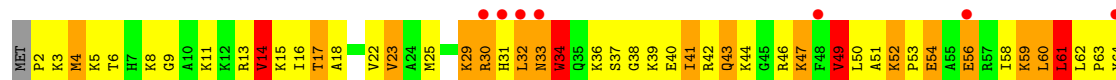
• Molecule 54: 50S RIBOSOMAL PROTEIN L34



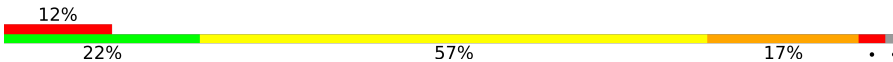
• Molecule 54: 50S RIBOSOMAL PROTEIN L34

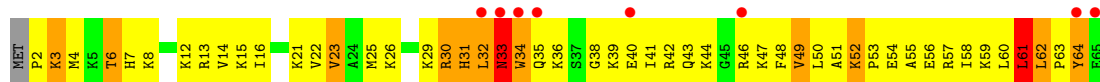


• Molecule 55: 50S RIBOSOMAL PROTEIN L35



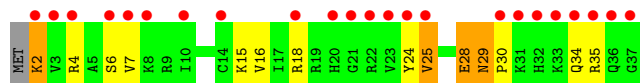
- Molecule 55: 50S RIBOSOMAL PROTEIN L35

Chain D8: 



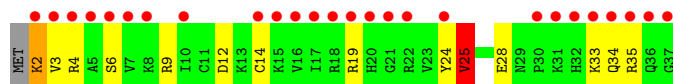
- Molecule 56: 50S RIBOSOMAL PROTEIN L36

Chain B9: 



- Molecule 56: 50S RIBOSOMAL PROTEIN L36

Chain D9: 





## 4 Data and refinement statistics

| Property                                                                | Value                                                             |
|-------------------------------------------------------------------------|-------------------------------------------------------------------|
| Space group                                                             | P 21 21 21                                                        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 210.46 Å   447.34 Å   622.30 Å<br>90.00°   90.00°   90.00°        |
| Resolution (Å)                                                          | 35.07 – 3.52<br>35.07 – 3.52                                      |
| % Data completeness<br>(in resolution range)                            | 99.9 (35.07-3.52)<br>99.8 (35.07-3.52)                            |
| $R_{merge}$                                                             | 0.44                                                              |
| $R_{sym}$                                                               | 0.46                                                              |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.81 (at 3.47 Å)                                                  |
| Refinement program                                                      | PHENIX (phenix.refine: 1.7_641), PHENIX (phenix.refine: 1.8_1069) |
| R, $R_{free}$                                                           | 0.210 , 0.249<br>0.214 , 0.253                                    |
| $R_{free}$ test set                                                     | 32826 reflections (4.56%)                                         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 91.1                                                              |
| Anisotropy                                                              | 0.109                                                             |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.28 , 81.4                                                       |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.25$       |
| Estimated twinning fraction                                             | No twinning to report.                                            |
| $F_o, F_c$ correlation                                                  | 0.91                                                              |
| Total number of atoms                                                   | 293977                                                            |
| Average B, all atoms (Å <sup>2</sup> )                                  | 79.0                                                              |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.60% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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   | AA    | 0.19         | 0/36189       | 0.44        | 0/56484        |
| 1   | CA    | 0.19         | 0/36189       | 0.43        | 0/56484        |
| 2   | AB    | 0.81         | 2/1936 (0.1%) | 1.03        | 6/2611 (0.2%)  |
| 2   | CB    | 0.89         | 0/1936        | 1.06        | 3/2611 (0.1%)  |
| 3   | AC    | 0.96         | 2/1637 (0.1%) | 1.09        | 7/2207 (0.3%)  |
| 3   | CC    | 1.05         | 3/1637 (0.2%) | 1.18        | 6/2207 (0.3%)  |
| 4   | AD    | 0.92         | 1/1733 (0.1%) | 1.17        | 13/2318 (0.6%) |
| 4   | CD    | 1.02         | 2/1733 (0.1%) | 1.18        | 13/2318 (0.6%) |
| 5   | AE    | 0.98         | 1/1163 (0.1%) | 1.27        | 9/1566 (0.6%)  |
| 5   | CE    | 0.96         | 0/1163        | 1.20        | 3/1566 (0.2%)  |
| 6   | AF    | 0.97         | 0/856         | 1.17        | 6/1154 (0.5%)  |
| 6   | CF    | 1.06         | 1/856 (0.1%)  | 1.17        | 4/1154 (0.3%)  |
| 7   | AG    | 1.04         | 4/1276 (0.3%) | 1.16        | 5/1709 (0.3%)  |
| 7   | CG    | 0.95         | 0/1276        | 1.13        | 12/1709 (0.7%) |
| 8   | AH    | 0.98         | 3/1136 (0.3%) | 1.13        | 2/1527 (0.1%)  |
| 8   | CH    | 0.97         | 1/1136 (0.1%) | 1.19        | 7/1527 (0.5%)  |
| 9   | AI    | 0.94         | 0/1029        | 1.16        | 6/1379 (0.4%)  |
| 9   | CI    | 0.95         | 0/1029        | 1.13        | 7/1379 (0.5%)  |
| 10  | AJ    | 1.03         | 2/808 (0.2%)  | 1.16        | 3/1087 (0.3%)  |
| 10  | CJ    | 0.89         | 0/808         | 1.08        | 5/1087 (0.5%)  |
| 11  | AK    | 0.93         | 0/900         | 1.18        | 5/1213 (0.4%)  |
| 11  | CK    | 0.95         | 0/900         | 1.25        | 8/1213 (0.7%)  |
| 12  | AL    | 1.17         | 1/987 (0.1%)  | 1.30        | 5/1322 (0.4%)  |
| 12  | CL    | 1.19         | 4/987 (0.4%)  | 1.39        | 8/1322 (0.6%)  |
| 13  | AM    | 0.88         | 0/999         | 1.07        | 4/1338 (0.3%)  |
| 13  | CM    | 0.55         | 1/1008 (0.1%) | 1.08        | 7/1347 (0.5%)  |
| 14  | AN    | 0.92         | 0/501         | 1.11        | 0/664          |
| 14  | CN    | 1.01         | 0/501         | 1.25        | 2/664 (0.3%)   |
| 15  | AO    | 1.08         | 2/745 (0.3%)  | 1.13        | 2/992 (0.2%)   |
| 15  | CO    | 1.00         | 1/745 (0.1%)  | 1.09        | 2/992 (0.2%)   |
| 16  | AP    | 0.94         | 0/717         | 1.15        | 4/965 (0.4%)   |
| 16  | CP    | 0.99         | 0/717         | 1.23        | 5/965 (0.5%)   |

| Mol | Chain | Bond lengths |                | Bond angles |                 |
|-----|-------|--------------|----------------|-------------|-----------------|
|     |       | RMSZ         | # Z  >5        | RMSZ        | # Z  >5         |
| 17  | AQ    | 0.95         | 0/837          | 1.18        | 6/1119 (0.5%)   |
| 17  | CQ    | 1.01         | 0/837          | 1.13        | 4/1119 (0.4%)   |
| 18  | AR    | 0.94         | 0/579          | 1.14        | 2/768 (0.3%)    |
| 18  | CR    | 1.03         | 1/579 (0.2%)   | 1.24        | 6/768 (0.8%)    |
| 19  | AS    | 1.02         | 3/643 (0.5%)   | 1.13        | 3/867 (0.3%)    |
| 19  | CS    | 1.03         | 1/643 (0.2%)   | 1.17        | 2/867 (0.2%)    |
| 20  | AT    | 1.04         | 3/765 (0.4%)   | 1.15        | 6/1007 (0.6%)   |
| 20  | CT    | 0.87         | 0/765          | 1.02        | 4/1007 (0.4%)   |
| 21  | AU    | 0.85         | 0/213          | 1.03        | 1/279 (0.4%)    |
| 21  | CU    | 0.85         | 0/213          | 1.03        | 0/279           |
| 22  | AV    | 0.64         | 0/1836         | 0.60        | 0/2859          |
| 22  | CV    | 0.61         | 0/1835         | 0.62        | 0/2859          |
| 23  | AW    | 0.52         | 0/1809         | 0.50        | 0/2819          |
| 23  | AY    | 0.61         | 0/408          | 0.56        | 0/634           |
| 23  | CW    | 0.53         | 0/1809         | 0.48        | 0/2819          |
| 23  | CY    | 0.72         | 0/408          | 0.68        | 0/634           |
| 24  | AX    | 0.82         | 1/285 (0.4%)   | 0.59        | 0/441           |
| 24  | CX    | 0.59         | 0/235          | 0.66        | 0/364           |
| 25  | BA    | 0.23         | 1/67788 (0.0%) | 0.48        | 1/105819 (0.0%) |
| 25  | DA    | 0.22         | 0/68124        | 0.49        | 1/106343 (0.0%) |
| 26  | BB    | 0.16         | 0/2853         | 0.36        | 0/4451          |
| 26  | DB    | 0.18         | 0/2853         | 0.40        | 0/4451          |
| 27  | BC    | 0.98         | 2/1145 (0.2%)  | 1.13        | 6/1556 (0.4%)   |
| 27  | DC    | 0.36         | 0/1145         | 0.80        | 0/1556          |
| 28  | BD    | 1.14         | 3/2155 (0.1%)  | 1.35        | 16/2907 (0.6%)  |
| 28  | DD    | 0.71         | 0/2155         | 1.13        | 14/2907 (0.5%)  |
| 29  | BE    | 1.06         | 3/1597 (0.2%)  | 1.31        | 16/2155 (0.7%)  |
| 29  | DE    | 0.68         | 1/1597 (0.1%)  | 1.12        | 12/2155 (0.6%)  |
| 30  | BF    | 1.07         | 1/1659 (0.1%)  | 1.20        | 6/2246 (0.3%)   |
| 30  | DF    | 0.61         | 0/1620         | 1.20        | 17/2194 (0.8%)  |
| 31  | BG    | 0.92         | 0/1499         | 1.11        | 7/2016 (0.3%)   |
| 31  | DG    | 0.51         | 1/1499 (0.1%)  | 0.98        | 10/2016 (0.5%)  |
| 32  | BH    | 0.87         | 0/1246         | 1.11        | 5/1684 (0.3%)   |
| 32  | DH    | 0.52         | 0/1315         | 1.15        | 9/1780 (0.5%)   |
| 33  | BI    | 0.94         | 1/1146 (0.1%)  | 1.16        | 5/1551 (0.3%)   |
| 33  | DI    | 0.49         | 1/1151 (0.1%)  | 1.08        | 10/1558 (0.6%)  |
| 34  | BN    | 1.04         | 1/1132 (0.1%)  | 1.21        | 7/1527 (0.5%)   |
| 34  | DN    | 0.57         | 0/1132         | 1.06        | 9/1527 (0.6%)   |
| 35  | BO    | 1.00         | 0/943          | 1.26        | 3/1269 (0.2%)   |
| 35  | DO    | 0.59         | 0/943          | 1.09        | 5/1269 (0.4%)   |
| 36  | BP    | 0.51         | 2/1162 (0.2%)  | 1.20        | 12/1544 (0.8%)  |
| 36  | DP    | 0.49         | 1/1162 (0.1%)  | 1.17        | 12/1544 (0.8%)  |
| 37  | BQ    | 1.03         | 1/1143 (0.1%)  | 1.19        | 5/1527 (0.3%)   |

| Mol | Chain | Bond lengths |                  | Bond angles |                   |
|-----|-------|--------------|------------------|-------------|-------------------|
|     |       | RMSZ         | # Z  >5          | RMSZ        | # Z  >5           |
| 37  | DQ    | 0.62         | 0/1143           | 0.99        | 3/1527 (0.2%)     |
| 38  | BR    | 1.15         | 4/974 (0.4%)     | 1.24        | 6/1302 (0.5%)     |
| 38  | DR    | 0.86         | 2/982 (0.2%)     | 1.07        | 3/1312 (0.2%)     |
| 39  | BS    | 1.00         | 1/779 (0.1%)     | 1.21        | 6/1038 (0.6%)     |
| 39  | DS    | 0.49         | 0/892            | 1.18        | 9/1187 (0.8%)     |
| 40  | BT    | 0.93         | 0/1156           | 1.33        | 19/1544 (1.2%)    |
| 40  | DT    | 0.80         | 1/1156 (0.1%)    | 1.27        | 20/1544 (1.3%)    |
| 41  | BU    | 1.10         | 3/982 (0.3%)     | 1.26        | 6/1306 (0.5%)     |
| 41  | DU    | 0.71         | 0/975            | 1.10        | 5/1297 (0.4%)     |
| 42  | BV    | 0.99         | 0/790            | 1.20        | 3/1057 (0.3%)     |
| 42  | DV    | 0.63         | 1/790 (0.1%)     | 1.12        | 5/1057 (0.5%)     |
| 43  | BW    | 1.13         | 2/907 (0.2%)     | 1.25        | 7/1216 (0.6%)     |
| 43  | DW    | 0.64         | 0/907            | 1.01        | 3/1216 (0.2%)     |
| 44  | BX    | 1.02         | 3/740 (0.4%)     | 1.25        | 6/995 (0.6%)      |
| 44  | DX    | 0.64         | 0/740            | 1.01        | 3/995 (0.3%)      |
| 45  | BY    | 0.99         | 2/789 (0.3%)     | 1.40        | 12/1053 (1.1%)    |
| 45  | DY    | 0.60         | 1/798 (0.1%)     | 1.17        | 5/1064 (0.5%)     |
| 46  | BZ    | 1.00         | 4/1436 (0.3%)    | 1.11        | 9/1951 (0.5%)     |
| 46  | DZ    | 0.47         | 0/1436           | 0.87        | 0/1951            |
| 47  | B0    | 1.01         | 2/671 (0.3%)     | 1.17        | 3/892 (0.3%)      |
| 47  | D0    | 0.59         | 0/671            | 1.00        | 3/892 (0.3%)      |
| 48  | B1    | 1.22         | 4/739 (0.5%)     | 1.30        | 3/983 (0.3%)      |
| 48  | D1    | 0.66         | 0/739            | 0.95        | 1/983 (0.1%)      |
| 49  | B2    | 0.98         | 0/600            | 1.09        | 1/793 (0.1%)      |
| 49  | D2    | 0.68         | 0/600            | 1.03        | 1/793 (0.1%)      |
| 50  | B3    | 1.07         | 1/473 (0.2%)     | 1.17        | 0/636             |
| 50  | D3    | 0.58         | 0/473            | 1.16        | 4/636 (0.6%)      |
| 51  | B4    | 1.00         | 0/229            | 1.16        | 3/311 (1.0%)      |
| 51  | D4    | 0.59         | 0/303            | 1.12        | 1/409 (0.2%)      |
| 52  | B5    | 1.28         | 3/473 (0.6%)     | 1.29        | 5/639 (0.8%)      |
| 52  | D5    | 0.59         | 0/473            | 1.06        | 2/639 (0.3%)      |
| 53  | B6    | 1.02         | 1/388 (0.3%)     | 1.38        | 8/520 (1.5%)      |
| 53  | D6    | 0.41         | 0/388            | 0.87        | 1/520 (0.2%)      |
| 54  | B7    | 1.12         | 0/427            | 1.32        | 2/563 (0.4%)      |
| 54  | D7    | 0.69         | 0/427            | 1.03        | 0/563             |
| 55  | B8    | 0.97         | 0/516            | 1.22        | 6/681 (0.9%)      |
| 55  | D8    | 0.65         | 0/516            | 1.21        | 5/681 (0.7%)      |
| 56  | B9    | 0.87         | 0/302            | 0.90        | 0/397             |
| 56  | D9    | 0.40         | 0/302            | 0.84        | 1/397 (0.3%)      |
| All | All   | 0.53         | 94/318178 (0.0%) | 0.72        | 571/475682 (0.1%) |

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 |
|-----|-------|---------------------|---------------------|
| 28  | BD    | 0                   | 1                   |

All (94) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|--------|-------------|----------|
| 25  | BA    | 1453 | U    | O3'-P   | 23.98  | 1.97        | 1.61     |
| 38  | DR    | 12   | ARG  | C-N     | 18.60  | 1.60        | 1.33     |
| 40  | DT    | 28   | VAL  | C-N     | 18.17  | 1.59        | 1.33     |
| 29  | DE    | 127  | ASP  | C-N     | 12.25  | 1.50        | 1.33     |
| 24  | AX    | 14   | A    | O3'-P   | -10.45 | 1.45        | 1.61     |
| 27  | BC    | 66   | HIS  | CG-CD2  | -8.85  | 1.26        | 1.35     |
| 42  | DV    | 1    | MET  | CG-SD   | 8.32   | 2.01        | 1.80     |
| 8   | AH    | 81   | HIS  | CG-CD2  | -8.16  | 1.26        | 1.35     |
| 52  | B5    | 23   | HIS  | CG-CD2  | -8.15  | 1.26        | 1.35     |
| 3   | CC    | 196  | LEU  | CA-C    | -8.11  | 1.49        | 1.53     |
| 7   | AG    | 122  | HIS  | ND1-CE1 | 8.01   | 1.40        | 1.32     |
| 19  | CS    | 31   | ILE  | CA-CB   | 8.01   | 1.62        | 1.53     |
| 7   | AG    | 122  | HIS  | CG-ND1  | -7.88  | 1.29        | 1.38     |
| 46  | BZ    | 85   | HIS  | ND1-CE1 | -7.69  | 1.24        | 1.32     |
| 19  | AS    | 57   | HIS  | CG-ND1  | -7.57  | 1.29        | 1.38     |
| 52  | B5    | 43   | HIS  | CG-CD2  | -7.56  | 1.27        | 1.35     |
| 27  | BC    | 66   | HIS  | CD2-NE2 | 7.52   | 1.46        | 1.37     |
| 30  | BF    | 31   | HIS  | CG-CD2  | -7.24  | 1.27        | 1.35     |
| 12  | AL    | 28   | LYS  | C-N     | -7.13  | 1.26        | 1.33     |
| 6   | CF    | 97   | PHE  | CA-C    | -7.08  | 1.45        | 1.53     |
| 52  | B5    | 23   | HIS  | CD2-NE2 | 6.94   | 1.45        | 1.37     |
| 38  | BR    | 13   | HIS  | C-N     | 6.88   | 1.43        | 1.33     |
| 48  | B1    | 66   | HIS  | CG-ND1  | 6.84   | 1.45        | 1.38     |
| 39  | BS    | 98   | VAL  | CA-CB   | 6.83   | 1.61        | 1.53     |
| 46  | BZ    | 85   | HIS  | CG-ND1  | 6.74   | 1.45        | 1.38     |
| 20  | AT    | 73   | HIS  | CG-CD2  | -6.68  | 1.28        | 1.35     |
| 19  | AS    | 57   | HIS  | ND1-CE1 | 6.61   | 1.39        | 1.32     |
| 38  | BR    | 61   | HIS  | CG-ND1  | 6.58   | 1.45        | 1.38     |
| 13  | CM    | 82   | MET  | CG-SD   | -6.46  | 1.64        | 1.80     |
| 12  | CL    | 31   | PRO  | C-N     | 6.46   | 1.41        | 1.33     |
| 2   | AB    | 40   | HIS  | CG-ND1  | 6.39   | 1.45        | 1.38     |
| 7   | AG    | 122  | HIS  | CE1-NE2 | -6.39  | 1.26        | 1.32     |
| 28  | BD    | 201  | HIS  | CG-ND1  | -6.37  | 1.31        | 1.38     |
| 20  | AT    | 49   | ALA  | C-O     | -6.36  | 1.16        | 1.24     |
| 2   | AB    | 40   | HIS  | ND1-CE1 | -6.22  | 1.26        | 1.32     |
| 20  | AT    | 49   | ALA  | CA-C    | 6.21   | 1.61        | 1.52     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 28  | BD    | 24  | ILE  | CA-CB   | 6.19  | 1.62        | 1.54     |
| 37  | BQ    | 123 | HIS  | ND1-CE1 | 6.19  | 1.38        | 1.32     |
| 4   | CD    | 123 | HIS  | CG-ND1  | 6.19  | 1.45        | 1.38     |
| 43  | BW    | 102 | HIS  | CG-ND1  | -6.13 | 1.31        | 1.38     |
| 10  | AJ    | 13  | HIS  | CG-CD2  | -6.13 | 1.29        | 1.35     |
| 31  | DG    | 86  | MET  | CG-SD   | -6.08 | 1.65        | 1.80     |
| 3   | CC    | 99  | VAL  | CA-CB   | 6.04  | 1.61        | 1.54     |
| 8   | AH    | 81  | HIS  | CD2-NE2 | 6.02  | 1.44        | 1.37     |
| 41  | BU    | 81  | HIS  | CD2-NE2 | 5.98  | 1.44        | 1.37     |
| 47  | B0    | 31  | VAL  | CA-CB   | -5.92 | 1.47        | 1.54     |
| 45  | DY    | 5   | MET  | CG-SD   | -5.87 | 1.66        | 1.80     |
| 33  | BI    | 92  | VAL  | CA-CB   | -5.79 | 1.46        | 1.54     |
| 10  | AJ    | 56  | HIS  | CG-CD2  | -5.78 | 1.29        | 1.35     |
| 29  | BE    | 41  | LYS  | CA-CB   | 5.76  | 1.62        | 1.53     |
| 8   | AH    | 97  | VAL  | CA-CB   | -5.74 | 1.48        | 1.54     |
| 29  | BE    | 120 | TRP  | CA-C    | 5.72  | 1.57        | 1.52     |
| 48  | B1    | 66  | HIS  | ND1-CE1 | -5.72 | 1.26        | 1.32     |
| 45  | BY    | 5   | MET  | C-N     | -5.70 | 1.26        | 1.33     |
| 48  | B1    | 51  | VAL  | CA-CB   | 5.69  | 1.62        | 1.54     |
| 41  | BU    | 81  | HIS  | ND1-CE1 | 5.59  | 1.38        | 1.32     |
| 15  | AO    | 50  | HIS  | CD2-NE2 | 5.58  | 1.44        | 1.37     |
| 48  | B1    | 66  | HIS  | CE1-NE2 | 5.54  | 1.38        | 1.32     |
| 8   | CH    | 48  | TYR  | CA-C    | -5.52 | 1.45        | 1.52     |
| 36  | DP    | 53  | GLY  | C-O     | 5.51  | 1.31        | 1.23     |
| 46  | BZ    | 55  | HIS  | CD2-NE2 | -5.49 | 1.31        | 1.37     |
| 18  | CR    | 75  | ILE  | CA-CB   | -5.46 | 1.48        | 1.54     |
| 7   | AG    | 153 | HIS  | CD2-NE2 | -5.46 | 1.31        | 1.37     |
| 45  | BY    | 83  | THR  | CA-C    | 5.46  | 1.59        | 1.52     |
| 53  | B6    | 48  | VAL  | CA-CB   | 5.42  | 1.61        | 1.54     |
| 19  | AS    | 57  | HIS  | CE1-NE2 | -5.42 | 1.27        | 1.32     |
| 15  | AO    | 50  | HIS  | CE1-NE2 | -5.42 | 1.27        | 1.32     |
| 44  | BX    | 58  | HIS  | ND1-CE1 | 5.40  | 1.38        | 1.32     |
| 47  | B0    | 81  | VAL  | CA-CB   | -5.39 | 1.47        | 1.54     |
| 36  | BP    | 1   | MET  | CG-SD   | -5.38 | 1.67        | 1.80     |
| 15  | CO    | 42  | HIS  | CG-CD2  | -5.38 | 1.29        | 1.35     |
| 46  | BZ    | 27  | VAL  | CA-CB   | -5.36 | 1.50        | 1.55     |
| 12  | CL    | 66  | VAL  | CA-CB   | -5.36 | 1.47        | 1.55     |
| 38  | DR    | 1   | MET  | SD-CE   | -5.33 | 1.66        | 1.79     |
| 38  | BR    | 61  | HIS  | ND1-CE1 | -5.27 | 1.27        | 1.32     |
| 34  | BN    | 48  | MET  | C-N     | 5.21  | 1.41        | 1.33     |
| 12  | CL    | 33  | ARG  | C-O     | -5.19 | 1.17        | 1.23     |
| 4   | CD    | 123 | HIS  | ND1-CE1 | -5.18 | 1.27        | 1.32     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3   | CC    | 89  | GLU  | C-N     | -5.18 | 1.27        | 1.33     |
| 41  | BU    | 81  | HIS  | CE1-NE2 | -5.18 | 1.27        | 1.32     |
| 5   | AE    | 31  | LEU  | CA-C    | -5.17 | 1.46        | 1.52     |
| 29  | BE    | 144 | ARG  | N-CA    | 5.16  | 1.49        | 1.46     |
| 3   | AC    | 69  | HIS  | CG-ND1  | 5.16  | 1.44        | 1.38     |
| 44  | BX    | 58  | HIS  | CE1-NE2 | -5.16 | 1.27        | 1.32     |
| 38  | BR    | 83  | ILE  | CA-CB   | 5.14  | 1.60        | 1.54     |
| 33  | DI    | 145 | VAL  | C-N     | 5.13  | 1.40        | 1.33     |
| 12  | CL    | 20  | LYS  | C-N     | -5.12 | 1.26        | 1.33     |
| 44  | BX    | 58  | HIS  | CG-ND1  | -5.11 | 1.32        | 1.38     |
| 50  | B3    | 56  | VAL  | CA-CB   | -5.10 | 1.48        | 1.54     |
| 43  | BW    | 102 | HIS  | ND1-CE1 | 5.09  | 1.37        | 1.32     |
| 3   | AC    | 6   | HIS  | CG-ND1  | -5.07 | 1.32        | 1.38     |
| 36  | BP    | 1   | MET  | SD-CE   | -5.05 | 1.67        | 1.79     |
| 28  | BD    | 242 | ARG  | CA-C    | -5.04 | 1.46        | 1.52     |
| 4   | AD    | 125 | HIS  | CG-ND1  | 5.03  | 1.43        | 1.38     |

All (571) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|--------|-------------|----------|
| 38  | DR    | 12   | ARG  | O-C-N     | 12.64  | 137.93      | 123.27   |
| 45  | BY    | 38   | ILE  | N-CA-C    | 12.17  | 121.97      | 110.53   |
| 36  | BP    | 14   | LYS  | N-CA-C    | -11.61 | 98.36       | 111.71   |
| 40  | DT    | 28   | VAL  | O-C-N     | 11.28  | 136.67      | 122.57   |
| 34  | DN    | 25   | ARG  | N-CA-C    | -10.76 | 99.55       | 111.28   |
| 12  | CL    | 26   | ALA  | N-CA-C    | -10.51 | 100.65      | 113.15   |
| 40  | BT    | 30   | VAL  | N-CA-C    | 10.49  | 122.06      | 110.21   |
| 30  | DF    | 163  | VAL  | N-CA-C    | -10.12 | 100.70      | 110.42   |
| 5   | AE    | 11   | ILE  | CB-CA-C   | -10.05 | 103.17      | 111.71   |
| 30  | DF    | 197  | ASP  | N-CA-C    | -9.85  | 98.29       | 110.41   |
| 51  | D4    | 6    | HIS  | N-CA-C    | 9.67   | 121.83      | 109.65   |
| 39  | DS    | 53   | SER  | N-CA-C    | -9.63  | 101.41      | 113.55   |
| 41  | BU    | 27   | LEU  | N-CA-C    | -9.63  | 101.22      | 113.16   |
| 32  | DH    | 124  | GLU  | N-CA-C    | -9.32  | 94.95       | 109.76   |
| 43  | BW    | 58   | ALA  | N-CA-C    | -9.31  | 99.83       | 111.75   |
| 41  | DU    | 109  | LEU  | N-CA-C    | -9.15  | 101.28      | 111.07   |
| 30  | DF    | 75   | HIS  | N-CA-C    | 9.04   | 122.02      | 109.18   |
| 4   | AD    | 110  | PHE  | N-CA-C    | -9.02  | 102.19      | 113.02   |
| 53  | B6    | 48   | VAL  | N-CA-C    | 8.88   | 119.68      | 110.62   |
| 25  | BA    | 1453 | U    | P-O3'-C3' | -8.86  | 106.91      | 120.20   |
| 30  | DF    | 84   | VAL  | N-CA-C    | -8.80  | 98.23       | 109.58   |
| 34  | BN    | 46   | VAL  | N-CA-C    | 8.79   | 119.59      | 110.62   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 39  | BS    | 98  | VAL  | N-CA-C  | 8.79  | 121.25      | 107.98   |
| 36  | BP    | 51  | PHE  | N-CA-C  | 8.75  | 121.89      | 110.43   |
| 27  | BC    | 208 | PHE  | N-CA-C  | 8.69  | 120.22      | 108.23   |
| 40  | BT    | 31  | SER  | N-CA-C  | 8.62  | 115.85      | 108.78   |
| 29  | BE    | 144 | ARG  | N-CA-C  | 8.56  | 115.80      | 108.78   |
| 34  | BN    | 41  | ASP  | N-CA-C  | -8.50 | 100.64      | 112.45   |
| 36  | DP    | 51  | PHE  | N-CA-C  | 8.50  | 121.91      | 110.35   |
| 31  | BG    | 54  | GLU  | N-CA-C  | -8.40 | 103.04      | 113.38   |
| 20  | AT    | 12  | ALA  | N-CA-C  | -8.36 | 102.85      | 113.72   |
| 34  | BN    | 25  | ARG  | N-CA-C  | -8.28 | 102.19      | 111.71   |
| 46  | BZ    | 54  | HIS  | N-CA-C  | -8.19 | 100.25      | 113.19   |
| 29  | BE    | 144 | ARG  | CA-C-O  | 8.17  | 122.68      | 117.94   |
| 45  | BY    | 12  | THR  | CA-C-N  | -8.12 | 111.87      | 122.51   |
| 45  | BY    | 12  | THR  | C-N-CA  | -8.12 | 111.87      | 122.51   |
| 53  | B6    | 50  | ARG  | CA-C-O  | 8.13  | 122.65      | 117.94   |
| 39  | BS    | 16  | ASN  | N-CA-C  | -8.11 | 102.27      | 112.90   |
| 18  | CR    | 25  | THR  | N-CA-C  | -7.99 | 101.27      | 113.89   |
| 41  | BU    | 49  | HIS  | N-CA-C  | 7.96  | 120.03      | 111.36   |
| 46  | BZ    | 124 | ILE  | N-CA-C  | 7.95  | 119.16      | 108.27   |
| 20  | AT    | 72  | LEU  | N-CA-C  | -7.94 | 100.05      | 110.53   |
| 40  | DT    | 76  | PHE  | CA-C-N  | 7.94  | 127.66      | 119.64   |
| 40  | DT    | 76  | PHE  | C-N-CA  | 7.94  | 127.66      | 119.64   |
| 32  | BH    | 97  | ARG  | CB-CA-C | -7.87 | 105.73      | 117.07   |
| 39  | DS    | 15  | ARG  | N-CA-C  | -7.81 | 102.71      | 111.14   |
| 8   | CH    | 4   | ASP  | CA-C-N  | 7.79  | 127.07      | 118.97   |
| 8   | CH    | 4   | ASP  | C-N-CA  | 7.79  | 127.07      | 118.97   |
| 40  | DT    | 30  | VAL  | N-CA-C  | 7.77  | 125.51      | 109.34   |
| 5   | AE    | 103 | GLY  | N-CA-C  | -7.76 | 102.61      | 112.54   |
| 29  | BE    | 40  | GLU  | N-CA-C  | 7.74  | 119.79      | 111.36   |
| 45  | BY    | 12  | THR  | O-C-N   | 7.73  | 131.99      | 123.10   |
| 53  | B6    | 45  | LYS  | N-CA-C  | 7.72  | 120.73      | 110.53   |
| 7   | AG    | 135 | VAL  | N-CA-C  | -7.72 | 105.17      | 111.81   |
| 31  | DG    | 167 | GLU  | N-CA-C  | -7.68 | 101.78      | 112.45   |
| 4   | AD    | 171 | GLY  | CA-C-N  | 7.63  | 127.29      | 119.82   |
| 4   | AD    | 171 | GLY  | C-N-CA  | 7.63  | 127.29      | 119.82   |
| 28  | DD    | 14  | ARG  | N-CA-C  | -7.58 | 103.86      | 113.72   |
| 55  | B8    | 38  | GLY  | N-CA-C  | -7.58 | 103.64      | 112.73   |
| 36  | DP    | 25  | SER  | N-CA-C  | -7.54 | 102.40      | 114.09   |
| 41  | BU    | 97  | ASP  | N-CA-C  | -7.50 | 103.02      | 113.37   |
| 35  | DO    | 3   | GLN  | CA-C-N  | -7.42 | 112.34      | 119.76   |
| 35  | DO    | 3   | GLN  | C-N-CA  | -7.42 | 112.34      | 119.76   |
| 16  | CP    | 5   | ARG  | N-CA-C  | 7.37  | 117.73      | 108.45   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 28  | BD    | 43  | ARG  | N-CA-C     | 7.32  | 118.90      | 111.07   |
| 11  | CK    | 25  | TYR  | N-CA-C     | -7.31 | 105.55      | 114.75   |
| 41  | BU    | 81  | HIS  | ND1-CG-CD2 | 7.28  | 113.38      | 106.10   |
| 40  | DT    | 29  | ARG  | N-CA-C     | 7.24  | 126.22      | 110.80   |
| 40  | BT    | 130 | ALA  | N-CA-C     | -7.23 | 104.03      | 112.92   |
| 40  | BT    | 89  | VAL  | N-CA-C     | 7.22  | 118.06      | 107.37   |
| 2   | CB    | 238 | LEU  | N-CA-C     | -7.21 | 104.06      | 112.92   |
| 36  | BP    | 139 | LYS  | N-CA-C     | -7.20 | 103.43      | 111.71   |
| 36  | DP    | 139 | LYS  | N-CA-C     | -7.20 | 103.43      | 111.71   |
| 50  | D3    | 11  | SER  | CA-C-N     | 7.18  | 128.15      | 120.47   |
| 50  | D3    | 11  | SER  | C-N-CA     | 7.18  | 128.15      | 120.47   |
| 6   | AF    | 61  | LEU  | CB-CA-C    | -7.13 | 105.49      | 114.40   |
| 39  | DS    | 6   | ALA  | N-CA-C     | -7.13 | 104.31      | 112.87   |
| 11  | CK    | 38  | ASN  | CA-C-N     | 7.11  | 128.22      | 119.98   |
| 11  | CK    | 38  | ASN  | C-N-CA     | 7.11  | 128.22      | 119.98   |
| 36  | BP    | 128 | HIS  | N-CA-C     | -7.08 | 105.26      | 114.04   |
| 32  | BH    | 97  | ARG  | CA-C-O     | 7.06  | 122.03      | 117.94   |
| 40  | BT    | 80  | SER  | CA-C-N     | -7.06 | 111.02      | 119.84   |
| 40  | BT    | 80  | SER  | C-N-CA     | -7.06 | 111.02      | 119.84   |
| 46  | BZ    | 157 | LEU  | CA-C-N     | 7.05  | 127.64      | 120.38   |
| 46  | BZ    | 157 | LEU  | C-N-CA     | 7.05  | 127.64      | 120.38   |
| 34  | DN    | 110 | GLY  | CA-C-N     | 7.04  | 126.67      | 119.56   |
| 34  | DN    | 110 | GLY  | C-N-CA     | 7.04  | 126.67      | 119.56   |
| 36  | DP    | 128 | HIS  | N-CA-C     | -7.03 | 105.32      | 114.04   |
| 11  | AK    | 40  | ILE  | N-CA-C     | -7.01 | 105.01      | 111.67   |
| 36  | DP    | 114 | ILE  | N-CA-C     | -6.99 | 100.56      | 109.30   |
| 3   | CC    | 195 | VAL  | CA-C-N     | -6.97 | 115.67      | 123.13   |
| 3   | CC    | 195 | VAL  | C-N-CA     | -6.97 | 115.67      | 123.13   |
| 6   | CF    | 55  | ASP  | CA-C-N     | 6.97  | 127.86      | 120.12   |
| 6   | CF    | 55  | ASP  | C-N-CA     | 6.97  | 127.86      | 120.12   |
| 36  | BP    | 114 | ILE  | N-CA-C     | -6.96 | 100.59      | 109.30   |
| 52  | B5    | 40  | LYS  | N-CA-C     | 6.96  | 114.48      | 108.22   |
| 13  | CM    | 82  | MET  | N-CA-C     | -6.92 | 99.64       | 110.36   |
| 29  | BE    | 168 | MET  | N-CA-C     | 6.92  | 119.26      | 108.96   |
| 45  | BY    | 7   | VAL  | N-CA-C     | 6.90  | 123.70      | 109.34   |
| 4   | AD    | 26  | CYS  | N-CA-C     | -6.90 | 103.97      | 112.38   |
| 13  | AM    | 70  | LEU  | N-CA-C     | -6.90 | 102.83      | 111.11   |
| 4   | CD    | 83  | SER  | N-CA-C     | -6.89 | 103.70      | 111.07   |
| 15  | AO    | 50  | HIS  | ND1-CG-CD2 | 6.87  | 112.97      | 106.10   |
| 28  | DD    | 218 | ARG  | CA-C-N     | 6.87  | 126.84      | 119.76   |
| 28  | DD    | 218 | ARG  | C-N-CA     | 6.87  | 126.84      | 119.76   |
| 2   | AB    | 53  | ARG  | N-CA-C     | -6.84 | 103.85      | 111.71   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 7   | CG    | 111 | ARG  | CA-C-N     | 6.83  | 126.29      | 118.85   |
| 7   | CG    | 111 | ARG  | C-N-CA     | 6.83  | 126.29      | 118.85   |
| 40  | BT    | 33  | LYS  | N-CA-C     | 6.81  | 119.74      | 110.55   |
| 16  | CP    | 20  | VAL  | N-CA-C     | 6.81  | 116.77      | 108.06   |
| 17  | AQ    | 46  | ASP  | CA-C-N     | 6.80  | 126.50      | 119.56   |
| 17  | AQ    | 46  | ASP  | C-N-CA     | 6.80  | 126.50      | 119.56   |
| 19  | AS    | 34  | TRP  | N-CA-C     | -6.80 | 103.69      | 113.21   |
| 37  | BQ    | 123 | HIS  | ND1-CG-CD2 | 6.80  | 112.90      | 106.10   |
| 36  | DP    | 14  | LYS  | N-CA-C     | -6.80 | 103.87      | 111.28   |
| 31  | BG    | 88  | ILE  | N-CA-C     | 6.78  | 118.06      | 108.36   |
| 30  | BF    | 75  | HIS  | N-CA-C     | 6.77  | 119.36      | 109.07   |
| 31  | BG    | 178 | PHE  | CA-C-N     | 6.76  | 127.83      | 119.98   |
| 31  | BG    | 178 | PHE  | C-N-CA     | 6.76  | 127.83      | 119.98   |
| 33  | DI    | 135 | GLU  | N-CA-C     | 6.76  | 125.21      | 110.80   |
| 33  | DI    | 27  | ARG  | N-CA-C     | 6.75  | 121.11      | 113.01   |
| 52  | B5    | 31  | VAL  | CA-C-N     | 6.74  | 125.98      | 118.97   |
| 52  | B5    | 31  | VAL  | C-N-CA     | 6.74  | 125.98      | 118.97   |
| 40  | DT    | 130 | ALA  | N-CA-C     | -6.74 | 103.93      | 111.28   |
| 4   | AD    | 114 | ARG  | N-CA-C     | -6.74 | 103.96      | 111.71   |
| 31  | DG    | 58  | GLN  | N-CA-C     | -6.73 | 105.20      | 113.41   |
| 9   | CI    | 54  | ASP  | N-CA-CB    | -6.73 | 107.37      | 114.10   |
| 52  | B5    | 23  | HIS  | ND1-CG-CD2 | 6.72  | 112.82      | 106.10   |
| 32  | BH    | 157 | TYR  | N-CA-C     | -6.72 | 104.14      | 112.47   |
| 35  | BO    | 118 | ALA  | CA-C-N     | 6.72  | 128.24      | 119.84   |
| 35  | BO    | 118 | ALA  | C-N-CA     | 6.72  | 128.24      | 119.84   |
| 12  | CL    | 38  | THR  | N-CA-C     | -6.69 | 104.59      | 112.89   |
| 33  | DI    | 41  | GLU  | N-CA-C     | -6.69 | 105.23      | 113.19   |
| 39  | DS    | 22  | GLY  | N-CA-C     | 6.68  | 123.91      | 115.42   |
| 5   | AE    | 48  | ALA  | N-CA-C     | 6.68  | 114.23      | 108.22   |
| 28  | DD    | 240 | ALA  | CA-C-N     | 6.68  | 128.19      | 119.84   |
| 28  | DD    | 240 | ALA  | C-N-CA     | 6.68  | 128.19      | 119.84   |
| 54  | B7    | 28  | ARG  | N-CA-C     | -6.66 | 104.10      | 111.36   |
| 7   | AG    | 122 | HIS  | CG-CD2-NE2 | -6.66 | 100.54      | 107.20   |
| 11  | AK    | 87  | THR  | N-CA-C     | -6.65 | 101.75      | 110.33   |
| 29  | BE    | 54  | GLN  | N-CA-C     | 6.64  | 119.72      | 108.90   |
| 17  | AQ    | 35  | VAL  | CB-CA-C    | -6.61 | 102.72      | 110.91   |
| 10  | CJ    | 14  | LYS  | N-CA-C     | -6.59 | 105.87      | 114.04   |
| 53  | B6    | 50  | ARG  | N-CA-C     | 6.58  | 114.18      | 108.78   |
| 28  | BD    | 166 | GLN  | N-CA-C     | -6.58 | 104.98      | 114.12   |
| 5   | AE    | 26  | PHE  | N-CA-C     | 6.57  | 115.05      | 108.75   |
| 7   | AG    | 122 | HIS  | ND1-CG-CD2 | 6.57  | 112.67      | 106.10   |
| 15  | CO    | 77  | ARG  | N-CA-C     | -6.57 | 105.26      | 113.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 28  | BD    | 127  | VAL  | N-CA-C      | 6.56  | 117.89      | 109.30   |
| 36  | BP    | 1    | MET  | CG-SD-CE    | 6.54  | 115.30      | 100.90   |
| 11  | AK    | 84   | VAL  | N-CA-C      | 6.54  | 117.77      | 108.42   |
| 29  | BE    | 10   | GLY  | CA-C-O      | -6.53 | 116.80      | 122.16   |
| 38  | BR    | 57   | ARG  | N-CA-C      | -6.51 | 100.27      | 110.36   |
| 38  | BR    | 38   | VAL  | CB-CA-C     | -6.48 | 107.55      | 113.70   |
| 45  | BY    | 46   | LYS  | N-CA-C      | 6.46  | 114.08      | 108.78   |
| 28  | BD    | 89   | SER  | N-CA-C      | -6.46 | 104.88      | 112.89   |
| 9   | AI    | 6    | GLY  | N-CA-C      | -6.45 | 103.28      | 110.96   |
| 9   | AI    | 17   | VAL  | N-CA-C      | 6.45  | 116.98      | 106.72   |
| 45  | DY    | 40   | GLU  | N-CA-C      | -6.43 | 103.97      | 113.61   |
| 53  | B6    | 42   | TRP  | N-CA-C      | -6.42 | 104.66      | 114.16   |
| 46  | BZ    | 100  | VAL  | CA-C-N      | 6.41  | 126.43      | 119.89   |
| 46  | BZ    | 100  | VAL  | C-N-CA      | 6.41  | 126.43      | 119.89   |
| 5   | CE    | 55   | VAL  | CB-CA-C     | -6.39 | 103.53      | 111.70   |
| 40  | DT    | 19   | LEU  | CA-C-N      | 6.36  | 126.31      | 119.76   |
| 40  | DT    | 19   | LEU  | C-N-CA      | 6.36  | 126.31      | 119.76   |
| 31  | DG    | 44   | GLY  | N-CA-C      | -6.35 | 105.87      | 113.99   |
| 33  | DI    | 15   | VAL  | N-CA-C      | 6.35  | 122.54      | 109.34   |
| 4   | AD    | 38   | TYR  | CA-C-N      | 6.33  | 126.90      | 120.38   |
| 4   | AD    | 38   | TYR  | C-N-CA      | 6.33  | 126.90      | 120.38   |
| 7   | CG    | 13   | GLN  | CA-C-N      | 6.31  | 127.72      | 119.84   |
| 7   | CG    | 13   | GLN  | C-N-CA      | 6.31  | 127.72      | 119.84   |
| 29  | BE    | 60   | ASN  | N-CA-C      | 6.30  | 116.77      | 108.07   |
| 20  | AT    | 74   | LYS  | CB-CA-C     | -6.30 | 108.30      | 115.79   |
| 12  | AL    | 9    | GLN  | N-CA-C      | -6.30 | 104.31      | 112.68   |
| 40  | BT    | 57   | PHE  | N-CA-C      | -6.29 | 100.60      | 110.36   |
| 31  | DG    | 38   | VAL  | N-CA-C      | 6.29  | 116.92      | 107.80   |
| 13  | AM    | 27   | LYS  | N-CA-C      | -6.26 | 105.61      | 113.18   |
| 9   | AI    | 64   | THR  | N-CA-C      | -6.25 | 100.72      | 110.42   |
| 25  | DA    | 1542 | A    | C2'-C3'-O3' | 6.25  | 118.88      | 109.50   |
| 38  | BR    | 9    | LYS  | N-CA-C      | 6.25  | 118.10      | 110.41   |
| 28  | BD    | 259  | THR  | N-CA-C      | 6.23  | 121.76      | 114.04   |
| 29  | DE    | 168  | MET  | N-CA-C      | 6.22  | 119.16      | 109.52   |
| 39  | DS    | 23   | ARG  | N-CA-C      | 6.22  | 117.90      | 110.19   |
| 40  | DT    | 31   | SER  | CA-C-N      | 6.22  | 128.90      | 120.44   |
| 40  | DT    | 31   | SER  | C-N-CA      | 6.22  | 128.90      | 120.44   |
| 14  | CN    | 42   | ILE  | CB-CA-C     | -6.21 | 104.02      | 111.97   |
| 17  | AQ    | 36   | ILE  | N-CA-C      | 6.21  | 117.78      | 108.96   |
| 2   | AB    | 166  | ASP  | CA-C-N      | 6.20  | 127.59      | 119.84   |
| 2   | AB    | 166  | ASP  | C-N-CA      | 6.20  | 127.59      | 119.84   |
| 36  | BP    | 24   | GLY  | N-CA-C      | -6.20 | 105.34      | 112.29   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 32  | DH    | 161 | GLY  | N-CA-C     | 6.19  | 119.63      | 111.70   |
| 17  | CQ    | 11  | VAL  | N-CA-C     | -6.19 | 107.25      | 113.20   |
| 37  | BQ    | 123 | HIS  | CG-CD2-NE2 | -6.19 | 101.01      | 107.20   |
| 37  | DQ    | 27  | VAL  | N-CA-C     | 6.19  | 116.36      | 110.42   |
| 9   | CI    | 118 | LYS  | N-CA-C     | 6.18  | 118.78      | 110.88   |
| 41  | DU    | 50  | ARG  | N-CA-C     | -6.17 | 104.64      | 111.36   |
| 34  | DN    | 43  | THR  | CA-C-N     | 6.17  | 127.55      | 119.84   |
| 34  | DN    | 43  | THR  | C-N-CA     | 6.17  | 127.55      | 119.84   |
| 29  | DE    | 38  | THR  | CA-C-N     | 6.16  | 127.54      | 119.84   |
| 29  | DE    | 38  | THR  | C-N-CA     | 6.16  | 127.54      | 119.84   |
| 4   | CD    | 208 | SER  | N-CA-C     | -6.16 | 103.93      | 112.30   |
| 45  | DY    | 90  | LEU  | N-CA-C     | -6.15 | 104.84      | 112.72   |
| 36  | DP    | 46  | LYS  | N-CA-C     | 6.14  | 117.64      | 111.07   |
| 42  | BV    | 5   | VAL  | N-CA-C     | 6.14  | 117.43      | 108.53   |
| 18  | CR    | 81  | PHE  | N-CA-C     | -6.14 | 106.33      | 113.88   |
| 33  | DI    | 14  | ASP  | N-CA-C     | 6.14  | 116.54      | 107.88   |
| 29  | DE    | 188 | VAL  | CA-C-N     | 6.13  | 127.51      | 119.84   |
| 29  | DE    | 188 | VAL  | C-N-CA     | 6.13  | 127.51      | 119.84   |
| 39  | DS    | 72  | ALA  | N-CA-C     | -6.13 | 104.51      | 111.07   |
| 43  | DW    | 86  | LEU  | CA-C-N     | -6.13 | 113.64      | 120.14   |
| 43  | DW    | 86  | LEU  | C-N-CA     | -6.13 | 113.64      | 120.14   |
| 28  | DD    | 212 | SER  | N-CA-C     | -6.12 | 104.67      | 111.71   |
| 16  | CP    | 33  | ILE  | CB-CA-C    | -6.12 | 104.00      | 112.02   |
| 56  | D9    | 12  | ASP  | N-CA-C     | -6.10 | 106.17      | 113.97   |
| 36  | BP    | 46  | LYS  | N-CA-C     | 6.09  | 117.59      | 111.07   |
| 40  | DT    | 28  | VAL  | CA-C-N     | -6.09 | 109.91      | 121.54   |
| 40  | DT    | 28  | VAL  | C-N-CA     | -6.09 | 109.91      | 121.54   |
| 30  | DF    | 80  | ALA  | CA-C-N     | 6.09  | 125.78      | 119.82   |
| 30  | DF    | 80  | ALA  | C-N-CA     | 6.09  | 125.78      | 119.82   |
| 3   | CC    | 155 | GLY  | N-CA-C     | 6.08  | 121.81      | 111.04   |
| 7   | CG    | 47  | CYS  | N-CA-C     | -6.08 | 104.21      | 111.69   |
| 14  | CN    | 3   | ARG  | N-CA-C     | -6.08 | 105.16      | 114.16   |
| 47  | B0    | 11  | ARG  | N-CA-C     | -6.08 | 105.44      | 112.92   |
| 40  | DT    | 110 | ILE  | CB-CA-C    | -6.07 | 103.94      | 112.14   |
| 8   | AH    | 129 | VAL  | N-CA-C     | 6.07  | 115.94      | 108.53   |
| 48  | B1    | 90  | ILE  | CB-CA-C    | -6.07 | 104.08      | 112.02   |
| 40  | DT    | 42  | ILE  | N-CA-C     | -6.06 | 98.39       | 107.37   |
| 28  | DD    | 118 | VAL  | N-CA-C     | 6.06  | 116.35      | 107.75   |
| 4   | CD    | 73  | ARG  | N-CA-C     | -6.05 | 103.64      | 111.02   |
| 12  | CL    | 39  | VAL  | N-CA-C     | 6.04  | 117.06      | 108.42   |
| 40  | BT    | 125 | ARG  | N-CA-C     | -6.04 | 105.89      | 113.20   |
| 40  | DT    | 25  | GLY  | N-CA-C     | -6.03 | 99.98       | 110.71   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 4   | AD    | 33  | MET  | N-CA-C  | -6.03 | 105.42      | 112.89   |
| 36  | DP    | 86  | LYS  | N-CA-C  | -6.03 | 104.63      | 111.14   |
| 30  | DF    | 130 | ALA  | N-CA-C  | -6.03 | 99.15       | 108.31   |
| 16  | AP    | 60  | LEU  | N-CA-C  | -6.02 | 105.42      | 112.89   |
| 46  | BZ    | 135 | GLU  | N-CA-C  | -6.02 | 106.27      | 113.97   |
| 36  | BP    | 86  | LYS  | N-CA-C  | -6.02 | 104.64      | 111.14   |
| 30  | DF    | 36  | VAL  | N-CA-C  | 6.02  | 116.19      | 110.53   |
| 33  | DI    | 129 | THR  | N-CA-C  | 6.02  | 118.29      | 110.53   |
| 7   | AG    | 133 | GLY  | N-CA-C  | -6.01 | 105.22      | 112.49   |
| 27  | BC    | 181 | PRO  | CA-C-N  | 6.01  | 127.36      | 119.84   |
| 27  | BC    | 181 | PRO  | C-N-CA  | 6.01  | 127.36      | 119.84   |
| 12  | CL    | 18  | VAL  | N-CA-C  | 6.01  | 116.07      | 110.42   |
| 28  | DD    | 136 | ILE  | CA-C-N  | 6.01  | 126.36      | 119.93   |
| 28  | DD    | 136 | ILE  | C-N-CA  | 6.01  | 126.36      | 119.93   |
| 28  | DD    | 250 | TRP  | N-CA-C  | -5.99 | 105.93      | 113.72   |
| 29  | DE    | 65  | GLY  | N-CA-C  | -5.99 | 105.34      | 115.34   |
| 40  | BT    | 19  | LEU  | CA-C-N  | 5.98  | 127.32      | 119.84   |
| 40  | BT    | 19  | LEU  | C-N-CA  | 5.98  | 127.32      | 119.84   |
| 9   | AI    | 35  | GLU  | N-CA-C  | -5.97 | 105.24      | 113.18   |
| 37  | BQ    | 12  | GLN  | N-CA-C  | 5.96  | 118.13      | 109.07   |
| 5   | CE    | 99  | GLY  | N-CA-C  | -5.96 | 103.22      | 112.45   |
| 19  | CS    | 52  | TYR  | N-CA-C  | -5.95 | 100.00      | 109.59   |
| 55  | B8    | 49  | VAL  | N-CA-C  | -5.95 | 99.71       | 108.99   |
| 45  | DY    | 4   | LYS  | N-CA-C  | 5.94  | 117.43      | 111.07   |
| 27  | BC    | 47  | LEU  | N-CA-C  | 5.94  | 116.08      | 108.24   |
| 8   | CH    | 73  | ASP  | CA-C-N  | 5.93  | 127.26      | 119.84   |
| 8   | CH    | 73  | ASP  | C-N-CA  | 5.93  | 127.26      | 119.84   |
| 41  | DU    | 35  | ALA  | N-CA-C  | -5.93 | 104.51      | 110.97   |
| 21  | AU    | 13  | ILE  | CB-CA-C | -5.92 | 104.30      | 111.88   |
| 44  | BX    | 73  | ARG  | CA-C-N  | 5.91  | 125.87      | 119.78   |
| 44  | BX    | 73  | ARG  | C-N-CA  | 5.91  | 125.87      | 119.78   |
| 45  | BY    | 94  | LYS  | N-CA-C  | 5.91  | 118.03      | 107.80   |
| 6   | CF    | 20  | ALA  | N-CA-C  | -5.91 | 105.17      | 112.38   |
| 12  | AL    | 36  | VAL  | N-CA-C  | 5.90  | 116.38      | 108.11   |
| 55  | D8    | 52  | LYS  | CA-C-N  | 5.86  | 125.40      | 119.19   |
| 55  | D8    | 52  | LYS  | C-N-CA  | 5.86  | 125.40      | 119.19   |
| 51  | B4    | 54  | LYS  | CA-C-N  | 5.86  | 126.63      | 120.12   |
| 51  | B4    | 54  | LYS  | C-N-CA  | 5.86  | 126.63      | 120.12   |
| 34  | BN    | 78  | TYR  | CA-C-N  | 5.86  | 126.05      | 119.90   |
| 34  | BN    | 78  | TYR  | C-N-CA  | 5.86  | 126.05      | 119.90   |
| 45  | BY    | 67  | LEU  | CB-CA-C | -5.86 | 109.84      | 116.63   |
| 20  | AT    | 27  | LYS  | N-CA-C  | -5.86 | 104.53      | 111.03   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 20  | CT    | 75  | ASN  | N-CA-C     | -5.85 | 105.25      | 112.38   |
| 10  | AJ    | 38  | ILE  | CA-C-N     | 5.84  | 127.14      | 119.84   |
| 10  | AJ    | 38  | ILE  | C-N-CA     | 5.84  | 127.14      | 119.84   |
| 40  | DT    | 89  | VAL  | N-CA-C     | 5.84  | 116.51      | 107.99   |
| 44  | BX    | 68  | ARG  | N-CA-C     | -5.83 | 106.39      | 112.93   |
| 28  | BD    | 14  | ARG  | N-CA-C     | -5.83 | 106.81      | 114.04   |
| 29  | DE    | 52  | LEU  | CA-C-N     | 5.83  | 127.13      | 119.84   |
| 29  | DE    | 52  | LEU  | C-N-CA     | 5.83  | 127.13      | 119.84   |
| 45  | BY    | 46  | LYS  | CA-C-O     | 5.83  | 121.32      | 117.94   |
| 32  | DH    | 164 | TYR  | N-CA-C     | -5.82 | 100.65      | 109.85   |
| 30  | DF    | 173 | VAL  | N-CA-C     | 5.81  | 116.24      | 107.75   |
| 45  | BY    | 37  | VAL  | N-CA-C     | 5.81  | 116.49      | 108.12   |
| 30  | DF    | 199 | TRP  | N-CA-C     | -5.81 | 105.69      | 112.89   |
| 13  | CM    | 98  | VAL  | N-CA-C     | 5.80  | 118.34      | 111.09   |
| 31  | DG    | 34  | LEU  | N-CA-C     | -5.80 | 101.31      | 109.96   |
| 39  | BS    | 54  | LEU  | N-CA-C     | -5.80 | 104.33      | 111.75   |
| 37  | DQ    | 125 | LEU  | CA-C-N     | 5.79  | 127.07      | 119.84   |
| 37  | DQ    | 125 | LEU  | C-N-CA     | 5.79  | 127.07      | 119.84   |
| 19  | CS    | 56  | GLN  | N-CA-C     | 5.78  | 115.87      | 108.24   |
| 45  | DY    | 7   | VAL  | N-CA-C     | 5.78  | 115.98      | 108.35   |
| 29  | BE    | 11  | MET  | N-CA-C     | 5.77  | 118.18      | 109.23   |
| 30  | DF    | 68  | LYS  | N-CA-C     | 5.77  | 118.86      | 109.06   |
| 34  | BN    | 43  | THR  | CA-C-N     | 5.76  | 126.52      | 120.12   |
| 34  | BN    | 43  | THR  | C-N-CA     | 5.76  | 126.52      | 120.12   |
| 46  | BZ    | 85  | HIS  | CG-CD2-NE2 | 5.76  | 112.96      | 107.20   |
| 6   | AF    | 87  | ARG  | CA-C-N     | -5.75 | 117.49      | 122.96   |
| 6   | AF    | 87  | ARG  | C-N-CA     | -5.75 | 117.49      | 122.96   |
| 13  | CM    | 11  | ARG  | N-CA-C     | 5.75  | 123.05      | 110.80   |
| 32  | DH    | 157 | TYR  | N-CA-C     | -5.75 | 105.93      | 113.17   |
| 42  | DV    | 43  | GLU  | N-CA-C     | -5.75 | 106.08      | 112.57   |
| 18  | CR    | 39  | VAL  | CB-CA-C    | -5.75 | 104.49      | 112.02   |
| 4   | CD    | 39  | PRO  | CA-C-N     | 5.73  | 125.72      | 120.21   |
| 4   | CD    | 39  | PRO  | C-N-CA     | 5.73  | 125.72      | 120.21   |
| 29  | BE    | 53  | PRO  | N-CA-C     | 5.72  | 121.07      | 113.40   |
| 42  | DV    | 44  | LYS  | N-CA-C     | 5.72  | 122.98      | 110.80   |
| 3   | AC    | 191 | THR  | CB-CA-C    | -5.72 | 107.25      | 114.40   |
| 20  | CT    | 33  | ILE  | CB-CA-C    | -5.72 | 103.70      | 112.05   |
| 37  | BQ    | 135 | ASP  | N-CA-C     | 5.71  | 122.95      | 110.80   |
| 28  | BD    | 148 | GLU  | N-CA-C     | -5.68 | 102.47      | 110.31   |
| 12  | AL    | 105 | TYR  | CB-CA-C    | -5.68 | 110.04      | 116.63   |
| 16  | AP    | 39  | TYR  | N-CA-C     | 5.68  | 117.22      | 107.28   |
| 17  | AQ    | 13  | ASP  | N-CA-C     | -5.68 | 105.55      | 112.88   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 4   | CD    | 38  | TYR  | N-CA-C     | 5.67  | 114.83      | 108.25   |
| 33  | BI    | 113 | ARG  | N-CA-C     | -5.67 | 106.97      | 112.97   |
| 10  | CJ    | 69  | ASN  | N-CA-C     | 5.66  | 118.01      | 109.23   |
| 28  | BD    | 136 | ILE  | CA-C-N     | 5.65  | 125.94      | 119.83   |
| 28  | BD    | 136 | ILE  | C-N-CA     | 5.65  | 125.94      | 119.83   |
| 30  | BF    | 101 | LEU  | CA-C-N     | 5.65  | 126.91      | 119.84   |
| 30  | BF    | 101 | LEU  | C-N-CA     | 5.65  | 126.91      | 119.84   |
| 28  | BD    | 116 | GLN  | N-CA-C     | -5.65 | 102.12      | 110.48   |
| 8   | CH    | 71  | GLY  | CA-C-N     | -5.65 | 113.96      | 119.78   |
| 8   | CH    | 71  | GLY  | C-N-CA     | -5.65 | 113.96      | 119.78   |
| 32  | DH    | 6   | ARG  | N-CA-C     | -5.65 | 105.66      | 113.18   |
| 42  | BV    | 65  | GLY  | N-CA-C     | 5.65  | 119.33      | 110.91   |
| 47  | D0    | 12  | ASN  | CB-CA-C    | -5.65 | 108.23      | 116.53   |
| 3   | CC    | 88  | ARG  | N-CA-C     | -5.64 | 104.53      | 111.75   |
| 43  | BW    | 101 | SER  | N-CA-C     | 5.63  | 118.87      | 110.14   |
| 27  | BC    | 66  | HIS  | ND1-CG-CD2 | 5.63  | 111.73      | 106.10   |
| 36  | DP    | 22  | GLY  | CA-C-N     | 5.63  | 125.61      | 120.03   |
| 36  | DP    | 22  | GLY  | C-N-CA     | 5.63  | 125.61      | 120.03   |
| 44  | BX    | 12  | VAL  | CB-CA-C    | -5.63 | 102.06      | 111.29   |
| 52  | B5    | 23  | HIS  | N-CA-C     | 5.63  | 119.25      | 112.38   |
| 17  | CQ    | 86  | GLU  | N-CA-C     | -5.63 | 104.83      | 110.97   |
| 45  | BY    | 46  | LYS  | CB-CA-C    | -5.62 | 108.97      | 117.07   |
| 44  | BX    | 58  | HIS  | ND1-CG-CD2 | 5.62  | 111.72      | 106.10   |
| 5   | AE    | 23  | GLY  | N-CA-C     | 5.61  | 118.71      | 110.80   |
| 47  | B0    | 22  | GLY  | N-CA-C     | 5.61  | 118.94      | 110.97   |
| 32  | DH    | 152 | ARG  | N-CA-C     | -5.60 | 98.87       | 110.80   |
| 3   | CC    | 29  | TYR  | N-CA-C     | -5.60 | 98.88       | 110.80   |
| 13  | CM    | 91  | ARG  | N-CA-C     | -5.59 | 105.57      | 112.90   |
| 4   | CD    | 174 | LEU  | N-CA-C     | 5.59  | 117.68      | 109.24   |
| 18  | CR    | 75  | ILE  | CB-CA-C    | -5.58 | 105.13      | 111.55   |
| 41  | BU    | 81  | HIS  | CG-CD2-NE2 | -5.58 | 101.62      | 107.20   |
| 4   | AD    | 38  | TYR  | N-CA-C     | 5.56  | 115.28      | 108.11   |
| 29  | DE    | 177 | PRO  | N-CA-C     | -5.56 | 106.15      | 113.65   |
| 6   | AF    | 36  | ARG  | N-CA-C     | -5.54 | 102.07      | 110.28   |
| 28  | BD    | 264 | LYS  | CA-C-N     | 5.54  | 125.38      | 119.28   |
| 28  | BD    | 264 | LYS  | C-N-CA     | 5.54  | 125.38      | 119.28   |
| 7   | CG    | 61  | VAL  | CB-CA-C    | -5.54 | 104.88      | 111.81   |
| 33  | DI    | 85  | GLU  | N-CA-C     | 5.54  | 117.42      | 108.34   |
| 6   | AF    | 81  | ILE  | CB-CA-C    | -5.54 | 103.58      | 112.16   |
| 28  | DD    | 43  | ARG  | N-CA-C     | 5.53  | 119.75      | 112.89   |
| 45  | BY    | 8   | LYS  | N-CA-C     | 5.53  | 118.06      | 109.60   |
| 5   | AE    | 32  | VAL  | N-CA-C     | 5.53  | 116.63      | 108.45   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 43  | BW    | 85  | VAL  | N-CA-C  | 5.53  | 115.81      | 107.80   |
| 11  | CK    | 80  | VAL  | CB-CA-C | -5.52 | 103.61      | 111.40   |
| 28  | DD    | 19  | ALA  | N-CA-C  | 5.52  | 117.86      | 110.35   |
| 5   | CE    | 109 | ILE  | CB-CA-C | -5.51 | 104.92      | 111.97   |
| 9   | AI    | 124 | GLN  | N-CA-C  | 5.50  | 118.90      | 110.20   |
| 11  | AK    | 40  | ILE  | CB-CA-C | -5.50 | 105.30      | 111.80   |
| 39  | DS    | 110 | LEU  | CB-CA-C | -5.50 | 109.74      | 117.23   |
| 12  | AL    | 11  | VAL  | N-CA-C  | -5.50 | 105.14      | 110.42   |
| 12  | CL    | 64  | TYR  | CB-CA-C | -5.50 | 107.52      | 114.40   |
| 4   | AD    | 180 | GLY  | N-CA-C  | -5.50 | 108.50      | 115.31   |
| 7   | CG    | 45  | ASP  | N-CA-C  | -5.49 | 105.45      | 111.82   |
| 11  | CK    | 118 | GLY  | N-CA-C  | 5.49  | 119.31      | 112.73   |
| 30  | DF    | 203 | GLN  | N-CA-C  | -5.49 | 106.43      | 113.01   |
| 16  | CP    | 35  | LYS  | CA-C-N  | -5.49 | 117.59      | 122.97   |
| 16  | CP    | 35  | LYS  | C-N-CA  | -5.49 | 117.59      | 122.97   |
| 43  | BW    | 72  | LYS  | N-CA-C  | -5.48 | 105.00      | 110.97   |
| 34  | DN    | 54  | VAL  | CB-CA-C | -5.48 | 104.11      | 110.91   |
| 9   | CI    | 83  | ARG  | N-CA-C  | -5.48 | 106.95      | 113.97   |
| 9   | CI    | 58  | HIS  | N-CA-C  | 5.47  | 117.24      | 111.28   |
| 30  | BF    | 8   | GLN  | N-CA-C  | 5.47  | 116.85      | 107.28   |
| 7   | CG    | 75  | VAL  | N-CA-C  | 5.47  | 115.41      | 106.72   |
| 2   | AB    | 164 | VAL  | N-CA-C  | 5.46  | 116.59      | 108.46   |
| 18  | CR    | 76  | LEU  | N-CA-C  | -5.46 | 106.93      | 113.21   |
| 11  | CK    | 127 | LYS  | N-CA-C  | -5.45 | 106.47      | 113.01   |
| 31  | DG    | 50  | ALA  | N-CA-C  | -5.45 | 105.34      | 111.28   |
| 4   | AD    | 6   | GLY  | CA-C-N  | 5.44  | 126.64      | 119.84   |
| 4   | AD    | 6   | GLY  | C-N-CA  | 5.44  | 126.64      | 119.84   |
| 3   | CC    | 68  | VAL  | N-CA-C  | 5.44  | 115.47      | 107.15   |
| 19  | AS    | 14  | HIS  | N-CA-C  | -5.44 | 105.46      | 111.71   |
| 3   | AC    | 198 | VAL  | N-CA-C  | 5.43  | 115.81      | 107.77   |
| 44  | DX    | 10  | ALA  | N-CA-C  | 5.43  | 112.91      | 108.07   |
| 42  | BV    | 69  | LYS  | N-CA-C  | 5.43  | 118.19      | 110.10   |
| 16  | AP    | 44  | THR  | N-CA-C  | -5.43 | 104.44      | 111.71   |
| 6   | CF    | 37  | VAL  | CB-CA-C | -5.42 | 104.74      | 111.08   |
| 40  | DT    | 99  | LEU  | N-CA-C  | 5.42  | 116.18      | 108.54   |
| 9   | CI    | 86  | VAL  | N-CA-C  | -5.41 | 105.43      | 113.39   |
| 39  | BS    | 58  | LEU  | N-CA-C  | 5.41  | 122.33      | 110.80   |
| 29  | BE    | 194 | GLY  | N-CA-C  | -5.41 | 105.35      | 112.82   |
| 30  | DF    | 183 | VAL  | N-CA-C  | 5.41  | 116.14      | 110.62   |
| 19  | AS    | 31  | ILE  | N-CA-C  | 5.40  | 115.83      | 107.78   |
| 42  | DV    | 14  | VAL  | N-CA-C  | 5.40  | 117.34      | 108.97   |
| 33  | BI    | 101 | LEU  | N-CA-C  | -5.40 | 105.43      | 112.23   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 28  | BD    | 62  | TYR  | N-CA-C     | 5.39  | 117.52      | 108.73   |
| 6   | AF    | 18  | GLN  | N-CA-C     | -5.39 | 105.30      | 111.07   |
| 43  | BW    | 12  | ILE  | N-CA-C     | -5.39 | 98.13       | 109.34   |
| 29  | DE    | 6   | GLY  | N-CA-C     | 5.38  | 118.43      | 110.63   |
| 13  | CM    | 123 | ALA  | N-CA-C     | 5.38  | 117.50      | 110.08   |
| 44  | DX    | 5   | TYR  | N-CA-C     | -5.38 | 106.31      | 112.92   |
| 47  | B0    | 63  | VAL  | CB-CA-C    | -5.38 | 103.82      | 111.40   |
| 20  | AT    | 14  | LYS  | N-CA-C     | -5.37 | 105.53      | 111.71   |
| 29  | BE    | 158 | GLY  | N-CA-C     | 5.37  | 118.00      | 110.38   |
| 4   | CD    | 87  | GLY  | N-CA-C     | -5.37 | 104.08      | 111.76   |
| 36  | BP    | 9   | ASN  | CA-C-N     | 5.37  | 126.55      | 119.84   |
| 36  | BP    | 9   | ASN  | C-N-CA     | 5.37  | 126.55      | 119.84   |
| 44  | BX    | 18  | TYR  | N-CA-C     | -5.36 | 104.68      | 111.11   |
| 35  | DO    | 25  | LEU  | N-CA-C     | 5.36  | 117.21      | 108.63   |
| 39  | BS    | 18  | ILE  | CB-CA-C    | 5.36  | 120.08      | 111.29   |
| 31  | BG    | 136 | ARG  | N-CA-C     | -5.36 | 106.88      | 113.41   |
| 17  | CQ    | 21  | VAL  | N-CA-C     | 5.35  | 115.57      | 107.75   |
| 30  | DF    | 139 | PHE  | N-CA-C     | -5.35 | 105.36      | 111.14   |
| 8   | CH    | 95  | VAL  | N-CA-C     | 5.34  | 115.97      | 108.17   |
| 55  | D8    | 62  | LEU  | CA-C-N     | -5.34 | 115.08      | 120.31   |
| 55  | D8    | 62  | LEU  | C-N-CA     | -5.34 | 115.08      | 120.31   |
| 54  | B7    | 22  | MET  | N-CA-C     | 5.33  | 122.15      | 110.80   |
| 28  | DD    | 209 | ALA  | N-CA-C     | -5.33 | 104.90      | 111.40   |
| 50  | D3    | 15  | TYR  | CA-C-N     | 5.33  | 125.27      | 119.78   |
| 50  | D3    | 15  | TYR  | C-N-CA     | 5.33  | 125.27      | 119.78   |
| 53  | B6    | 50  | ARG  | CB-CA-C    | -5.33 | 109.40      | 117.07   |
| 5   | AE    | 105 | VAL  | CB-CA-C    | -5.32 | 108.71      | 114.35   |
| 33  | BI    | 79  | ILE  | CA-C-N     | 5.32  | 126.49      | 119.84   |
| 33  | BI    | 79  | ILE  | C-N-CA     | 5.32  | 126.49      | 119.84   |
| 47  | D0    | 31  | VAL  | CB-CA-C    | -5.31 | 103.94      | 111.38   |
| 8   | AH    | 44  | PHE  | N-CA-C     | -5.30 | 106.70      | 114.39   |
| 32  | BH    | 115 | VAL  | CB-CA-C    | -5.30 | 105.20      | 111.09   |
| 37  | BQ    | 133 | ARG  | N-CA-C     | 5.30  | 119.07      | 111.02   |
| 4   | CD    | 88  | VAL  | N-CA-C     | 5.30  | 114.93      | 106.88   |
| 12  | AL    | 49  | ASN  | N-CA-C     | 5.29  | 117.90      | 109.81   |
| 33  | DI    | 62  | LYS  | N-CA-C     | -5.29 | 105.69      | 111.82   |
| 7   | CG    | 105 | VAL  | CB-CA-C    | -5.28 | 105.01      | 112.14   |
| 15  | CO    | 42  | HIS  | ND1-CG-CD2 | 5.28  | 111.38      | 106.10   |
| 28  | BD    | 215 | LEU  | N-CA-C     | -5.28 | 106.69      | 113.02   |
| 35  | DO    | 46  | ALA  | N-CA-C     | 5.28  | 116.83      | 108.96   |
| 18  | AR    | 86  | VAL  | N-CA-C     | 5.27  | 115.37      | 107.51   |
| 51  | B4    | 57  | ILE  | N-CA-C     | 5.27  | 115.98      | 106.61   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 28  | DD    | 60  | ARG  | N-CA-C  | 5.26  | 116.61      | 107.93   |
| 38  | DR    | 12  | ARG  | CA-C-N  | -5.26 | 111.45      | 122.03   |
| 38  | DR    | 12  | ARG  | C-N-CA  | -5.26 | 111.45      | 122.03   |
| 17  | AQ    | 9   | VAL  | N-CA-C  | 5.25  | 116.15      | 108.53   |
| 2   | CB    | 76  | GLN  | N-CA-C  | -5.25 | 105.16      | 112.30   |
| 11  | CK    | 50  | TYR  | N-CA-C  | 5.25  | 116.39      | 108.46   |
| 40  | BT    | 66  | VAL  | N-CA-C  | 5.24  | 115.06      | 106.72   |
| 3   | AC    | 191 | THR  | N-CA-C  | 5.24  | 116.68      | 109.29   |
| 12  | CL    | 39  | VAL  | CA-C-N  | -5.24 | 116.11      | 123.13   |
| 12  | CL    | 39  | VAL  | C-N-CA  | -5.24 | 116.11      | 123.13   |
| 9   | CI    | 75  | ASP  | N-CA-C  | -5.24 | 106.74      | 113.23   |
| 10  | CJ    | 20  | ALA  | N-CA-C  | -5.23 | 107.06      | 113.50   |
| 16  | AP    | 20  | VAL  | N-CA-C  | 5.23  | 115.26      | 108.35   |
| 30  | BF    | 17  | ARG  | N-CA-C  | 5.23  | 116.76      | 108.96   |
| 2   | CB    | 140 | HIS  | N-CA-C  | -5.23 | 105.58      | 111.28   |
| 11  | AK    | 102 | GLY  | N-CA-C  | -5.23 | 106.85      | 114.90   |
| 53  | B6    | 40  | CYS  | CA-C-N  | 5.22  | 126.37      | 119.84   |
| 53  | B6    | 40  | CYS  | C-N-CA  | 5.22  | 126.37      | 119.84   |
| 27  | BC    | 52  | ARG  | CB-CA-C | -5.22 | 110.13      | 117.23   |
| 17  | CQ    | 73  | VAL  | N-CA-C  | 5.22  | 115.37      | 107.80   |
| 47  | D0    | 40  | GLN  | N-CA-C  | 5.22  | 117.19      | 108.99   |
| 20  | AT    | 9   | ASN  | N-CA-C  | 5.22  | 117.95      | 109.24   |
| 7   | CG    | 87  | VAL  | N-CA-C  | 5.22  | 113.58      | 107.89   |
| 40  | DT    | 29  | ARG  | CA-C-N  | 5.21  | 131.34      | 121.97   |
| 40  | DT    | 29  | ARG  | C-N-CA  | 5.21  | 131.34      | 121.97   |
| 5   | AE    | 80  | ILE  | CB-CA-C | -5.20 | 102.90      | 110.81   |
| 40  | BT    | 31  | SER  | CA-C-O  | 5.20  | 120.96      | 117.94   |
| 9   | CI    | 99  | LEU  | N-CA-C  | -5.20 | 106.93      | 113.28   |
| 20  | CT    | 91  | LEU  | N-CA-C  | -5.20 | 107.59      | 114.04   |
| 49  | D2    | 47  | ASN  | N-CA-C  | 5.20  | 121.88      | 110.80   |
| 41  | BU    | 98  | LEU  | N-CA-C  | -5.20 | 105.61      | 111.28   |
| 30  | DF    | 48  | THR  | N-CA-C  | 5.20  | 120.27      | 113.30   |
| 18  | AR    | 75  | ILE  | CB-CA-C | -5.20 | 105.11      | 111.92   |
| 33  | DI    | 94  | ALA  | N-CA-C  | -5.20 | 105.70      | 111.36   |
| 18  | CR    | 50  | ILE  | CB-CA-C | -5.19 | 102.78      | 111.29   |
| 41  | DU    | 34  | LYS  | N-CA-C  | -5.19 | 105.80      | 111.82   |
| 33  | DI    | 89  | TYR  | N-CA-C  | -5.18 | 105.32      | 111.69   |
| 28  | BD    | 240 | ALA  | CA-C-N  | 5.18  | 126.31      | 119.84   |
| 28  | BD    | 240 | ALA  | C-N-CA  | 5.18  | 126.31      | 119.84   |
| 55  | B8    | 41  | ILE  | N-CA-C  | 5.17  | 115.39      | 110.53   |
| 31  | DG    | 89  | GLY  | N-CA-C  | 5.17  | 118.49      | 111.72   |
| 29  | BE    | 144 | ARG  | CB-CA-C | -5.17 | 109.63      | 117.07   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 52  | D5    | 31  | VAL  | CA-C-N     | 5.17  | 126.30      | 119.84   |
| 52  | D5    | 31  | VAL  | C-N-CA     | 5.17  | 126.30      | 119.84   |
| 38  | BR    | 61  | HIS  | CG-CD2-NE2 | 5.16  | 112.36      | 107.20   |
| 40  | BT    | 31  | SER  | CB-CA-C    | -5.16 | 109.64      | 117.07   |
| 40  | BT    | 15  | VAL  | N-CA-C     | 5.16  | 116.71      | 108.87   |
| 32  | BH    | 97  | ARG  | N-CA-C     | 5.16  | 113.01      | 108.78   |
| 48  | B1    | 92  | LYS  | N-CA-C     | -5.16 | 105.35      | 110.97   |
| 15  | AO    | 42  | HIS  | N-CA-C     | -5.16 | 105.66      | 111.28   |
| 44  | DX    | 80  | ILE  | CB-CA-C    | 5.15  | 116.29      | 110.41   |
| 40  | BT    | 93  | ARG  | N-CA-C     | -5.15 | 105.89      | 113.72   |
| 7   | CG    | 24  | THR  | N-CA-C     | -5.15 | 105.66      | 111.28   |
| 29  | BE    | 113 | PHE  | CB-CA-C    | -5.15 | 104.40      | 112.12   |
| 34  | DN    | 10  | GLU  | CA-C-N     | 5.15  | 126.27      | 119.84   |
| 34  | DN    | 10  | GLU  | C-N-CA     | 5.15  | 126.27      | 119.84   |
| 36  | BP    | 49  | ARG  | N-CA-C     | -5.14 | 99.84       | 110.80   |
| 4   | CD    | 195 | ALA  | N-CA-C     | -5.14 | 100.86      | 109.24   |
| 39  | DS    | 28  | VAL  | N-CA-C     | 5.14  | 115.36      | 108.17   |
| 45  | DY    | 84  | ARG  | N-CA-C     | -5.14 | 101.50      | 109.72   |
| 29  | BE    | 63  | LEU  | N-CA-C     | -5.12 | 105.61      | 111.14   |
| 3   | AC    | 29  | TYR  | N-CA-C     | -5.12 | 99.89       | 110.80   |
| 35  | DO    | 15  | GLY  | N-CA-C     | -5.12 | 108.60      | 114.69   |
| 55  | B8    | 54  | GLU  | N-CA-C     | -5.11 | 105.79      | 111.36   |
| 32  | DH    | 20  | ALA  | CA-C-N     | -5.11 | 113.45      | 119.84   |
| 32  | DH    | 20  | ALA  | C-N-CA     | -5.11 | 113.45      | 119.84   |
| 11  | CK    | 74  | ALA  | N-CA-C     | -5.11 | 106.89      | 113.02   |
| 31  | BG    | 146 | TYR  | N-CA-C     | -5.11 | 107.60      | 113.88   |
| 20  | CT    | 73  | HIS  | N-CA-C     | 5.11  | 115.08      | 107.88   |
| 36  | DP    | 49  | ARG  | N-CA-C     | -5.11 | 99.92       | 110.80   |
| 42  | DV    | 28  | GLU  | CA-C-N     | 5.11  | 126.22      | 119.84   |
| 42  | DV    | 28  | GLU  | C-N-CA     | 5.11  | 126.22      | 119.84   |
| 53  | D6    | 48  | VAL  | N-CA-C     | 5.11  | 115.88      | 110.72   |
| 33  | BI    | 130 | TYR  | N-CA-C     | 5.11  | 115.08      | 107.88   |
| 12  | CL    | 84  | LEU  | N-CA-C     | 5.10  | 117.81      | 109.59   |
| 2   | AB    | 40  | HIS  | CG-CD2-NE2 | 5.10  | 112.30      | 107.20   |
| 31  | BG    | 36  | LYS  | N-CA-C     | 5.10  | 116.28      | 108.52   |
| 48  | B1    | 74  | VAL  | CB-CA-C    | -5.10 | 105.36      | 112.04   |
| 13  | CM    | 40  | ASN  | CA-C-N     | 5.10  | 124.71      | 119.05   |
| 13  | CM    | 40  | ASN  | C-N-CA     | 5.10  | 124.71      | 119.05   |
| 48  | D1    | 4   | VAL  | N-CA-C     | 5.10  | 117.07      | 108.81   |
| 46  | BZ    | 109 | ALA  | N-CA-C     | -5.09 | 106.77      | 112.87   |
| 40  | DT    | 38  | ASN  | N-CA-C     | 5.08  | 116.90      | 111.36   |
| 7   | AG    | 106 | GLN  | N-CA-C     | -5.08 | 105.82      | 111.36   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 35  | BO    | 46  | ALA  | N-CA-C  | 5.08  | 116.01      | 108.60   |
| 30  | DF    | 170 | LEU  | CA-C-N  | 5.08  | 125.15      | 119.87   |
| 30  | DF    | 170 | LEU  | C-N-CA  | 5.08  | 125.15      | 119.87   |
| 31  | DG    | 31  | VAL  | CA-C-N  | 5.07  | 126.18      | 119.84   |
| 31  | DG    | 31  | VAL  | C-N-CA  | 5.07  | 126.18      | 119.84   |
| 2   | AB    | 219 | VAL  | CB-CA-C | -5.07 | 105.38      | 112.02   |
| 34  | DN    | 80  | GLY  | N-CA-C  | -5.07 | 108.26      | 115.30   |
| 7   | CG    | 132 | GLY  | N-CA-C  | 5.07  | 119.46      | 112.37   |
| 55  | D8    | 23  | VAL  | CB-CA-C | -5.07 | 103.58      | 110.77   |
| 3   | AC    | 57  | ILE  | N-CA-C  | 5.05  | 115.19      | 108.27   |
| 29  | BE    | 52  | LEU  | CA-C-N  | 5.05  | 124.36      | 118.85   |
| 29  | BE    | 52  | LEU  | C-N-CA  | 5.05  | 124.36      | 118.85   |
| 40  | BT    | 29  | ARG  | CA-C-N  | 5.05  | 128.32      | 120.34   |
| 40  | BT    | 29  | ARG  | C-N-CA  | 5.05  | 128.32      | 120.34   |
| 29  | DE    | 92  | THR  | N-CA-C  | 5.05  | 116.66      | 109.14   |
| 13  | AM    | 65  | LYS  | CA-C-N  | 5.05  | 130.79      | 121.70   |
| 13  | AM    | 65  | LYS  | C-N-CA  | 5.05  | 130.79      | 121.70   |
| 38  | BR    | 38  | VAL  | CA-C-N  | -5.05 | 113.53      | 119.84   |
| 38  | BR    | 38  | VAL  | C-N-CA  | -5.05 | 113.53      | 119.84   |
| 43  | DW    | 85  | VAL  | N-CA-C  | 5.05  | 115.58      | 108.36   |
| 39  | BS    | 97  | ARG  | N-CA-C  | 5.04  | 121.55      | 110.80   |
| 39  | DS    | 19  | LYS  | N-CA-C  | -5.04 | 100.06      | 110.80   |
| 31  | DG    | 123 | ASN  | N-CA-C  | -5.04 | 107.79      | 114.04   |
| 36  | DP    | 71  | VAL  | CB-CA-C | -5.04 | 109.01      | 114.35   |
| 41  | DU    | 70  | ARG  | N-CA-C  | -5.03 | 106.65      | 112.89   |
| 3   | AC    | 72  | LYS  | CA-C-N  | 5.03  | 125.30      | 119.47   |
| 3   | AC    | 72  | LYS  | C-N-CA  | 5.03  | 125.30      | 119.47   |
| 32  | DH    | 145 | ALA  | N-CA-C  | -5.02 | 105.70      | 111.07   |
| 9   | AI    | 127 | LYS  | N-CA-C  | -5.02 | 105.41      | 113.28   |
| 5   | AE    | 113 | ALA  | N-CA-C  | -5.01 | 105.33      | 111.75   |
| 43  | BW    | 13  | SER  | CA-C-N  | 5.01  | 126.11      | 119.84   |
| 43  | BW    | 13  | SER  | C-N-CA  | 5.01  | 126.11      | 119.84   |
| 55  | B8    | 23  | VAL  | CB-CA-C | -5.01 | 104.03      | 110.84   |
| 55  | B8    | 49  | VAL  | CA-C-O  | -5.01 | 115.84      | 121.75   |
| 30  | BF    | 38  | ARG  | N-CA-C  | -5.01 | 104.91      | 111.02   |
| 40  | BT    | 82  | LEU  | N-CA-C  | -5.01 | 101.13      | 108.79   |
| 4   | CD    | 6   | GLY  | CA-C-N  | 5.01  | 125.01      | 119.90   |
| 4   | CD    | 6   | GLY  | C-N-CA  | 5.01  | 125.01      | 119.90   |
| 29  | DE    | 141 | ILE  | CB-CA-C | -5.00 | 105.75      | 110.70   |
| 4   | AD    | 108 | LEU  | N-CA-C  | -5.00 | 106.92      | 112.57   |
| 49  | B2    | 47  | ASN  | N-CA-C  | 5.00  | 121.46      | 110.80   |
| 4   | CD    | 204 | ILE  | N-CA-C  | -5.00 | 105.72      | 110.42   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 10  | CJ    | 36  | GLY  | CA-C-N | 5.00  | 126.09      | 119.84   |
| 10  | CJ    | 36  | GLY  | C-N-CA | 5.00  | 126.09      | 119.84   |
| 10  | AJ    | 17  | ASP  | N-CA-C | -5.00 | 107.22      | 113.72   |

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 28  | BD    | 222 | 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   | AA    | 32328 | 0        | 16317    | 801     | 0            |
| 1   | CA    | 32328 | 0        | 16317    | 876     | 1            |
| 2   | AB    | 1901  | 0        | 1951     | 255     | 0            |
| 2   | CB    | 1901  | 0        | 1951     | 253     | 0            |
| 3   | AC    | 1613  | 0        | 1677     | 216     | 0            |
| 3   | CC    | 1613  | 0        | 1677     | 162     | 0            |
| 4   | AD    | 1703  | 0        | 1765     | 199     | 0            |
| 4   | CD    | 1703  | 0        | 1764     | 188     | 0            |
| 5   | AE    | 1147  | 0        | 1207     | 152     | 0            |
| 5   | CE    | 1147  | 0        | 1207     | 171     | 0            |
| 6   | AF    | 843   | 0        | 857      | 92      | 0            |
| 6   | CF    | 843   | 0        | 857      | 67      | 0            |
| 7   | AG    | 1257  | 0        | 1296     | 125     | 0            |
| 7   | CG    | 1257  | 0        | 1296     | 111     | 0            |
| 8   | AH    | 1116  | 0        | 1177     | 117     | 0            |
| 8   | CH    | 1116  | 0        | 1177     | 114     | 0            |
| 9   | AI    | 1010  | 0        | 1037     | 138     | 0            |
| 9   | CI    | 1010  | 0        | 1037     | 149     | 0            |
| 10  | AJ    | 795   | 0        | 840      | 128     | 0            |
| 10  | CJ    | 795   | 0        | 840      | 136     | 0            |
| 11  | AK    | 885   | 0        | 904      | 103     | 0            |
| 11  | CK    | 885   | 0        | 904      | 115     | 0            |
| 12  | AL    | 971   | 0        | 1057     | 130     | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 12  | CL    | 971   | 0        | 1057     | 130     | 0            |
| 13  | AM    | 988   | 0        | 1059     | 156     | 0            |
| 13  | CM    | 997   | 0        | 1072     | 175     | 0            |
| 14  | AN    | 492   | 0        | 529      | 96      | 0            |
| 14  | CN    | 492   | 0        | 531      | 77      | 0            |
| 15  | AO    | 734   | 0        | 771      | 64      | 0            |
| 15  | CO    | 734   | 0        | 771      | 54      | 0            |
| 16  | AP    | 701   | 0        | 720      | 64      | 0            |
| 16  | CP    | 701   | 0        | 720      | 105     | 0            |
| 17  | AQ    | 824   | 0        | 891      | 70      | 0            |
| 17  | CQ    | 824   | 0        | 891      | 89      | 0            |
| 18  | AR    | 574   | 0        | 644      | 67      | 0            |
| 18  | CR    | 574   | 0        | 644      | 72      | 0            |
| 19  | AS    | 630   | 0        | 652      | 123     | 0            |
| 19  | CS    | 630   | 0        | 652      | 112     | 0            |
| 20  | AT    | 763   | 0        | 861      | 137     | 0            |
| 20  | CT    | 763   | 0        | 861      | 172     | 0            |
| 21  | AU    | 209   | 0        | 221      | 13      | 0            |
| 21  | CU    | 209   | 0        | 221      | 22      | 0            |
| 22  | AV    | 1644  | 0        | 836      | 110     | 0            |
| 22  | CV    | 1643  | 0        | 836      | 143     | 0            |
| 23  | AW    | 1619  | 0        | 822      | 122     | 0            |
| 23  | AY    | 365   | 0        | 185      | 29      | 0            |
| 23  | CW    | 1619  | 0        | 822      | 108     | 0            |
| 23  | CY    | 365   | 0        | 185      | 37      | 0            |
| 24  | AX    | 255   | 0        | 129      | 49      | 0            |
| 24  | CX    | 210   | 0        | 109      | 23      | 0            |
| 25  | BA    | 60527 | 0        | 30515    | 1620    | 1            |
| 25  | DA    | 60827 | 0        | 30663    | 1380    | 0            |
| 26  | BB    | 2551  | 0        | 1295     | 56      | 1            |
| 26  | DB    | 2551  | 0        | 1295     | 55      | 0            |
| 27  | BC    | 1142  | 0        | 865      | 85      | 0            |
| 27  | DC    | 1142  | 0        | 865      | 76      | 0            |
| 28  | BD    | 2105  | 0        | 2182     | 326     | 0            |
| 28  | DD    | 2105  | 0        | 2182     | 289     | 0            |
| 29  | BE    | 1564  | 0        | 1629     | 226     | 0            |
| 29  | DE    | 1564  | 0        | 1629     | 218     | 0            |
| 30  | BF    | 1624  | 0        | 1677     | 258     | 0            |
| 30  | DF    | 1585  | 0        | 1632     | 199     | 0            |
| 31  | BG    | 1474  | 0        | 1535     | 272     | 0            |
| 31  | DG    | 1474  | 0        | 1535     | 223     | 0            |
| 32  | BH    | 1223  | 0        | 1282     | 138     | 1            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 32  | DH    | 1290  | 0        | 1364     | 242     | 0            |
| 33  | BI    | 1131  | 0        | 1218     | 159     | 0            |
| 33  | DI    | 1136  | 0        | 1223     | 243     | 0            |
| 34  | BN    | 1105  | 0        | 1180     | 191     | 0            |
| 34  | DN    | 1105  | 0        | 1180     | 156     | 0            |
| 35  | BO    | 933   | 0        | 996      | 119     | 0            |
| 35  | DO    | 933   | 0        | 996      | 95      | 0            |
| 36  | BP    | 1145  | 0        | 1228     | 285     | 0            |
| 36  | DP    | 1145  | 0        | 1228     | 289     | 3            |
| 37  | BQ    | 1122  | 0        | 1179     | 138     | 0            |
| 37  | DQ    | 1122  | 0        | 1179     | 129     | 0            |
| 38  | BR    | 960   | 0        | 1021     | 153     | 0            |
| 38  | DR    | 968   | 0        | 1033     | 117     | 0            |
| 39  | BS    | 771   | 0        | 832      | 129     | 0            |
| 39  | DS    | 882   | 0        | 943      | 151     | 0            |
| 40  | BT    | 1142  | 0        | 1202     | 245     | 0            |
| 40  | DT    | 1142  | 0        | 1202     | 274     | 0            |
| 41  | BU    | 964   | 0        | 1022     | 162     | 0            |
| 41  | DU    | 958   | 0        | 1014     | 204     | 0            |
| 42  | BV    | 779   | 0        | 852      | 138     | 0            |
| 42  | DV    | 779   | 0        | 852      | 155     | 3            |
| 43  | BW    | 896   | 0        | 953      | 110     | 0            |
| 43  | DW    | 896   | 0        | 953      | 91      | 0            |
| 44  | BX    | 726   | 0        | 778      | 67      | 0            |
| 44  | DX    | 726   | 0        | 778      | 69      | 0            |
| 45  | BY    | 776   | 0        | 870      | 181     | 0            |
| 45  | DY    | 785   | 0        | 878      | 182     | 0            |
| 46  | BZ    | 1404  | 0        | 1432     | 154     | 0            |
| 46  | DZ    | 1404  | 0        | 1432     | 223     | 0            |
| 47  | B0    | 662   | 0        | 688      | 63      | 0            |
| 47  | D0    | 662   | 0        | 688      | 63      | 0            |
| 48  | B1    | 732   | 0        | 808      | 81      | 0            |
| 48  | D1    | 732   | 0        | 808      | 70      | 0            |
| 49  | B2    | 598   | 0        | 653      | 70      | 0            |
| 49  | D2    | 598   | 0        | 653      | 56      | 0            |
| 50  | B3    | 468   | 0        | 523      | 43      | 3            |
| 50  | D3    | 468   | 0        | 523      | 55      | 0            |
| 51  | B4    | 226   | 0        | 229      | 40      | 0            |
| 51  | D4    | 298   | 0        | 312      | 45      | 0            |
| 52  | B5    | 459   | 0        | 480      | 51      | 0            |
| 52  | D5    | 459   | 0        | 480      | 53      | 3            |
| 53  | B6    | 381   | 0        | 391      | 51      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 53  | D6    | 381   | 0        | 391      | 104     | 0            |
| 54  | B7    | 419   | 0        | 467      | 38      | 0            |
| 54  | D7    | 419   | 0        | 467      | 35      | 0            |
| 55  | B8    | 508   | 0        | 576      | 115     | 0            |
| 55  | D8    | 508   | 0        | 576      | 89      | 0            |
| 56  | B9    | 299   | 0        | 326      | 14      | 0            |
| 56  | D9    | 299   | 0        | 326      | 14      | 0            |
| 57  | AA    | 110   | 0        | 0        | 0       | 0            |
| 57  | AE    | 1     | 0        | 0        | 0       | 0            |
| 57  | AV    | 5     | 0        | 0        | 0       | 0            |
| 57  | AX    | 1     | 0        | 0        | 0       | 0            |
| 57  | B5    | 1     | 0        | 0        | 0       | 0            |
| 57  | B7    | 1     | 0        | 0        | 0       | 0            |
| 57  | BA    | 323   | 0        | 0        | 0       | 0            |
| 57  | BB    | 5     | 0        | 0        | 0       | 0            |
| 57  | BD    | 2     | 0        | 0        | 0       | 0            |
| 57  | BE    | 3     | 0        | 0        | 0       | 0            |
| 57  | BF    | 1     | 0        | 0        | 0       | 0            |
| 57  | BN    | 1     | 0        | 0        | 0       | 0            |
| 57  | BO    | 1     | 0        | 0        | 0       | 0            |
| 57  | BP    | 1     | 0        | 0        | 0       | 0            |
| 57  | BU    | 1     | 0        | 0        | 0       | 0            |
| 57  | CA    | 141   | 0        | 0        | 0       | 0            |
| 57  | CE    | 2     | 0        | 0        | 0       | 0            |
| 57  | CV    | 5     | 0        | 0        | 0       | 0            |
| 57  | CW    | 1     | 0        | 0        | 0       | 0            |
| 57  | CX    | 1     | 0        | 0        | 0       | 0            |
| 57  | CY    | 1     | 0        | 0        | 0       | 0            |
| 57  | D0    | 2     | 0        | 0        | 0       | 0            |
| 57  | D1    | 2     | 0        | 0        | 0       | 0            |
| 57  | D2    | 1     | 0        | 0        | 0       | 0            |
| 57  | D5    | 2     | 0        | 0        | 0       | 0            |
| 57  | D8    | 1     | 0        | 0        | 0       | 0            |
| 57  | DA    | 397   | 0        | 0        | 0       | 0            |
| 57  | DB    | 5     | 0        | 0        | 0       | 0            |
| 57  | DD    | 3     | 0        | 0        | 0       | 0            |
| 57  | DE    | 2     | 0        | 0        | 0       | 0            |
| 57  | DF    | 1     | 0        | 0        | 0       | 0            |
| 57  | DP    | 3     | 0        | 0        | 0       | 0            |
| 57  | DQ    | 1     | 0        | 0        | 0       | 0            |
| 57  | DU    | 3     | 0        | 0        | 0       | 0            |
| 57  | DW    | 1     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 57  | DX    | 1      | 0        | 0        | 0       | 0            |
| 58  | AA    | 42     | 0        | 45       | 3       | 0            |
| 58  | CA    | 42     | 0        | 45       | 2       | 0            |
| 59  | AD    | 1      | 0        | 0        | 0       | 0            |
| 59  | AN    | 1      | 0        | 0        | 1       | 0            |
| 59  | CD    | 1      | 0        | 0        | 0       | 0            |
| 59  | CN    | 1      | 0        | 0        | 3       | 0            |
| All | All   | 293977 | 0        | 199058   | 16999   | 8            |

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 35.

All (16999) 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:BS:34:HIS:CE1  | 39:BS:54:LEU:HB2   | 1.32                     | 1.58              |
| 42:DV:1:MET:SD    | 42:DV:1:MET:CG     | 2.01                     | 1.47              |
| 40:BT:28:VAL:CG1  | 40:BT:46:GLU:HA    | 1.42                     | 1.44              |
| 1:CA:748:C:H1'    | 1:CA:749:C:C5      | 1.53                     | 1.44              |
| 34:BN:62:VAL:HG22 | 34:BN:66:LYS:CD    | 1.49                     | 1.42              |
| 1:AA:1049:U:H1'   | 1:AA:1201:A:N7     | 1.33                     | 1.41              |
| 40:BT:29:ARG:HG3  | 40:BT:85:LYS:CA    | 1.49                     | 1.41              |
| 19:AS:5:LEU:HD12  | 19:AS:10:PHE:CD1   | 1.56                     | 1.41              |
| 1:CA:1065:U:C4'   | 1:CA:1066:C:H5''   | 1.49                     | 1.41              |
| 5:CE:78:HIS:CD2   | 8:CH:104:ARG:HG3   | 1.50                     | 1.40              |
| 20:AT:37:SER:HB3  | 20:AT:84:LEU:CD2   | 1.54                     | 1.36              |
| 39:BS:34:HIS:HE1  | 39:BS:54:LEU:CB    | 1.38                     | 1.36              |
| 33:BI:77:LEU:CD2  | 33:BI:101:LEU:HD13 | 1.52                     | 1.36              |
| 7:AG:14:PRO:HG3   | 7:AG:21:VAL:CG1    | 1.56                     | 1.36              |
| 5:CE:102:ALA:CB   | 5:CE:106:PRO:HB2   | 1.56                     | 1.36              |
| 45:BY:28:LYS:CB   | 45:BY:37:VAL:HB    | 1.54                     | 1.35              |
| 25:DA:887:A:H1'   | 25:DA:889:C:N4     | 1.38                     | 1.35              |
| 12:CL:11:VAL:HG13 | 17:CQ:29:HIS:CD2   | 1.61                     | 1.34              |
| 4:CD:108:LEU:HB3  | 4:CD:110:PHE:CD1   | 1.60                     | 1.34              |
| 1:CA:1064:G:H4'   | 1:CA:1065:U:C5'    | 1.56                     | 1.34              |
| 1:CA:1065:U:H4'   | 1:CA:1066:C:C5'    | 1.56                     | 1.34              |
| 31:BG:43:LEU:CB   | 31:BG:88:ILE:HD11  | 1.56                     | 1.33              |
| 14:AN:12:ARG:C    | 14:AN:14:PRO:HD2   | 1.51                     | 1.32              |
| 45:BY:28:LYS:HB2  | 45:BY:37:VAL:CB    | 1.58                     | 1.32              |
| 28:BD:80:ALA:HB2  | 28:BD:96:HIS:CD2   | 1.62                     | 1.31              |
| 31:BG:72:ARG:CB   | 31:BG:86:MET:HA    | 1.61                     | 1.31              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 38:BR:10:LEU:CB   | 38:BR:17:ARG:HD3   | 1.62                     | 1.29              |
| 40:DT:32:TYR:HB3  | 40:DT:81:PRO:CB    | 1.61                     | 1.29              |
| 31:BG:43:LEU:HB2  | 31:BG:88:ILE:CD1   | 1.62                     | 1.28              |
| 36:BP:59:LEU:HA   | 36:BP:61:ARG:NH1   | 1.48                     | 1.28              |
| 40:BT:29:ARG:CG   | 40:BT:85:LYS:HA    | 1.63                     | 1.27              |
| 30:BF:64:ILE:HG23 | 30:BF:65:TRP:CD1   | 1.69                     | 1.26              |
| 5:AE:121:LYS:CG   | 5:AE:122:GLU:H     | 1.45                     | 1.25              |
| 22:CV:29:C:C2'    | 22:CV:30:G:H5'     | 1.64                     | 1.25              |
| 55:B8:31:HIS:ND1  | 55:B8:32:LEU:HA    | 1.50                     | 1.24              |
| 5:CE:102:ALA:HB1  | 5:CE:106:PRO:CB    | 1.68                     | 1.24              |
| 13:CM:124:PRO:HB3 | 13:CM:125:ARG:CG   | 1.68                     | 1.24              |
| 19:AS:9:VAL:CG1   | 19:AS:11:VAL:HG12  | 1.67                     | 1.24              |
| 31:BG:72:ARG:HH11 | 31:BG:86:MET:CB    | 1.51                     | 1.24              |
| 1:CA:251:G:H1'    | 1:CA:252:U:C5      | 1.73                     | 1.23              |
| 31:BG:142:PRO:HG2 | 31:BG:143:GLU:OE1  | 1.39                     | 1.23              |
| 38:BR:10:LEU:HB3  | 38:BR:17:ARG:CD    | 1.69                     | 1.23              |
| 25:BA:887:A:H1'   | 25:BA:889:C:N4     | 1.53                     | 1.22              |
| 25:DA:1693:U:H2'  | 28:DD:14:ARG:NH2   | 1.51                     | 1.22              |
| 1:AA:1049:U:H1'   | 1:AA:1201:A:C8     | 1.75                     | 1.22              |
| 25:BA:1453:U:O3'  | 25:BA:1455:G:P     | 1.97                     | 1.22              |
| 40:BT:28:VAL:HG22 | 40:BT:47:GLY:N     | 1.51                     | 1.22              |
| 23:AW:34:G:C4     | 24:AX:14:A:C2      | 2.27                     | 1.22              |
| 39:DS:106:ARG:HA  | 39:DS:110:LEU:CD1  | 1.69                     | 1.22              |
| 5:CE:102:ALA:O    | 5:CE:106:PRO:HG3   | 1.37                     | 1.21              |
| 45:DY:76:CYS:SG   | 45:DY:77:PRO:HD2   | 1.80                     | 1.21              |
| 32:DH:98:LEU:HB2  | 32:DH:125:VAL:HG21 | 1.21                     | 1.21              |
| 5:CE:78:HIS:HD2   | 8:CH:104:ARG:CG    | 1.53                     | 1.20              |
| 19:AS:5:LEU:CD1   | 19:AS:10:PHE:HD1   | 1.53                     | 1.20              |
| 1:CA:251:G:C1'    | 1:CA:252:U:H5      | 1.55                     | 1.20              |
| 20:CT:56:MET:CG   | 20:CT:84:LEU:HD12  | 1.71                     | 1.20              |
| 4:CD:108:LEU:HG   | 4:CD:110:PHE:CE1   | 1.76                     | 1.19              |
| 30:DF:62:ARG:HH11 | 30:DF:62:ARG:HG2   | 1.03                     | 1.19              |
| 41:DU:92:ARG:HD2  | 42:DV:11:GLN:CD    | 1.66                     | 1.19              |
| 1:AA:1049:U:H1'   | 1:AA:1201:A:C5     | 1.78                     | 1.18              |
| 31:BG:72:ARG:HB3  | 31:BG:86:MET:CA    | 1.72                     | 1.18              |
| 19:AS:9:VAL:HG12  | 19:AS:11:VAL:CG1   | 1.72                     | 1.18              |
| 28:BD:267:SER:O   | 28:BD:268:ARG:CG   | 1.91                     | 1.18              |
| 20:CT:56:MET:HG3  | 20:CT:84:LEU:HD12  | 1.18                     | 1.18              |
| 1:CA:251:G:C1'    | 1:CA:252:U:C5      | 2.25                     | 1.18              |
| 36:DP:59:LEU:HA   | 36:DP:61:ARG:CZ    | 1.73                     | 1.18              |
| 36:BP:59:LEU:HA   | 36:BP:61:ARG:CZ    | 1.71                     | 1.18              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 34:BN:123:TYR:HE1  | 34:BN:130:HIS:CE1  | 1.62                     | 1.18              |
| 10:CJ:78:ASN:HD21  | 10:CJ:80:LYS:HB2   | 1.03                     | 1.18              |
| 5:AE:103:GLY:O     | 5:AE:106:PRO:HD2   | 1.43                     | 1.17              |
| 28:BD:267:SER:O    | 28:BD:268:ARG:HG3  | 0.99                     | 1.17              |
| 36:DP:63:PRO:HB3   | 55:D8:13:ARG:HB3   | 1.23                     | 1.17              |
| 13:CM:57:ARG:HH21  | 51:D4:34:GLU:HG3   | 1.03                     | 1.17              |
| 39:DS:106:ARG:CA   | 39:DS:110:LEU:HD11 | 1.73                     | 1.17              |
| 13:AM:65:LYS:HA    | 13:AM:66:LEU:HB2   | 1.25                     | 1.17              |
| 20:CT:49:ALA:HB1   | 20:CT:100:ILE:CD1  | 1.73                     | 1.17              |
| 25:BA:2171:A:H4'   | 25:BA:2172:U:OP1   | 1.45                     | 1.17              |
| 11:CK:21:ILE:HG23  | 11:CK:30:VAL:HG12  | 1.24                     | 1.17              |
| 20:CT:49:ALA:CB    | 20:CT:100:ILE:HD11 | 1.74                     | 1.16              |
| 20:CT:49:ALA:HB1   | 20:CT:100:ILE:HD11 | 1.17                     | 1.16              |
| 12:AL:47:LYS:HB2   | 12:AL:48:PRO:HD3   | 1.26                     | 1.16              |
| 1:AA:60:A:H4'      | 1:AA:61:G:O5'      | 1.41                     | 1.16              |
| 5:CE:78:HIS:CD2    | 8:CH:104:ARG:CG    | 2.26                     | 1.16              |
| 5:AE:121:LYS:HG3   | 5:AE:122:GLU:N     | 1.47                     | 1.15              |
| 40:DT:38:ASN:O     | 40:DT:39:ARG:HG2   | 1.46                     | 1.15              |
| 4:CD:108:LEU:HG    | 4:CD:110:PHE:HE1   | 1.00                     | 1.15              |
| 33:BI:72:LEU:HD11  | 33:BI:138:ILE:HB   | 1.21                     | 1.15              |
| 1:AA:250:A:H4'     | 1:AA:251:G:O5'     | 1.45                     | 1.15              |
| 28:BD:80:ALA:HB2   | 28:BD:96:HIS:NE2   | 1.62                     | 1.15              |
| 20:CT:50:GLU:OE2   | 20:CT:50:GLU:HA    | 1.46                     | 1.15              |
| 40:BT:29:ARG:HA    | 40:BT:29:ARG:NE    | 1.55                     | 1.15              |
| 3:AC:79:ARG:HH12   | 11:CK:100:ALA:HB2  | 1.12                     | 1.14              |
| 35:DO:104:ARG:NH1  | 40:DT:35:LYS:HE2   | 1.63                     | 1.14              |
| 4:AD:11:LEU:N      | 4:AD:11:LEU:HD23   | 1.60                     | 1.14              |
| 4:CD:108:LEU:CB    | 4:CD:110:PHE:HD1   | 1.58                     | 1.14              |
| 20:CT:43:LEU:CD1   | 20:CT:51:GLU:CG    | 2.25                     | 1.14              |
| 25:DA:1453:U:H4'   | 25:DA:1455:G:OP1   | 1.39                     | 1.14              |
| 38:BR:4:LEU:HD13   | 38:BR:4:LEU:O      | 1.41                     | 1.14              |
| 13:CM:124:PRO:HB2  | 13:CM:125:ARG:HB2  | 1.22                     | 1.14              |
| 24:AX:21:C:H2'     | 24:AX:22:A:H8      | 1.10                     | 1.14              |
| 29:BE:39:PRO:O     | 29:BE:43:GLY:HA2   | 1.44                     | 1.14              |
| 32:BH:107:VAL:HG23 | 32:BH:109:PHE:CZ   | 1.83                     | 1.13              |
| 28:BD:31:LYS:HG3   | 28:BD:33:LEU:HD13  | 1.28                     | 1.13              |
| 30:BF:64:ILE:CG2   | 30:BF:65:TRP:CD1   | 2.30                     | 1.13              |
| 43:BW:4:LYS:HE3    | 43:BW:6:ILE:HD11   | 1.30                     | 1.13              |
| 1:CA:748:C:C1'     | 1:CA:749:C:C5      | 2.30                     | 1.13              |
| 40:DT:36:GLU:HB3   | 40:DT:38:ASN:ND2   | 1.63                     | 1.13              |
| 41:DU:92:ARG:NH1   | 42:DV:11:GLN:HB2   | 1.64                     | 1.13              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:AA:1226:C:H4'    | 1:AA:1227:A:OP1   | 1.39                     | 1.13              |
| 23:AW:34:G:C5      | 24:AX:14:A:C2     | 2.37                     | 1.12              |
| 15:AO:24:SER:O     | 15:AO:28:GLN:HG3  | 1.46                     | 1.12              |
| 36:DP:75:ILE:HD13  | 36:DP:75:ILE:H    | 1.06                     | 1.12              |
| 39:DS:106:ARG:HB2  | 39:DS:106:ARG:NH1 | 1.62                     | 1.12              |
| 1:AA:983:A:H2      | 1:AA:984:C:C5     | 1.67                     | 1.12              |
| 1:AA:1285:A:H1'    | 1:AA:1286:A:OP2   | 1.50                     | 1.12              |
| 29:BE:36:ARG:NH2   | 29:BE:88:GLY:HA3  | 1.63                     | 1.12              |
| 20:CT:56:MET:HG3   | 20:CT:84:LEU:CD1  | 1.79                     | 1.12              |
| 1:AA:992:U:H4'     | 1:AA:993:G:O5'    | 1.47                     | 1.12              |
| 51:B4:40:ILE:HG13  | 51:B4:57:ILE:HG21 | 1.32                     | 1.12              |
| 13:CM:125:ARG:HD3  | 13:CM:126:LYS:H   | 0.99                     | 1.12              |
| 25:DA:84:A:H5'     | 45:DY:8:LYS:HG2   | 1.31                     | 1.12              |
| 41:DU:92:ARG:HD2   | 42:DV:11:GLN:NE2  | 1.65                     | 1.12              |
| 5:CE:102:ALA:C     | 5:CE:106:PRO:HG3  | 1.75                     | 1.11              |
| 20:CT:52:ALA:O     | 20:CT:56:MET:HB2  | 1.48                     | 1.11              |
| 25:DA:1653:G:H4'   | 25:DA:1654:A:OP1  | 1.45                     | 1.11              |
| 2:AB:61:LEU:HD21   | 2:AB:68:ILE:HD11  | 1.19                     | 1.11              |
| 43:BW:4:LYS:HE3    | 43:BW:6:ILE:CD1   | 1.79                     | 1.11              |
| 25:DA:768:G:H2'    | 25:DA:769:G:H8    | 1.04                     | 1.11              |
| 1:AA:1201:A:H4'    | 1:AA:1202:G:O5'   | 1.46                     | 1.11              |
| 25:BA:614(C):A:H4' | 25:BA:615:G:OP1   | 1.42                     | 1.11              |
| 25:BA:1966:A:H1'   | 25:BA:2593:U:H5'  | 1.28                     | 1.11              |
| 12:AL:28:LYS:HG2   | 12:AL:28:LYS:O    | 1.47                     | 1.11              |
| 25:BA:2317:C:H2'   | 25:BA:2318:G:H5'  | 1.31                     | 1.11              |
| 34:BN:42:TRP:CZ3   | 34:BN:48:MET:HE1  | 1.85                     | 1.11              |
| 36:BP:75:ILE:H     | 36:BP:75:ILE:HD13 | 1.06                     | 1.10              |
| 22:CV:41:C:O2'     | 22:CV:42:C:H5'    | 1.51                     | 1.10              |
| 41:DU:92:ARG:CZ    | 42:DV:11:GLN:HB2  | 1.81                     | 1.10              |
| 48:D1:86:SER:HB2   | 48:D1:89:GLU:HB2  | 1.32                     | 1.10              |
| 25:BA:241:A:H4'    | 25:BA:242:G:OP1   | 1.51                     | 1.10              |
| 25:BA:2457:U:H2'   | 25:BA:2458:G:H5'  | 1.34                     | 1.10              |
| 40:DT:129:ARG:NE   | 40:DT:131:ALA:HB3 | 1.67                     | 1.10              |
| 1:AA:968:A:H4'     | 1:AA:969:A:OP2    | 1.42                     | 1.10              |
| 25:BA:1385:G:H4'   | 25:BA:1386:C:OP1  | 1.46                     | 1.10              |
| 1:CA:1226:C:H4'    | 1:CA:1227:A:OP1   | 1.39                     | 1.10              |
| 12:CL:47:LYS:HB3   | 12:CL:48:PRO:CD   | 1.82                     | 1.10              |
| 25:DA:1799:G:H4'   | 25:DA:1800:C:O5'  | 1.47                     | 1.10              |
| 53:D6:41:PRO:HD2   | 53:D6:46:HIS:H    | 1.07                     | 1.10              |
| 1:AA:738:C:H5''    | 6:AF:69:GLU:HB2   | 1.33                     | 1.10              |
| 9:AI:58:HIS:C      | 9:AI:59:PHE:CD1   | 2.30                     | 1.10              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:AW:33:U:H2'     | 23:AW:35:A:OP2     | 1.52                     | 1.10              |
| 31:BG:72:ARG:HH11  | 31:BG:86:MET:HB3   | 1.02                     | 1.10              |
| 36:BP:63:PRO:HB3   | 55:B8:13:ARG:HB3   | 1.23                     | 1.10              |
| 39:BS:35:ILE:HD11  | 39:BS:69:VAL:HG11  | 1.31                     | 1.10              |
| 12:CL:46:LYS:HG2   | 12:CL:47:LYS:H     | 1.00                     | 1.10              |
| 22:CV:29:C:H2'     | 22:CV:30:G:H5'     | 1.20                     | 1.10              |
| 25:DA:1963:U:H4'   | 25:DA:1964:G:OP1   | 1.51                     | 1.10              |
| 40:BT:28:VAL:HG13  | 40:BT:46:GLU:CA    | 1.81                     | 1.09              |
| 1:CA:251:G:O2'     | 1:CA:252:U:H5''    | 1.47                     | 1.09              |
| 5:CE:100:VAL:HB    | 5:CE:118:ILE:HG22  | 1.12                     | 1.09              |
| 36:DP:65:ARG:HH12  | 55:D8:15:LYS:HB2   | 1.15                     | 1.09              |
| 40:DT:125:ARG:O    | 40:DT:128:GLU:HG3  | 1.52                     | 1.09              |
| 19:AS:6:LYS:HG2    | 19:AS:7:LYS:HD3    | 1.32                     | 1.09              |
| 25:BA:448:U:H1'    | 30:BF:84:VAL:CG1   | 1.82                     | 1.09              |
| 38:BR:100:LEU:HB2  | 38:BR:111:LEU:O    | 1.52                     | 1.09              |
| 40:BT:25:GLY:O     | 40:BT:48:ILE:HG23  | 1.53                     | 1.09              |
| 46:BZ:5:LEU:HD21   | 46:BZ:43:GLU:HB3   | 1.18                     | 1.09              |
| 55:B8:32:LEU:H     | 55:B8:32:LEU:HD12  | 1.06                     | 1.09              |
| 34:DN:4:TYR:HB2    | 41:DU:64:ARG:HH22  | 1.16                     | 1.09              |
| 36:DP:59:LEU:HA    | 36:DP:61:ARG:NH1   | 1.67                     | 1.09              |
| 40:DT:33:LYS:HE3   | 40:DT:43:GLN:NE2   | 1.66                     | 1.09              |
| 25:BA:1342:A:N6    | 25:BA:1397:U:C5    | 2.20                     | 1.09              |
| 40:BT:83:ILE:HG13  | 40:BT:84:GLN:H     | 1.08                     | 1.09              |
| 25:DA:1645:G:H5''  | 25:DA:1646:C:H5'   | 1.30                     | 1.09              |
| 33:DI:131:LYS:HB3  | 33:DI:132:PRO:HA   | 1.25                     | 1.09              |
| 35:DO:104:ARG:HH12 | 40:DT:35:LYS:CE    | 1.63                     | 1.09              |
| 40:DT:32:TYR:HB3   | 40:DT:81:PRO:HB2   | 1.19                     | 1.09              |
| 25:BA:1549:C:H2'   | 25:BA:1550:C:C6    | 1.87                     | 1.09              |
| 51:D4:9:LEU:HA     | 51:D4:26:SER:O     | 1.50                     | 1.09              |
| 1:CA:1305:G:H22    | 1:CA:1331:G:H2'    | 1.09                     | 1.09              |
| 39:DS:106:ARG:HB2  | 39:DS:106:ARG:HH11 | 1.10                     | 1.09              |
| 9:CI:15:ALA:HB2    | 9:CI:65:VAL:HG23   | 1.33                     | 1.08              |
| 9:CI:55:ALA:HB1    | 9:CI:58:HIS:HB2    | 1.34                     | 1.08              |
| 32:DH:89:ILE:HD11  | 32:DH:129:THR:HB   | 1.27                     | 1.08              |
| 19:AS:12:ASP:HB3   | 19:AS:14:HIS:CE1   | 1.89                     | 1.08              |
| 25:BA:434:U:H4'    | 25:BA:435:C:OP1    | 1.43                     | 1.08              |
| 30:BF:51:THR:HG21  | 30:BF:92:PRO:HD2   | 1.33                     | 1.08              |
| 1:CA:1054:C:N4     | 23:CY:34:G:H1'     | 1.67                     | 1.08              |
| 25:DA:995:C:C6     | 41:DU:57:PHE:CE1   | 2.42                     | 1.08              |
| 39:DS:59:LYS:HG2   | 39:DS:60:GLY:H     | 1.18                     | 1.08              |
| 2:CB:21:ARG:HB3    | 2:CB:39:ILE:HA     | 1.32                     | 1.08              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:DA:2701:C:H3'  | 25:DA:2702:U:H5''  | 1.30                     | 1.08              |
| 38:DR:55:ALA:HA   | 38:DR:80:PHE:HE1   | 1.16                     | 1.08              |
| 38:BR:13:HIS:HE1  | 38:BR:16:HIS:HB2   | 1.18                     | 1.08              |
| 45:BY:75:ILE:HG13 | 45:BY:79:CYS:HA    | 1.30                     | 1.08              |
| 20:CT:53:LEU:HD23 | 20:CT:100:ILE:HG21 | 1.14                     | 1.08              |
| 25:DA:221:A:H4'   | 25:DA:222:A:O5'    | 1.47                     | 1.08              |
| 33:DI:115:ALA:HB3 | 33:DI:128:LEU:HD11 | 1.12                     | 1.08              |
| 2:AB:97:TRP:HZ2   | 2:AB:102:LEU:HD13  | 1.19                     | 1.07              |
| 4:AD:11:LEU:HD23  | 4:AD:11:LEU:H      | 0.96                     | 1.07              |
| 25:BA:448:U:O2'   | 30:BF:84:VAL:HG13  | 1.54                     | 1.07              |
| 34:BN:62:VAL:HG22 | 34:BN:66:LYS:HD3   | 1.34                     | 1.07              |
| 40:BT:60:THR:HG22 | 40:BT:77:PRO:HA    | 1.35                     | 1.07              |
| 13:CM:124:PRO:CB  | 13:CM:125:ARG:HG2  | 1.82                     | 1.07              |
| 13:CM:125:ARG:HD3 | 13:CM:126:LYS:N    | 1.68                     | 1.07              |
| 25:BA:2320:A:N7   | 25:BA:2333:A:C6    | 2.23                     | 1.07              |
| 33:BI:77:LEU:HD22 | 33:BI:101:LEU:HD13 | 1.35                     | 1.07              |
| 55:B8:33:ASN:O    | 55:B8:34:TRP:HB3   | 1.28                     | 1.07              |
| 25:DA:768:G:H2'   | 25:DA:769:G:C8     | 1.90                     | 1.07              |
| 40:DT:23:ARG:HG2  | 40:DT:120:ARG:NH1  | 1.69                     | 1.07              |
| 25:BA:1966:A:H4'  | 25:BA:1967:C:OP1   | 1.52                     | 1.07              |
| 43:BW:51:LEU:C    | 43:BW:51:LEU:HD13  | 1.79                     | 1.07              |
| 1:CA:819:A:H5'    | 1:CA:820:U:OP2     | 1.50                     | 1.07              |
| 25:DA:84:A:OP2    | 45:DY:8:LYS:HD3    | 1.52                     | 1.07              |
| 22:AV:18:U:H4'    | 22:AV:19:G:OP2     | 1.52                     | 1.07              |
| 25:BA:448:U:H1'   | 30:BF:84:VAL:HG11  | 1.12                     | 1.07              |
| 40:BT:34:VAL:HG22 | 40:BT:39:ARG:HB3   | 1.34                     | 1.07              |
| 42:DV:58:VAL:HB   | 42:DV:98:GLU:HB2   | 1.28                     | 1.07              |
| 39:BS:24:LEU:HB3  | 39:BS:85:VAL:HG12  | 1.37                     | 1.07              |
| 29:DE:77:ILE:HG22 | 29:DE:78:LEU:H     | 1.17                     | 1.07              |
| 31:DG:56:ALA:HB2  | 31:DG:153:ARG:HE   | 1.16                     | 1.07              |
| 25:BA:559:G:H22   | 41:BU:49:HIS:CE1   | 1.72                     | 1.06              |
| 20:CT:43:LEU:HD13 | 20:CT:51:GLU:CG    | 1.84                     | 1.06              |
| 30:DF:32:LEU:HD11 | 30:DF:105:VAL:HG13 | 1.35                     | 1.06              |
| 31:DG:67:LYS:HG2  | 51:D4:5:ILE:HG22   | 1.32                     | 1.06              |
| 10:AJ:38:ILE:HD11 | 10:AJ:71:LEU:HD23  | 1.33                     | 1.06              |
| 25:BA:995:C:N4    | 34:BN:1:MET:HG3    | 1.68                     | 1.06              |
| 25:BA:1300:U:H4'  | 25:BA:1301:A:O5'   | 1.53                     | 1.06              |
| 41:BU:108:GLU:OE2 | 42:BV:44:LYS:HD3   | 1.55                     | 1.06              |
| 45:BY:55:TYR:HB2  | 45:BY:56:PRO:HD2   | 1.17                     | 1.06              |
| 9:CI:13:ALA:HB2   | 9:CI:68:GLY:HA3    | 1.37                     | 1.06              |
| 27:DC:58:VAL:HG21 | 27:DC:166:ASP:H    | 1.12                     | 1.06              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 20:AT:37:SER:HB3   | 20:AT:84:LEU:HD22 | 1.09                     | 1.06              |
| 25:BA:1453:U:H4'   | 25:BA:1455:G:P    | 1.96                     | 1.06              |
| 1:CA:820:U:H4'     | 1:CA:821:G:OP2    | 1.53                     | 1.06              |
| 25:BA:2198:A:H4'   | 25:BA:2199:A:OP1  | 1.56                     | 1.06              |
| 9:CI:19:LEU:HD22   | 9:CI:59:PHE:CB    | 1.84                     | 1.06              |
| 1:AA:1300:G:O2'    | 1:AA:1301:U:H5''  | 1.55                     | 1.05              |
| 40:BT:28:VAL:CG1   | 40:BT:46:GLU:CA   | 2.32                     | 1.05              |
| 52:D5:57:VAL:C     | 52:D5:58:LEU:HD23 | 1.79                     | 1.05              |
| 7:AG:15:ASP:O      | 7:AG:19:GLY:HA2   | 1.55                     | 1.05              |
| 20:AT:26:ASN:HB3   | 20:AT:71:THR:OG1  | 1.57                     | 1.05              |
| 24:CX:16:A:H2'     | 24:CX:17:U:H6     | 1.19                     | 1.05              |
| 25:BA:1453:U:H4'   | 25:BA:1455:G:OP1  | 1.53                     | 1.05              |
| 41:BU:34:LYS:HA    | 41:BU:34:LYS:CE   | 1.79                     | 1.05              |
| 13:CM:57:ARG:NH2   | 51:D4:34:GLU:HG3  | 1.70                     | 1.05              |
| 25:DA:913:U:H4'    | 25:DA:914:C:OP1   | 1.49                     | 1.05              |
| 30:DF:95:ARG:NE    | 30:DF:97:TYR:CE1  | 2.24                     | 1.05              |
| 41:DU:108:GLU:HG3  | 42:DV:44:LYS:HE3  | 1.10                     | 1.05              |
| 45:DY:95:LYS:HB3   | 45:DY:100:ALA:HA  | 1.34                     | 1.05              |
| 40:BT:28:VAL:HG21  | 40:BT:46:GLU:HG3  | 1.12                     | 1.05              |
| 42:BV:77:ALA:O     | 42:BV:79:VAL:HG12 | 1.55                     | 1.05              |
| 1:CA:913:A:H4'     | 1:CA:914:A:O5'    | 1.53                     | 1.05              |
| 52:D5:57:VAL:O     | 52:D5:58:LEU:HD23 | 1.55                     | 1.05              |
| 1:AA:1049:U:C1'    | 1:AA:1201:A:N7    | 2.20                     | 1.05              |
| 25:BA:1342:A:C6    | 25:BA:1397:U:C5   | 2.43                     | 1.05              |
| 22:CV:17:C:H3'     | 22:CV:18:U:H5'    | 1.39                     | 1.05              |
| 4:AD:49:ARG:HD3    | 4:AD:50:ARG:H     | 1.20                     | 1.04              |
| 5:AE:76:ILE:HD11   | 5:AE:142:LEU:HD11 | 1.37                     | 1.04              |
| 19:AS:9:VAL:CG1    | 19:AS:11:VAL:CG1  | 2.30                     | 1.04              |
| 42:BV:72:VAL:HG23  | 42:BV:85:LYS:HB3  | 1.37                     | 1.04              |
| 32:DH:153:LYS:HB3  | 32:DH:154:PRO:HD2 | 1.05                     | 1.04              |
| 1:AA:1049:U:C1'    | 1:AA:1201:A:C8    | 2.40                     | 1.04              |
| 5:AE:50:GLU:HB3    | 5:AE:53:LEU:HD13  | 1.38                     | 1.04              |
| 27:BC:58:VAL:HG21  | 27:BC:166:ASP:H   | 1.14                     | 1.04              |
| 30:BF:154:VAL:HG22 | 30:BF:191:ARG:HB2 | 1.38                     | 1.04              |
| 32:BH:107:VAL:CG2  | 32:BH:109:PHE:CZ  | 2.40                     | 1.04              |
| 25:BA:2126:A:H4'   | 25:BA:2127:G:O5'  | 1.54                     | 1.04              |
| 13:CM:124:PRO:CB   | 13:CM:125:ARG:CB  | 2.36                     | 1.04              |
| 28:DD:10:THR:HG23  | 28:DD:13:ARG:HB3  | 1.40                     | 1.04              |
| 53:D6:41:PRO:HD2   | 53:D6:46:HIS:N    | 1.73                     | 1.04              |
| 1:AA:913:A:H4'     | 1:AA:914:A:O5'    | 1.58                     | 1.04              |
| 1:CA:1065:U:H4'    | 1:CA:1066:C:H5''  | 1.08                     | 1.04              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 13:CM:124:PRO:HB3  | 13:CM:125:ARG:HG2  | 1.04                     | 1.04              |
| 1:AA:686:U:H1'     | 11:AK:42:TRP:HE1   | 1.22                     | 1.04              |
| 20:AT:53:LEU:HD12  | 20:AT:102:GLY:HA3  | 1.40                     | 1.04              |
| 52:B5:16:ARG:HH11  | 52:B5:16:ARG:HG2   | 1.21                     | 1.04              |
| 1:CA:1064:G:H4'    | 1:CA:1065:U:H5''   | 1.05                     | 1.04              |
| 1:CA:1285:A:H4'    | 1:CA:1286:A:O5'    | 1.54                     | 1.04              |
| 20:CT:43:LEU:HD13  | 20:CT:51:GLU:CB    | 1.86                     | 1.04              |
| 22:CV:43:G:H2'     | 22:CV:44:A:H5'     | 1.35                     | 1.04              |
| 42:DV:11:GLN:NE2   | 42:DV:39:LEU:HD23  | 1.72                     | 1.04              |
| 25:DA:1558:A:H4'   | 25:DA:1559:G:O5'   | 1.58                     | 1.03              |
| 40:DT:129:ARG:CZ   | 40:DT:131:ALA:HB3  | 1.87                     | 1.03              |
| 44:DX:63:LYS:HE3   | 44:DX:72:LYS:HE3   | 1.40                     | 1.03              |
| 53:D6:40:CYS:SG    | 53:D6:45:LYS:HE3   | 1.97                     | 1.03              |
| 25:BA:1300:U:H4'   | 25:BA:1301:A:C5'   | 1.88                     | 1.03              |
| 25:DA:1693:U:C2'   | 28:DD:14:ARG:HH21  | 1.71                     | 1.03              |
| 29:DE:49:LEU:H     | 29:DE:49:LEU:HD12  | 1.20                     | 1.03              |
| 4:CD:7:PRO:HB2     | 4:CD:10:ARG:HD2    | 1.41                     | 1.03              |
| 38:BR:13:HIS:O     | 38:BR:14:SER:HB3   | 1.59                     | 1.03              |
| 39:BS:12:PHE:HE1   | 39:BS:14:VAL:CG2   | 1.71                     | 1.03              |
| 10:CJ:38:ILE:HD11  | 10:CJ:71:LEU:HD23  | 1.40                     | 1.03              |
| 12:CL:11:VAL:CG1   | 17:CQ:29:HIS:HD2   | 1.70                     | 1.03              |
| 28:DD:49:ILE:HD11  | 28:DD:52:ARG:HA    | 1.40                     | 1.03              |
| 29:BE:134:ILE:HD13 | 29:BE:134:ILE:H    | 1.24                     | 1.03              |
| 4:CD:108:LEU:CB    | 4:CD:110:PHE:CD1   | 2.34                     | 1.03              |
| 40:DT:25:GLY:HA3   | 40:DT:120:ARG:HH22 | 1.20                     | 1.03              |
| 46:DZ:11:GLU:CD    | 46:DZ:11:GLU:H     | 1.60                     | 1.03              |
| 25:BA:2449:U:H4'   | 25:BA:2450:A:OP1   | 1.59                     | 1.02              |
| 55:B8:50:LEU:HD12  | 55:B8:51:ALA:H     | 1.22                     | 1.02              |
| 1:CA:428:G:H4'     | 1:CA:429:U:O5'     | 1.57                     | 1.02              |
| 41:DU:92:ARG:NH2   | 41:DU:94:ASN:HD22  | 1.55                     | 1.02              |
| 7:AG:10:ARG:HH11   | 7:AG:10:ARG:HG3    | 1.21                     | 1.02              |
| 25:BA:559:G:N2     | 41:BU:49:HIS:CE1   | 2.27                     | 1.02              |
| 41:BU:34:LYS:HA    | 41:BU:34:LYS:HE2   | 1.07                     | 1.02              |
| 42:BV:18:LEU:HD13  | 42:BV:19:LYS:H     | 1.23                     | 1.02              |
| 1:CA:250:A:H4'     | 1:CA:251:G:O5'     | 1.56                     | 1.02              |
| 1:CA:484:G:H4'     | 1:CA:485:G:O5'     | 1.59                     | 1.02              |
| 25:DA:660:G:H21    | 36:DP:12:ALA:HA    | 1.18                     | 1.02              |
| 41:DU:104:GLN:HE22 | 41:DU:105:VAL:HG23 | 1.21                     | 1.02              |
| 10:AJ:40:LEU:HB2   | 10:AJ:41:PRO:HD2   | 1.39                     | 1.02              |
| 30:BF:51:THR:HG21  | 30:BF:92:PRO:CD    | 1.90                     | 1.02              |
| 31:BG:45:GLU:H     | 31:BG:88:ILE:HD13  | 1.21                     | 1.02              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 28:DD:31:LYS:HG3   | 28:DD:33:LEU:HD13  | 1.38                     | 1.02              |
| 33:DI:77:LEU:HD11  | 33:DI:140:LEU:HB2  | 1.37                     | 1.02              |
| 39:DS:107:GLU:H    | 39:DS:110:LEU:CD1  | 1.70                     | 1.02              |
| 10:AJ:50:ILE:HG12  | 14:AN:41:ARG:HD3   | 1.41                     | 1.02              |
| 14:AN:13:THR:N     | 14:AN:14:PRO:HD2   | 1.71                     | 1.02              |
| 28:BD:44:ASN:HB3   | 28:BD:49:ILE:HA    | 1.40                     | 1.02              |
| 34:BN:62:VAL:HG22  | 34:BN:66:LYS:HD2   | 1.35                     | 1.02              |
| 9:CI:19:LEU:HD22   | 9:CI:59:PHE:HB3    | 1.39                     | 1.02              |
| 19:CS:63:THR:HG22  | 19:CS:66:MET:CE    | 1.90                     | 1.02              |
| 34:DN:56:ASN:HA    | 34:DN:125:GLY:H    | 1.19                     | 1.02              |
| 42:DV:35:LEU:HD21  | 42:DV:57:VAL:HG22  | 1.39                     | 1.02              |
| 25:BA:1645:G:H5''  | 25:BA:1646:C:H5'   | 1.05                     | 1.01              |
| 29:BE:33:VAL:HG13  | 29:BE:69:LYS:HE3   | 1.38                     | 1.01              |
| 40:BT:24:PRO:O     | 40:BT:49:VAL:HB    | 1.59                     | 1.01              |
| 1:CA:748:C:H1'     | 1:CA:749:C:H5      | 1.20                     | 1.01              |
| 1:CA:1502:A:H2     | 1:CA:1505:G:N2     | 1.57                     | 1.01              |
| 19:CS:63:THR:CG2   | 19:CS:66:MET:HG2   | 1.91                     | 1.01              |
| 25:DA:2835:A:H4'   | 25:DA:2836:U:OP1   | 1.56                     | 1.01              |
| 32:DH:4:ILE:HG13   | 32:DH:6:ARG:NE     | 1.75                     | 1.01              |
| 42:DV:35:LEU:HB2   | 42:DV:37:VAL:HG22  | 1.37                     | 1.01              |
| 30:BF:123:LEU:HD12 | 30:BF:124:LEU:H    | 1.23                     | 1.01              |
| 20:AT:49:ALA:HB1   | 20:AT:100:ILE:HD11 | 1.42                     | 1.01              |
| 20:AT:84:LEU:O     | 20:AT:84:LEU:HD12  | 1.59                     | 1.01              |
| 30:BF:9:ILE:HA     | 30:BF:13:SER:O     | 1.60                     | 1.01              |
| 36:BP:19:VAL:HG22  | 36:BP:20:GLY:H     | 1.23                     | 1.01              |
| 5:CE:102:ALA:HB1   | 5:CE:106:PRO:HB2   | 1.01                     | 1.01              |
| 25:DA:2171:A:H4'   | 25:DA:2172:U:OP1   | 1.60                     | 1.01              |
| 36:DP:57:THR:O     | 36:DP:60:MET:HG2   | 1.59                     | 1.01              |
| 10:AJ:49:VAL:HG23  | 14:AN:41:ARG:HB2   | 1.41                     | 1.01              |
| 36:BP:64:LYS:HB3   | 55:B8:25:MET:HG3   | 1.38                     | 1.01              |
| 22:CV:18:U:H4'     | 22:CV:19:G:OP2     | 1.60                     | 1.01              |
| 39:DS:107:GLU:N    | 39:DS:110:LEU:HD11 | 1.74                     | 1.01              |
| 38:BR:13:HIS:CE1   | 38:BR:16:HIS:HB2   | 1.95                     | 1.01              |
| 45:BY:55:TYR:CB    | 45:BY:56:PRO:HD2   | 1.89                     | 1.01              |
| 1:CA:128:G:H2'     | 1:CA:129:U:H5'     | 1.42                     | 1.01              |
| 13:CM:88:ARG:HH11  | 13:CM:88:ARG:HB3   | 1.19                     | 1.01              |
| 30:DF:107:LYS:HD2  | 30:DF:206:ILE:HD13 | 1.43                     | 1.01              |
| 39:DS:106:ARG:HA   | 39:DS:110:LEU:HD11 | 1.02                     | 1.01              |
| 43:DW:5:ALA:HB2    | 43:DW:54:ALA:HB2   | 1.37                     | 1.01              |
| 7:AG:14:PRO:HG3    | 7:AG:21:VAL:HG13   | 1.01                     | 1.00              |
| 12:AL:6:THR:HG23   | 12:AL:9:GLN:HG3    | 1.42                     | 1.00              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 40:BT:83:ILE:HG13 | 40:BT:84:GLN:HG3   | 1.44                     | 1.00              |
| 1:CA:1348:U:H4'   | 9:CI:120:ARG:HD2   | 1.43                     | 1.00              |
| 1:CA:1502:A:C2    | 1:CA:1505:G:N2     | 2.27                     | 1.00              |
| 9:CI:58:HIS:HB3   | 9:CI:59:PHE:CE1    | 1.96                     | 1.00              |
| 9:CI:78:LYS:HE3   | 9:CI:101:PHE:HE2   | 1.24                     | 1.00              |
| 1:AA:243:A:H4'    | 1:AA:244:U:O5'     | 1.57                     | 1.00              |
| 25:BA:1645:G:H5'' | 25:BA:1646:C:C5'   | 1.92                     | 1.00              |
| 31:BG:44:GLY:HA2  | 31:BG:88:ILE:HG21  | 1.43                     | 1.00              |
| 13:AM:3:ARG:CZ    | 31:BG:113:ARG:HH21 | 1.74                     | 1.00              |
| 29:BE:36:ARG:HH22 | 29:BE:88:GLY:CA    | 1.75                     | 1.00              |
| 32:BH:144:VAL:HA  | 32:BH:147:ASN:HB2  | 1.43                     | 1.00              |
| 40:BT:30:VAL:HG11 | 40:BT:83:ILE:CG1   | 1.90                     | 1.00              |
| 40:BT:30:VAL:CG1  | 40:BT:83:ILE:HG12  | 1.92                     | 1.00              |
| 8:CH:91:ARG:HH11  | 8:CH:91:ARG:HG2    | 1.21                     | 1.00              |
| 19:CS:63:THR:HG22 | 19:CS:66:MET:CG    | 1.90                     | 1.00              |
| 25:DA:1204:A:H1'  | 25:DA:1206:G:N7    | 1.76                     | 1.00              |
| 25:DA:2681:C:H5   | 25:DA:2725:A:N6    | 1.58                     | 1.00              |
| 29:DE:59:VAL:HG22 | 29:DE:60:ASN:H     | 1.26                     | 1.00              |
| 53:D6:47:THR:HB   | 53:D6:49:HIS:CE1   | 1.96                     | 1.00              |
| 25:BA:1504:C:O2'  | 25:BA:1505:C:H5'   | 1.59                     | 1.00              |
| 31:BG:72:ARG:HD3  | 31:BG:86:MET:HB3   | 1.44                     | 1.00              |
| 9:CI:96:LEU:HD11  | 9:CI:102:LEU:HD23  | 1.43                     | 1.00              |
| 31:BG:41:GLN:HB3  | 31:BG:43:LEU:HD11  | 1.43                     | 1.00              |
| 45:BY:8:LYS:HD2   | 45:BY:8:LYS:H      | 1.23                     | 1.00              |
| 19:CS:63:THR:CG2  | 19:CS:66:MET:CG    | 2.40                     | 1.00              |
| 1:CA:344:A:H5''   | 1:CA:345:C:OP2     | 1.61                     | 1.00              |
| 41:DU:104:GLN:NE2 | 41:DU:105:VAL:H    | 1.59                     | 1.00              |
| 31:DG:67:LYS:HE2  | 51:D4:6:HIS:CE1    | 1.97                     | 0.99              |
| 45:DY:63:LYS:HZ2  | 45:DY:64:GLU:H     | 1.04                     | 0.99              |
| 25:DA:1697:G:H3'  | 25:DA:1698:A:C5'   | 1.91                     | 0.99              |
| 25:DA:644:A:H4'   | 25:DA:645:C:C5     | 1.96                     | 0.99              |
| 35:BO:85:VAL:HG11 | 35:BO:114:ILE:HD12 | 1.42                     | 0.99              |
| 25:DA:1693:U:C2'  | 28:DD:14:ARG:NH2   | 2.24                     | 0.99              |
| 46:BZ:93:ASP:HA   | 46:BZ:130:PRO:HG2  | 1.42                     | 0.99              |
| 25:BA:995:C:O2'   | 41:BU:61:TRP:CZ2   | 2.16                     | 0.99              |
| 25:BA:1666:G:C2'  | 25:BA:1667:G:H5'   | 1.93                     | 0.99              |
| 31:BG:43:LEU:N    | 31:BG:43:LEU:HD13  | 1.77                     | 0.99              |
| 45:BY:40:GLU:HA   | 45:BY:40:GLU:OE2   | 1.61                     | 0.99              |
| 25:DA:2681:C:H5   | 25:DA:2725:A:H62   | 1.00                     | 0.99              |
| 33:BI:77:LEU:CD2  | 33:BI:101:LEU:CD1  | 2.41                     | 0.99              |
| 25:BA:1820:U:H4'  | 25:BA:1821:A:OP2   | 1.61                     | 0.99              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 31:BG:72:ARG:HB3  | 31:BG:86:MET:HA    | 1.00                     | 0.99              |
| 40:BT:32:TYR:HB2  | 40:BT:81:PRO:HB2   | 1.45                     | 0.99              |
| 1:CA:968:A:H4'    | 1:CA:969:A:OP2     | 1.56                     | 0.99              |
| 1:CA:992:U:H4'    | 1:CA:993:G:O5'     | 1.60                     | 0.99              |
| 1:AA:983:A:C2     | 1:AA:984:C:C5      | 2.50                     | 0.99              |
| 10:CJ:49:VAL:HG23 | 14:CN:41:ARG:HB2   | 1.40                     | 0.99              |
| 43:DW:9:TYR:H     | 43:DW:102:HIS:CD2  | 1.81                     | 0.99              |
| 25:BA:1645:G:C5'  | 25:BA:1646:C:H5'   | 1.93                     | 0.99              |
| 1:AA:595:G:H4'    | 1:AA:596:C:OP1     | 1.62                     | 0.98              |
| 16:AP:82:GLN:HG2  | 16:AP:83:GLU:H     | 1.27                     | 0.98              |
| 25:BA:1929:G:H4'  | 25:BA:1930:G:OP1   | 1.63                     | 0.98              |
| 1:CA:1054:C:H42   | 23:CY:34:G:H1'     | 1.19                     | 0.98              |
| 32:DH:153:LYS:CB  | 32:DH:154:PRO:HD2  | 1.93                     | 0.98              |
| 40:DT:28:VAL:HG22 | 40:DT:47:GLY:H     | 1.26                     | 0.98              |
| 40:DT:33:LYS:CE   | 40:DT:43:GLN:CD    | 2.37                     | 0.98              |
| 25:BA:1301:A:H5'' | 25:BA:1301:A:N3    | 1.76                     | 0.98              |
| 25:BA:1342:A:C5   | 25:BA:1397:U:C6    | 2.52                     | 0.98              |
| 34:BN:62:VAL:CG2  | 34:BN:66:LYS:CD    | 2.39                     | 0.98              |
| 10:CJ:63:PHE:HB3  | 14:CN:58:LYS:HA    | 1.45                     | 0.98              |
| 25:BA:865:C:H4'   | 25:BA:866:A:OP1    | 1.61                     | 0.98              |
| 28:DD:44:ASN:HB3  | 28:DD:49:ILE:HA    | 1.44                     | 0.98              |
| 25:BA:1653:G:H4'  | 25:BA:1654:A:O5'   | 1.60                     | 0.98              |
| 12:CL:47:LYS:HB3  | 12:CL:48:PRO:HD3   | 0.98                     | 0.98              |
| 1:CA:1064:G:C4'   | 1:CA:1065:U:H5''   | 1.93                     | 0.98              |
| 33:DI:92:VAL:HG13 | 33:DI:120:ILE:HG23 | 1.44                     | 0.98              |
| 25:BA:2320:A:C8   | 25:BA:2333:A:N6    | 2.32                     | 0.98              |
| 1:CA:1064:G:C4'   | 1:CA:1065:U:C5'    | 2.42                     | 0.98              |
| 3:CC:20:SER:HB2   | 3:CC:40:ARG:HH22   | 1.27                     | 0.98              |
| 45:DY:97:ARG:HH21 | 45:DY:98:VAL:HB    | 1.27                     | 0.98              |
| 40:BT:32:TYR:CB   | 40:BT:81:PRO:HB2   | 1.93                     | 0.97              |
| 45:BY:67:LEU:HD12 | 45:BY:71:LYS:HG3   | 1.46                     | 0.97              |
| 53:D6:46:HIS:HD2  | 53:D6:47:THR:N     | 1.61                     | 0.97              |
| 25:BA:995:C:N3    | 34:BN:1:MET:HG2    | 1.79                     | 0.97              |
| 31:BG:85:GLY:C    | 31:BG:87:PRO:HD2   | 1.88                     | 0.97              |
| 48:B1:90:ILE:HG22 | 48:B1:94:LEU:HD12  | 1.43                     | 0.97              |
| 30:DF:103:LYS:HA  | 30:DF:106:ARG:HG3  | 1.45                     | 0.97              |
| 23:AW:34:G:C6     | 24:AX:14:A:N3      | 2.31                     | 0.97              |
| 24:AX:21:C:H2'    | 24:AX:22:A:C8      | 1.98                     | 0.97              |
| 25:BA:1251:C:H5'  | 25:BA:1251:C:H6    | 1.27                     | 0.97              |
| 45:BY:42:VAL:HB   | 45:BY:65:ALA:HB3   | 1.45                     | 0.97              |
| 1:CA:1201:A:H4'   | 1:CA:1202:G:O5'    | 1.61                     | 0.97              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:CJ:78:ASN:ND2   | 10:CJ:80:LYS:HB2   | 1.78                     | 0.97              |
| 11:CK:21:ILE:HG23  | 11:CK:30:VAL:CG1   | 1.93                     | 0.97              |
| 31:BG:39:ILE:HD11  | 31:BG:155:MET:HB2  | 1.46                     | 0.97              |
| 25:DA:1497:U:H3'   | 25:DA:1497:U:O2    | 1.65                     | 0.97              |
| 53:D6:46:HIS:CD2   | 53:D6:46:HIS:C     | 2.41                     | 0.97              |
| 25:BA:483:A:H1'    | 45:BY:60:PHE:HZ    | 1.27                     | 0.97              |
| 41:BU:34:LYS:HE2   | 41:BU:34:LYS:CA    | 1.94                     | 0.97              |
| 45:BY:10:GLY:HA2   | 45:BY:27:VAL:HG13  | 1.47                     | 0.97              |
| 40:DT:88:ILE:HG22  | 40:DT:89:VAL:HG23  | 1.44                     | 0.97              |
| 2:AB:97:TRP:CZ2    | 2:AB:102:LEU:HD13  | 1.99                     | 0.97              |
| 4:CD:109:GLY:HA3   | 4:CD:165:MET:SD    | 2.04                     | 0.97              |
| 28:DD:35:LYS:NZ    | 28:DD:103:ARG:HA   | 1.79                     | 0.97              |
| 40:DT:28:VAL:O     | 40:DT:29:ARG:HB2   | 1.65                     | 0.97              |
| 40:DT:33:LYS:HE2   | 40:DT:43:GLN:HB3   | 1.44                     | 0.97              |
| 34:BN:123:TYR:CE1  | 34:BN:130:HIS:CE1  | 2.52                     | 0.97              |
| 20:CT:53:LEU:HD23  | 20:CT:100:ILE:CG2  | 1.94                     | 0.97              |
| 2:AB:14:GLY:O      | 2:AB:15:VAL:HG13   | 1.65                     | 0.97              |
| 12:CL:47:LYS:CB    | 12:CL:48:PRO:HD3   | 1.94                     | 0.97              |
| 17:CQ:67:LYS:HA    | 17:CQ:70:ARG:HH12  | 1.29                     | 0.97              |
| 19:CS:63:THR:HG22  | 19:CS:66:MET:HE3   | 1.47                     | 0.97              |
| 39:DS:88:ASP:O     | 39:DS:89:ARG:HB3   | 1.61                     | 0.97              |
| 4:AD:189:PRO:HB2   | 4:AD:194:LEU:HD21  | 1.46                     | 0.96              |
| 32:DH:98:LEU:CB    | 32:DH:125:VAL:HG21 | 1.94                     | 0.96              |
| 40:DT:80:SER:HB3   | 40:DT:81:PRO:CD    | 1.94                     | 0.96              |
| 40:DT:89:VAL:HG11  | 40:DT:91:ARG:HE    | 1.25                     | 0.96              |
| 25:DA:598:G:H1'    | 36:DP:12:ALA:HB2   | 1.46                     | 0.96              |
| 25:BA:1666:G:H2'   | 25:BA:1667:G:H5'   | 1.47                     | 0.96              |
| 1:AA:251:G:O2'     | 1:AA:252:U:H5''    | 1.66                     | 0.96              |
| 25:BA:311:A:C8     | 25:BA:332:A:C5     | 2.52                     | 0.96              |
| 25:BA:1966:A:H1'   | 25:BA:2593:U:C5'   | 1.96                     | 0.96              |
| 20:CT:40:ALA:HB2   | 20:CT:55:ILE:CG2   | 1.96                     | 0.96              |
| 25:BA:311:A:H4'    | 25:BA:312:G:OP1    | 1.61                     | 0.96              |
| 25:BA:1549:C:H2'   | 25:BA:1550:C:H6    | 1.21                     | 0.96              |
| 25:BA:2701:C:H3'   | 25:BA:2702:U:H5''  | 1.45                     | 0.96              |
| 25:BA:2848:G:H4'   | 25:BA:2849:U:OP1   | 1.64                     | 0.96              |
| 30:BF:64:ILE:HG23  | 30:BF:65:TRP:NE1   | 1.78                     | 0.96              |
| 45:BY:81:LYS:HD3   | 45:BY:97:ARG:HB3   | 1.46                     | 0.96              |
| 1:CA:1065:U:H1'    | 1:CA:1066:C:OP2    | 1.66                     | 0.96              |
| 3:CC:165:THR:HG22  | 3:CC:165:THR:O     | 1.64                     | 0.96              |
| 33:BI:77:LEU:HD22  | 33:BI:101:LEU:CD1  | 1.95                     | 0.96              |
| 46:BZ:124:ILE:HD11 | 46:BZ:165:VAL:HG21 | 1.47                     | 0.96              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 50:B3:10:LYS:HB3   | 50:B3:53:LEU:HB3   | 1.47                     | 0.96              |
| 28:DD:181:GLU:HA   | 28:DD:272:ALA:HB3  | 1.48                     | 0.96              |
| 28:BD:267:SER:C    | 28:BD:268:ARG:HG3  | 1.87                     | 0.96              |
| 20:CT:53:LEU:CD2   | 20:CT:100:ILE:HG21 | 1.95                     | 0.96              |
| 36:DP:70:GLN:HB3   | 36:DP:72:PRO:HD2   | 1.45                     | 0.96              |
| 39:DS:107:GLU:H    | 39:DS:110:LEU:HD11 | 1.18                     | 0.96              |
| 40:DT:32:TYR:HB3   | 40:DT:81:PRO:HB3   | 1.43                     | 0.96              |
| 1:AA:1158:C:H3'    | 1:AA:1158:C:O2     | 1.64                     | 0.96              |
| 1:AA:1267:C:O2     | 1:AA:1267:C:H2'    | 1.66                     | 0.96              |
| 40:BT:30:VAL:HG11  | 40:BT:83:ILE:HG12  | 0.98                     | 0.96              |
| 25:DA:2311:A:H8    | 31:DG:88:ILE:HG13  | 1.29                     | 0.96              |
| 25:DA:2406:U:O4    | 36:DP:70:GLN:HB2   | 1.66                     | 0.96              |
| 36:BP:70:GLN:C     | 36:BP:72:PRO:HD2   | 1.90                     | 0.96              |
| 2:CB:61:LEU:HD21   | 2:CB:68:ILE:HD11   | 1.48                     | 0.96              |
| 19:CS:31:ILE:HG23  | 19:CS:49:ILE:HA    | 1.43                     | 0.96              |
| 1:AA:983:A:H2      | 1:AA:984:C:C4      | 1.84                     | 0.95              |
| 5:CE:100:VAL:HB    | 5:CE:118:ILE:CG2   | 1.94                     | 0.95              |
| 33:DI:78:THR:HA    | 33:DI:141:LYS:HB2  | 1.46                     | 0.95              |
| 35:DO:104:ARG:HH12 | 40:DT:35:LYS:HE2   | 0.80                     | 0.95              |
| 1:AA:1054:C:H42    | 23:AY:34:G:H1'     | 1.30                     | 0.95              |
| 38:BR:10:LEU:CB    | 38:BR:17:ARG:CD    | 2.36                     | 0.95              |
| 1:CA:748:C:C1'     | 1:CA:749:C:H5      | 1.72                     | 0.95              |
| 22:CV:17:C:H3'     | 22:CV:18:U:C5'     | 1.96                     | 0.95              |
| 22:CV:29:C:O2'     | 22:CV:30:G:H5'     | 1.65                     | 0.95              |
| 41:DU:92:ARG:HH11  | 41:DU:92:ARG:HG2   | 1.31                     | 0.95              |
| 23:AW:34:G:C6      | 24:AX:14:A:C4      | 2.54                     | 0.95              |
| 31:BG:4:ASP:HA     | 31:BG:8:LYS:HD2    | 1.48                     | 0.95              |
| 40:BT:83:ILE:HG13  | 40:BT:84:GLN:N     | 1.66                     | 0.95              |
| 28:DD:80:ALA:HB3   | 28:DD:94:LEU:HD13  | 1.46                     | 0.95              |
| 41:DU:108:GLU:HG3  | 42:DV:44:LYS:CE    | 1.96                     | 0.95              |
| 2:AB:77:ALA:O      | 2:AB:80:ILE:HG23   | 1.65                     | 0.95              |
| 55:B8:33:ASN:O     | 55:B8:34:TRP:CB    | 2.15                     | 0.95              |
| 1:CA:251:G:H4'     | 1:CA:252:U:O5'     | 1.63                     | 0.95              |
| 12:CL:46:LYS:HG2   | 12:CL:47:LYS:N     | 1.82                     | 0.95              |
| 20:CT:43:LEU:CD1   | 20:CT:51:GLU:HG3   | 1.95                     | 0.95              |
| 1:CA:1108:G:H5'    | 3:CC:176:HIS:HD1   | 1.29                     | 0.95              |
| 8:CH:25:ASP:OD2    | 8:CH:60:ARG:HG3    | 1.67                     | 0.95              |
| 13:CM:93:ARG:NH1   | 25:DA:888:C:O4'    | 2.00                     | 0.95              |
| 25:BA:2320:A:N6    | 25:BA:2333:A:C4    | 2.34                     | 0.95              |
| 1:CA:342:C:C2'     | 1:CA:343:U:H5'     | 1.97                     | 0.95              |
| 5:CE:126:ARG:HH11  | 5:CE:126:ARG:HG3   | 1.31                     | 0.95              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 20:CT:43:LEU:CD1   | 20:CT:51:GLU:CB   | 2.43                     | 0.95              |
| 23:CW:68:C:H2'     | 23:CW:69:G:H8     | 1.30                     | 0.95              |
| 7:AG:23:VAL:HG13   | 7:AG:43:PHE:HE2   | 1.32                     | 0.95              |
| 31:BG:86:MET:HG3   | 31:BG:87:PRO:CD   | 1.96                     | 0.95              |
| 1:CA:49:U:C4       | 1:CA:364:A:C5     | 2.55                     | 0.95              |
| 1:CA:1067:A:H4'    | 1:CA:1068:G:O5'   | 1.67                     | 0.95              |
| 22:CV:15:G:H22     | 22:CV:49:C:H41    | 1.10                     | 0.95              |
| 42:DV:52:VAL:HG21  | 42:DV:55:ALA:HB3  | 1.48                     | 0.95              |
| 36:BP:71:VAL:N     | 36:BP:72:PRO:HD2  | 1.80                     | 0.95              |
| 42:BV:82:ARG:HH11  | 42:BV:82:ARG:HG2  | 1.29                     | 0.95              |
| 55:B8:32:LEU:HD12  | 55:B8:32:LEU:N    | 1.82                     | 0.95              |
| 5:CE:105:VAL:N     | 5:CE:106:PRO:HD2  | 1.79                     | 0.95              |
| 33:DI:95:LYS:HA    | 33:DI:111:PRO:HG3 | 1.49                     | 0.94              |
| 25:BA:221:A:C8     | 25:BA:266:G:O6    | 2.21                     | 0.94              |
| 25:BA:2126:A:H1'   | 25:BA:2127:G:O4'  | 1.66                     | 0.94              |
| 31:BG:72:ARG:NH1   | 31:BG:86:MET:HB3  | 1.82                     | 0.94              |
| 39:BS:12:PHE:HE1   | 39:BS:14:VAL:HG22 | 1.32                     | 0.94              |
| 31:BG:144:ILE:HD12 | 31:BG:145:THR:H   | 1.30                     | 0.94              |
| 12:CL:11:VAL:CG1   | 17:CQ:29:HIS:CD2  | 2.47                     | 0.94              |
| 20:CT:81:LYS:O     | 20:CT:85:MET:HG3  | 1.65                     | 0.94              |
| 30:BF:2:LYS:HD3    | 30:BF:2:LYS:H     | 1.27                     | 0.94              |
| 33:BI:118:LYS:HD2  | 33:BI:119:PRO:HD2 | 1.45                     | 0.94              |
| 34:BN:14:VAL:HG13  | 34:BN:137:LYS:HG3 | 1.49                     | 0.94              |
| 25:DA:242:G:H5''   | 55:D8:62:LEU:HD13 | 1.49                     | 0.94              |
| 30:DF:188:ARG:HG2  | 36:DP:3:LEU:HD11  | 1.49                     | 0.94              |
| 36:DP:79:ARG:HG3   | 36:DP:109:GLY:O   | 1.66                     | 0.94              |
| 40:DT:65:LYS:HZ2   | 40:DT:66:VAL:H    | 1.16                     | 0.94              |
| 34:BN:62:VAL:CG2   | 34:BN:66:LYS:HD3  | 1.97                     | 0.94              |
| 43:BW:4:LYS:CE     | 43:BW:6:ILE:HD11  | 1.98                     | 0.94              |
| 1:CA:60:A:H4'      | 1:CA:61:G:O5'     | 1.65                     | 0.94              |
| 51:D4:8:LYS:O      | 51:D4:27:THR:HG22 | 1.67                     | 0.94              |
| 3:AC:113:ALA:HB2   | 3:AC:202:ILE:HG13 | 1.48                     | 0.94              |
| 33:DI:38:LEU:HD12  | 33:DI:38:LEU:H    | 1.30                     | 0.94              |
| 28:BD:80:ALA:CB    | 28:BD:96:HIS:NE2  | 2.30                     | 0.94              |
| 40:BT:34:VAL:HG13  | 40:BT:39:ARG:HG2  | 1.50                     | 0.94              |
| 45:BY:14:LEU:HD12  | 45:BY:15:VAL:H    | 1.32                     | 0.94              |
| 41:DU:62:ILE:HD11  | 41:DU:93:LYS:HG2  | 1.47                     | 0.94              |
| 36:DP:65:ARG:NH1   | 55:D8:15:LYS:HB2  | 1.82                     | 0.94              |
| 36:BP:79:ARG:HG3   | 36:BP:109:GLY:O   | 1.66                     | 0.94              |
| 2:CB:213:LEU:HD23  | 2:CB:214:ILE:HG12 | 1.50                     | 0.94              |
| 43:DW:9:TYR:H      | 43:DW:102:HIS:HD2 | 1.12                     | 0.94              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:AA:1297:C:O2'    | 7:AG:114:ARG:NH2  | 2.00                     | 0.93              |
| 3:AC:43:LEU:HD22   | 3:AC:47:LEU:HD22  | 1.46                     | 0.93              |
| 25:BA:1719:G:O2'   | 25:BA:1720:U:H5'  | 1.68                     | 0.93              |
| 55:B8:31:HIS:ND1   | 55:B8:32:LEU:CA   | 2.30                     | 0.93              |
| 1:CA:49:U:C5       | 1:CA:364:A:C6     | 2.56                     | 0.93              |
| 1:CA:1445:C:H2'    | 1:CA:1446:U:H5'   | 1.51                     | 0.93              |
| 13:CM:124:PRO:CB   | 13:CM:125:ARG:HB2 | 1.94                     | 0.93              |
| 45:DY:76:CYS:HG    | 45:DY:77:PRO:HD2  | 1.15                     | 0.93              |
| 25:BA:242:G:C6     | 55:B8:5:LYS:HE2   | 2.03                     | 0.93              |
| 1:CA:1065:U:C4'    | 1:CA:1066:C:C5'   | 2.30                     | 0.93              |
| 29:DE:73:GLU:HG3   | 29:DE:74:PRO:HD2  | 1.49                     | 0.93              |
| 39:DS:83:LYS:C     | 39:DS:109:GLY:HA3 | 1.93                     | 0.93              |
| 40:BT:29:ARG:NE    | 40:BT:29:ARG:CA   | 2.31                     | 0.93              |
| 55:B8:32:LEU:H     | 55:B8:32:LEU:CD1  | 1.81                     | 0.93              |
| 10:CJ:78:ASN:ND2   | 10:CJ:80:LYS:H    | 1.67                     | 0.93              |
| 30:DF:46:ARG:HH11  | 30:DF:46:ARG:HG2  | 1.32                     | 0.93              |
| 40:DT:33:LYS:HE2   | 40:DT:43:GLN:CD   | 1.93                     | 0.93              |
| 36:BP:59:LEU:CA    | 36:BP:61:ARG:NH1  | 2.32                     | 0.93              |
| 40:BT:28:VAL:HG22  | 40:BT:46:GLU:C    | 1.93                     | 0.93              |
| 41:BU:95:LEU:HD13  | 42:BV:4:ILE:HD13  | 1.47                     | 0.93              |
| 17:CQ:59:ILE:HG22  | 17:CQ:71:PHE:HB3  | 1.48                     | 0.93              |
| 25:BA:125:G:H5''   | 25:BA:126:A:OP2   | 1.69                     | 0.93              |
| 28:BD:223:GLY:HA2  | 28:BD:231:HIS:HD2 | 1.31                     | 0.93              |
| 4:CD:176:LEU:HD12  | 4:CD:177:ASP:H    | 1.30                     | 0.93              |
| 4:AD:8:VAL:HA      | 4:AD:11:LEU:HD21  | 1.48                     | 0.93              |
| 13:AM:65:LYS:HA    | 13:AM:66:LEU:CB   | 1.95                     | 0.93              |
| 1:CA:49:U:C4       | 1:CA:364:A:C6     | 2.57                     | 0.93              |
| 1:CA:1305:G:H22    | 1:CA:1331:G:C2'   | 1.80                     | 0.93              |
| 14:AN:48:ALA:HB2   | 14:AN:53:LEU:HD12 | 1.51                     | 0.93              |
| 20:AT:53:LEU:HD12  | 20:AT:102:GLY:CA  | 1.99                     | 0.93              |
| 48:B1:52:ARG:HD2   | 48:B1:53:VAL:H    | 1.33                     | 0.93              |
| 30:DF:136:THR:HG22 | 30:DF:166:ALA:O   | 1.69                     | 0.93              |
| 40:DT:129:ARG:C    | 40:DT:129:ARG:HD2 | 1.94                     | 0.93              |
| 7:AG:14:PRO:CG     | 7:AG:21:VAL:CG1   | 2.46                     | 0.93              |
| 12:AL:39:VAL:HB    | 12:AL:57:LYS:HB2  | 1.48                     | 0.93              |
| 25:BA:995:C:H42    | 34:BN:1:MET:HG3   | 1.33                     | 0.93              |
| 16:CP:8:ARG:CG     | 16:CP:8:ARG:HH11  | 1.81                     | 0.93              |
| 32:DH:153:LYS:HB3  | 32:DH:154:PRO:CD  | 1.97                     | 0.93              |
| 41:DU:90:VAL:HG12  | 41:DU:91:ASP:H    | 1.32                     | 0.93              |
| 13:CM:10:PRO:HB2   | 13:CM:18:ALA:HB1  | 1.51                     | 0.93              |
| 25:DA:887:A:C1'    | 25:DA:889:C:N4    | 2.29                     | 0.93              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:AD:11:LEU:H      | 4:AD:11:LEU:CD2    | 1.74                     | 0.92              |
| 40:BT:29:ARG:CG    | 40:BT:85:LYS:C     | 2.42                     | 0.92              |
| 37:DQ:134:ARG:HH21 | 46:DZ:122:ARG:HH21 | 1.16                     | 0.92              |
| 40:DT:50:ILE:HD11  | 40:DT:102:ILE:HD11 | 1.50                     | 0.92              |
| 1:AA:1275:A:H2'    | 1:AA:1276:G:H8     | 1.33                     | 0.92              |
| 1:AA:1423:G:H5'    | 35:BO:49:ARG:HH22  | 1.33                     | 0.92              |
| 13:AM:3:ARG:NH1    | 31:BG:113:ARG:HH21 | 1.66                     | 0.92              |
| 25:BA:995:C:N3     | 34:BN:1:MET:CG     | 2.31                     | 0.92              |
| 40:BT:28:VAL:HG13  | 40:BT:46:GLU:HA    | 0.95                     | 0.92              |
| 3:CC:150:LYS:HE3   | 3:CC:152:ILE:HD11  | 1.51                     | 0.92              |
| 9:AI:58:HIS:C      | 9:AI:59:PHE:HD1    | 1.75                     | 0.92              |
| 20:AT:37:SER:CB    | 20:AT:84:LEU:HD22  | 1.99                     | 0.92              |
| 33:BI:38:LEU:H     | 33:BI:38:LEU:HD12  | 1.34                     | 0.92              |
| 13:CM:124:PRO:HB2  | 13:CM:125:ARG:CB   | 1.96                     | 0.92              |
| 29:DE:36:ARG:HH22  | 29:DE:88:GLY:HA3   | 1.28                     | 0.92              |
| 19:AS:6:LYS:H      | 19:AS:6:LYS:HE3    | 1.34                     | 0.92              |
| 19:AS:6:LYS:CG     | 19:AS:7:LYS:HD3    | 1.98                     | 0.92              |
| 30:BF:22:ALA:O     | 30:BF:26:ALA:HB2   | 1.69                     | 0.92              |
| 33:BI:72:LEU:HD11  | 33:BI:138:ILE:CB   | 2.00                     | 0.92              |
| 33:BI:133:HIS:HB2  | 33:BI:134:PRO:HD2  | 1.49                     | 0.92              |
| 41:BU:88:ILE:HG22  | 42:BV:47:VAL:HG23  | 1.49                     | 0.92              |
| 13:CM:124:PRO:HB3  | 13:CM:125:ARG:CB   | 1.99                     | 0.92              |
| 22:CV:43:G:C2'     | 22:CV:44:A:H5'     | 2.00                     | 0.92              |
| 44:DX:60:ARG:HH12  | 54:D7:47:ARG:NH2   | 1.67                     | 0.92              |
| 25:BA:2519:U:H4'   | 25:BA:2520:C:OP1   | 1.68                     | 0.92              |
| 34:BN:56:ASN:HA    | 34:BN:125:GLY:H    | 1.32                     | 0.92              |
| 31:DG:47:LYS:HD3   | 31:DG:81:LYS:HB2   | 1.50                     | 0.92              |
| 25:BA:2503:A:H4'   | 25:BA:2504:U:OP1   | 1.68                     | 0.92              |
| 40:DT:25:GLY:CA    | 40:DT:120:ARG:HH22 | 1.82                     | 0.92              |
| 1:AA:1279:A:C2'    | 1:AA:1282:C:N4     | 2.33                     | 0.92              |
| 5:AE:103:GLY:C     | 5:AE:106:PRO:HD2   | 1.95                     | 0.92              |
| 22:AV:55:U:O2'     | 22:AV:56:U:H5'     | 1.69                     | 0.92              |
| 30:BF:46:ARG:HH11  | 30:BF:46:ARG:HG3   | 1.35                     | 0.92              |
| 4:CD:108:LEU:O     | 4:CD:165:MET:HE2   | 1.69                     | 0.92              |
| 34:DN:67:LEU:O     | 34:DN:68:GLU:HB2   | 1.66                     | 0.92              |
| 34:BN:42:TRP:CE3   | 34:BN:48:MET:HE1   | 2.03                     | 0.92              |
| 37:BQ:30:GLY:HA2   | 37:BQ:107:ALA:HB2  | 1.52                     | 0.92              |
| 40:BT:88:ILE:HG22  | 40:BT:89:VAL:HG23  | 1.51                     | 0.92              |
| 5:CE:76:ILE:HG12   | 5:CE:77:PRO:HD2    | 1.50                     | 0.92              |
| 9:CI:28:VAL:HG22   | 9:CI:63:ILE:HB     | 1.49                     | 0.92              |
| 12:CL:46:LYS:CG    | 12:CL:47:LYS:H     | 1.77                     | 0.92              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 28:DD:108:PRO:HB3  | 28:DD:143:HIS:CE1  | 2.05                     | 0.92              |
| 53:D6:40:CYS:SG    | 53:D6:45:LYS:CE    | 2.57                     | 0.92              |
| 2:AB:55:PHE:HA     | 2:AB:58:ILE:HG13   | 1.50                     | 0.92              |
| 25:BA:2614:A:H4'   | 25:BA:2615:U:OP1   | 1.67                     | 0.92              |
| 39:BS:12:PHE:CE1   | 39:BS:14:VAL:HG22  | 2.05                     | 0.92              |
| 23:CW:36:A:H2'     | 23:CW:37:A:H5''    | 1.52                     | 0.92              |
| 40:DT:25:GLY:HA3   | 40:DT:120:ARG:NH2  | 1.85                     | 0.92              |
| 25:BA:2500:U:O2    | 25:BA:2504:U:C5    | 2.23                     | 0.91              |
| 33:DI:115:ALA:CB   | 33:DI:128:LEU:HD11 | 1.99                     | 0.91              |
| 3:AC:79:ARG:NH1    | 11:CK:100:ALA:HB2  | 1.84                     | 0.91              |
| 13:AM:108:ARG:HG3  | 13:AM:108:ARG:HH11 | 1.34                     | 0.91              |
| 25:BA:995:C:C4     | 34:BN:1:MET:HG3    | 2.05                     | 0.91              |
| 31:BG:22:ARG:HH11  | 31:BG:22:ARG:HB3   | 1.33                     | 0.91              |
| 1:CA:636:U:H5'     | 17:CQ:2:PRO:HG3    | 1.50                     | 0.91              |
| 21:CU:6:ARG:HE     | 21:CU:15:ARG:HH22  | 1.11                     | 0.91              |
| 25:DA:614(C):A:H4' | 25:DA:615:G:OP1    | 1.67                     | 0.91              |
| 38:DR:55:ALA:HA    | 38:DR:80:PHE:CE1   | 2.05                     | 0.91              |
| 20:AT:63:ILE:HD12  | 20:AT:81:LYS:HG2   | 1.52                     | 0.91              |
| 30:BF:51:THR:OG1   | 30:BF:88:VAL:HG11  | 1.69                     | 0.91              |
| 1:CA:566:G:OP1     | 1:CA:566:G:H8      | 1.53                     | 0.91              |
| 5:CE:102:ALA:C     | 5:CE:106:PRO:CG    | 2.43                     | 0.91              |
| 40:DT:42:ILE:HD12  | 40:DT:42:ILE:H     | 1.34                     | 0.91              |
| 5:CE:102:ALA:CB    | 5:CE:106:PRO:CB    | 2.38                     | 0.91              |
| 11:CK:21:ILE:CG2   | 11:CK:30:VAL:HG12  | 2.01                     | 0.91              |
| 25:DA:83:G:N2      | 25:DA:102:G:H2'    | 1.86                     | 0.91              |
| 33:DI:77:LEU:HD11  | 33:DI:140:LEU:CB   | 2.00                     | 0.91              |
| 36:DP:70:GLN:C     | 36:DP:72:PRO:HD2   | 1.95                     | 0.91              |
| 2:AB:75:LYS:O      | 2:AB:75:LYS:HD3    | 1.70                     | 0.91              |
| 30:BF:34:TRP:CA    | 36:BP:6:LEU:HD12   | 2.01                     | 0.91              |
| 4:CD:108:LEU:CG    | 4:CD:110:PHE:CE1   | 2.53                     | 0.91              |
| 37:DQ:69:PHE:CD1   | 37:DQ:70:PRO:HD2   | 2.05                     | 0.91              |
| 44:BX:64:LYS:HZ3   | 44:BX:73:ARG:HE    | 0.92                     | 0.91              |
| 53:B6:43:CYS:O     | 53:B6:44:ARG:O     | 1.87                     | 0.91              |
| 2:CB:24:TRP:CZ3    | 2:CB:26:PRO:HA     | 2.06                     | 0.91              |
| 39:DS:71:ARG:HG2   | 39:DS:104:GLY:HA2  | 1.48                     | 0.91              |
| 40:DT:81:PRO:O     | 40:DT:82:LEU:HD12  | 1.69                     | 0.91              |
| 19:AS:5:LEU:HD12   | 19:AS:10:PHE:HD1   | 0.75                     | 0.91              |
| 23:AW:68:C:H2'     | 23:AW:69:G:H8      | 1.36                     | 0.91              |
| 33:BI:121:LYS:O    | 33:BI:122:GLU:HB2  | 1.69                     | 0.91              |
| 39:BS:20:ARG:HH11  | 39:BS:20:ARG:HG2   | 1.33                     | 0.91              |
| 5:CE:102:ALA:HB3   | 5:CE:106:PRO:HB2   | 1.53                     | 0.91              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:CV:7:G:O2'      | 22:CV:50:G:H5'     | 1.70                     | 0.91              |
| 25:DA:887:A:H1'    | 25:DA:889:C:H41    | 1.30                     | 0.91              |
| 25:BA:2320:A:C6    | 25:BA:2333:A:C5    | 2.59                     | 0.91              |
| 36:BP:70:GLN:HB3   | 36:BP:72:PRO:HD2   | 1.51                     | 0.91              |
| 45:BY:76:CYS:SG    | 45:BY:77:PRO:HD2   | 2.11                     | 0.91              |
| 22:CV:15:G:H1      | 22:CV:49:C:H5      | 0.94                     | 0.91              |
| 25:DA:888:C:H5''   | 25:DA:889:C:OP2    | 1.69                     | 0.91              |
| 31:DG:37:VAL:HG22  | 31:DG:159:VAL:HA   | 1.53                     | 0.91              |
| 32:DH:13:LYS:HE2   | 32:DH:13:LYS:HA    | 1.51                     | 0.91              |
| 37:DQ:54:MET:HB3   | 37:DQ:64:ILE:HD13  | 1.50                     | 0.91              |
| 47:D0:53:MET:HB3   | 47:D0:59:LEU:HD23  | 1.51                     | 0.91              |
| 32:BH:25:LYS:HD3   | 32:BH:25:LYS:H     | 1.34                     | 0.91              |
| 41:BU:14:HIS:HD2   | 41:BU:32:PHE:CD1   | 1.88                     | 0.91              |
| 1:CA:913:A:O2'     | 1:CA:914:A:H5''    | 1.71                     | 0.91              |
| 13:CM:120:LYS:N    | 13:CM:120:LYS:HD3  | 1.84                     | 0.91              |
| 1:AA:1067:A:O2'    | 1:AA:1068:G:H8     | 1.54                     | 0.91              |
| 37:BQ:34:LEU:HB2   | 37:BQ:118:LEU:HD13 | 1.53                     | 0.91              |
| 38:BR:10:LEU:HB2   | 38:BR:17:ARG:NE    | 1.85                     | 0.91              |
| 20:CT:48:LYS:NZ    | 20:CT:48:LYS:CB    | 2.34                     | 0.91              |
| 25:DA:2750:A:H4'   | 25:DA:2751:G:OP2   | 1.69                     | 0.91              |
| 40:DT:129:ARG:CD   | 40:DT:131:ALA:CB   | 2.48                     | 0.91              |
| 53:D6:46:HIS:CD2   | 53:D6:47:THR:N     | 2.38                     | 0.91              |
| 1:AA:839:U:H3'     | 1:AA:839:U:O2      | 1.71                     | 0.90              |
| 6:AF:7:ASN:HD21    | 18:AR:34:TYR:HE1   | 1.03                     | 0.90              |
| 36:BP:146:VAL:HG22 | 36:BP:147:LEU:H    | 1.36                     | 0.90              |
| 42:BV:21:ARG:HG2   | 42:BV:91:TYR:CD2   | 2.06                     | 0.90              |
| 36:DP:71:VAL:N     | 36:DP:72:PRO:HD2   | 1.85                     | 0.90              |
| 41:DU:79:PHE:HE2   | 41:DU:83:LEU:HD21  | 1.34                     | 0.90              |
| 19:AS:48:THR:HG22  | 19:AS:61:TYR:HA    | 1.49                     | 0.90              |
| 20:AT:71:THR:HG22  | 20:AT:72:LEU:H     | 1.36                     | 0.90              |
| 25:BA:768:G:H21    | 25:BA:1379:A:H8    | 1.19                     | 0.90              |
| 4:CD:114:ARG:HG3   | 4:CD:114:ARG:HH11  | 1.35                     | 0.90              |
| 25:DA:1820:U:H4'   | 25:DA:1821:A:OP2   | 1.66                     | 0.90              |
| 35:DO:119:PRO:HB2  | 40:DT:68:TYR:CE1   | 2.06                     | 0.90              |
| 40:DT:28:VAL:HG13  | 40:DT:46:GLU:HA    | 1.53                     | 0.90              |
| 40:DT:129:ARG:HD2  | 40:DT:129:ARG:O    | 1.72                     | 0.90              |
| 55:D8:50:LEU:HD12  | 55:D8:51:ALA:H     | 1.33                     | 0.90              |
| 2:AB:74:LYS:H      | 2:AB:74:LYS:HD2    | 1.33                     | 0.90              |
| 25:BA:1819:A:H1'   | 25:BA:1821:A:C6    | 2.06                     | 0.90              |
| 40:BT:30:VAL:HG23  | 40:BT:84:GLN:O     | 1.72                     | 0.90              |
| 25:DA:2835:A:C4'   | 25:DA:2836:U:OP1   | 2.20                     | 0.90              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 33:DI:87:LYS:HA   | 33:DI:122:GLU:HA   | 1.52                     | 0.90              |
| 41:BU:27:LEU:HB3  | 41:BU:31:SER:HB3   | 1.54                     | 0.90              |
| 45:BY:54:LYS:O    | 45:BY:55:TYR:CG    | 2.25                     | 0.90              |
| 13:CM:39:ILE:HD12 | 13:CM:56:LEU:HD23  | 1.52                     | 0.90              |
| 30:DF:9:ILE:HD11  | 30:DF:125:LEU:HG   | 1.52                     | 0.90              |
| 44:BX:80:ILE:HD13 | 44:BX:80:ILE:O     | 1.71                     | 0.90              |
| 11:CK:124:LYS:HB3 | 11:CK:125:PHE:CD1  | 2.06                     | 0.90              |
| 42:DV:89:GLN:HE21 | 42:DV:89:GLN:HA    | 1.37                     | 0.90              |
| 6:AF:72:VAL:HG13  | 6:AF:73:ASN:H      | 1.37                     | 0.90              |
| 25:BA:1962:C:H4'  | 25:BA:1963:U:OP1   | 1.70                     | 0.90              |
| 25:BA:2576:G:H3'  | 25:BA:2576:G:N3    | 1.86                     | 0.90              |
| 31:BG:85:GLY:O    | 31:BG:87:PRO:HG2   | 1.72                     | 0.90              |
| 33:DI:74:ASN:ND2  | 33:DI:75:LEU:H     | 1.69                     | 0.90              |
| 42:DV:35:LEU:HD22 | 42:DV:35:LEU:H     | 1.35                     | 0.90              |
| 36:BP:75:ILE:HD13 | 36:BP:75:ILE:N     | 1.87                     | 0.90              |
| 36:BP:79:ARG:HD3  | 36:BP:109:GLY:CA   | 2.01                     | 0.90              |
| 38:BR:9:LYS:C     | 38:BR:10:LEU:HG    | 1.97                     | 0.90              |
| 2:CB:18:GLY:H     | 2:CB:42:ILE:CG2    | 1.84                     | 0.90              |
| 2:CB:185:ILE:HG12 | 2:CB:199:TYR:HB2   | 1.53                     | 0.90              |
| 5:CE:72:GLN:O     | 5:CE:73:ASN:HB3    | 1.71                     | 0.90              |
| 16:CP:8:ARG:HH11  | 16:CP:8:ARG:HG2    | 1.35                     | 0.90              |
| 25:DA:2457:U:C2'  | 25:DA:2458:G:H5'   | 2.02                     | 0.90              |
| 31:DG:7:LEU:HD21  | 31:DG:176:LEU:HD22 | 1.52                     | 0.90              |
| 41:DU:79:PHE:O    | 41:DU:83:LEU:HD13  | 1.71                     | 0.90              |
| 5:AE:83:GLU:HG2   | 5:AE:88:LYS:HG3    | 1.51                     | 0.90              |
| 25:DA:1798:U:H5'  | 28:DD:259:THR:HG22 | 1.54                     | 0.90              |
| 36:DP:75:ILE:HD13 | 36:DP:75:ILE:N     | 1.87                     | 0.90              |
| 46:BZ:151:HIS:HB3 | 46:BZ:170:THR:HA   | 1.52                     | 0.90              |
| 1:CA:128:G:C2'    | 1:CA:129:U:H5'     | 2.02                     | 0.90              |
| 7:CG:23:VAL:HG13  | 7:CG:43:PHE:CE2    | 2.07                     | 0.90              |
| 40:DT:32:TYR:CB   | 40:DT:81:PRO:HB2   | 2.02                     | 0.90              |
| 9:CI:4:TYR:HB2    | 9:CI:19:LEU:HB2    | 1.54                     | 0.89              |
| 31:DG:56:ALA:CB   | 31:DG:153:ARG:HE   | 1.84                     | 0.89              |
| 36:DP:79:ARG:HD3  | 36:DP:109:GLY:CA   | 2.01                     | 0.89              |
| 43:DW:9:TYR:HD2   | 43:DW:102:HIS:HE2  | 1.17                     | 0.89              |
| 52:B5:16:ARG:HG2  | 52:B5:16:ARG:NH1   | 1.81                     | 0.89              |
| 2:CB:7:VAL:O      | 2:CB:11:LEU:HD12   | 1.70                     | 0.89              |
| 2:CB:22:LYS:O     | 2:CB:24:TRP:HD1    | 1.54                     | 0.89              |
| 25:BA:448:U:C1'   | 30:BF:84:VAL:HG11  | 2.01                     | 0.89              |
| 25:BA:1602:U:H3'  | 25:BA:1603:A:H5'   | 1.54                     | 0.89              |
| 25:BA:2780:G:H5'' | 25:BA:2781:A:OP2   | 1.71                     | 0.89              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:CH:68:ARG:CG    | 8:CH:68:ARG:HH11  | 1.84                     | 0.89              |
| 20:CT:52:ALA:O    | 20:CT:56:MET:CB   | 2.21                     | 0.89              |
| 25:DA:1272:A:H1'  | 25:DA:1618:A:N7   | 1.87                     | 0.89              |
| 23:AW:42:C:H2'    | 23:AW:43:C:H6     | 1.37                     | 0.89              |
| 34:BN:62:VAL:HG13 | 34:BN:62:VAL:O    | 1.72                     | 0.89              |
| 35:BO:4:PRO:O     | 35:BO:5:GLN:HB2   | 1.72                     | 0.89              |
| 5:AE:102:ALA:HB1  | 5:AE:106:PRO:HG2  | 1.54                     | 0.89              |
| 25:BA:2168:G:C2   | 25:BA:2171:A:N7   | 2.41                     | 0.89              |
| 40:BT:28:VAL:HG11 | 40:BT:46:GLU:HA   | 1.52                     | 0.89              |
| 30:DF:62:ARG:HG2  | 30:DF:62:ARG:NH1  | 1.74                     | 0.89              |
| 42:DV:38:LEU:HD12 | 42:DV:56:SER:HA   | 1.54                     | 0.89              |
| 25:BA:2689:U:H4'  | 25:BA:2690:C:H5'  | 1.55                     | 0.89              |
| 45:BY:54:LYS:O    | 45:BY:55:TYR:CD2  | 2.26                     | 0.89              |
| 1:CA:49:U:O4      | 1:CA:364:A:C5     | 2.26                     | 0.89              |
| 35:DO:77:ILE:HD13 | 40:DT:74:ARG:HG2  | 1.51                     | 0.89              |
| 25:DA:886:C:H2'   | 25:DA:887:A:H4'   | 1.52                     | 0.89              |
| 28:DD:31:LYS:O    | 28:DD:35:LYS:HB2  | 1.73                     | 0.89              |
| 31:DG:16:ARG:HH11 | 31:DG:16:ARG:HG2  | 1.37                     | 0.89              |
| 40:DT:65:LYS:NZ   | 40:DT:66:VAL:H    | 1.69                     | 0.89              |
| 1:AA:1152:A:H5''  | 10:AJ:13:HIS:HD2  | 1.35                     | 0.89              |
| 2:AB:91:PRO:HG3   | 2:AB:154:LEU:HB2  | 1.54                     | 0.89              |
| 25:DA:1455:G:H8   | 38:DR:60:LEU:HD11 | 1.36                     | 0.89              |
| 46:DZ:118:GLN:HG2 | 46:DZ:119:GLU:H   | 1.38                     | 0.89              |
| 5:AE:121:LYS:HG3  | 5:AE:122:GLU:H    | 0.74                     | 0.89              |
| 20:AT:71:THR:HG22 | 20:AT:72:LEU:N    | 1.85                     | 0.89              |
| 24:AX:13:A:H3'    | 24:AX:13:A:N3     | 1.88                     | 0.89              |
| 20:CT:43:LEU:HD11 | 20:CT:51:GLU:HG3  | 1.54                     | 0.89              |
| 40:DT:27:THR:O    | 40:DT:87:ASP:HA   | 1.73                     | 0.89              |
| 40:DT:36:GLU:CD   | 40:DT:38:ASN:HD21 | 1.80                     | 0.89              |
| 6:AF:8:ILE:HD13   | 6:AF:26:ILE:HD13  | 1.53                     | 0.89              |
| 36:BP:52:GLU:CD   | 36:BP:55:ARG:HH21 | 1.81                     | 0.89              |
| 38:BR:3:HIS:O     | 38:BR:5:LYS:HD2   | 1.72                     | 0.89              |
| 1:CA:1065:U:O4'   | 1:CA:1066:C:H5''  | 1.72                     | 0.89              |
| 1:CA:1286:A:H2'   | 1:CA:1287:A:H4'   | 1.55                     | 0.89              |
| 16:CP:22:THR:HA   | 16:CP:33:ILE:HG12 | 1.55                     | 0.89              |
| 20:CT:48:LYS:NZ   | 20:CT:48:LYS:HB2  | 1.88                     | 0.89              |
| 25:DA:221:A:H5'   | 25:DA:222:A:H5'   | 1.52                     | 0.89              |
| 32:DH:89:ILE:CD1  | 32:DH:129:THR:HB  | 2.02                     | 0.89              |
| 39:DS:26:LEU:HB3  | 39:DS:87:PHE:HA   | 1.55                     | 0.89              |
| 8:CH:118:VAL:O    | 8:CH:119:LEU:HD23 | 1.72                     | 0.88              |
| 17:CQ:6:LEU:HD23  | 17:CQ:23:VAL:HG11 | 1.53                     | 0.88              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 33:DI:131:LYS:HB3  | 33:DI:132:PRO:CA   | 2.03                     | 0.88              |
| 52:D5:4:HIS:HB3    | 52:D5:5:PRO:HD3    | 1.54                     | 0.88              |
| 25:BA:2873:A:N3    | 38:BR:6:SER:HB2    | 1.88                     | 0.88              |
| 32:BH:98:LEU:HB2   | 32:BH:125:VAL:HG21 | 1.54                     | 0.88              |
| 1:CA:243:A:C2      | 1:CA:246:A:C8      | 2.61                     | 0.88              |
| 24:CX:16:A:H2'     | 24:CX:17:U:C6      | 2.05                     | 0.88              |
| 25:DA:1819:A:OP1   | 28:DD:158:ALA:CB   | 2.21                     | 0.88              |
| 36:DP:47:ASP:HB3   | 36:DP:48:PRO:C     | 1.98                     | 0.88              |
| 7:AG:14:PRO:CG     | 7:AG:21:VAL:HG13   | 1.96                     | 0.88              |
| 19:AS:5:LEU:CD1    | 19:AS:10:PHE:CD1   | 2.38                     | 0.88              |
| 31:BG:72:ARG:CG    | 31:BG:86:MET:HA    | 2.03                     | 0.88              |
| 33:BI:77:LEU:HD23  | 33:BI:101:LEU:HD13 | 1.55                     | 0.88              |
| 34:BN:134:ARG:H    | 34:BN:135:PRO:HD3  | 1.38                     | 0.88              |
| 36:BP:52:GLU:CD    | 36:BP:55:ARG:NH2   | 2.31                     | 0.88              |
| 53:B6:12:GLU:HB2   | 53:B6:23:THR:H     | 1.36                     | 0.88              |
| 4:CD:111:ALA:HB2   | 4:CD:120:LEU:HD12  | 1.53                     | 0.88              |
| 11:CK:124:LYS:HB3  | 11:CK:125:PHE:HD1  | 1.38                     | 0.88              |
| 12:AL:86:ARG:HB2   | 12:AL:101:VAL:CG2  | 2.04                     | 0.88              |
| 14:AN:15:LYS:HB3   | 14:AN:16:PHE:CD2   | 2.09                     | 0.88              |
| 25:BA:1301:A:H4'   | 25:BA:1302:A:OP1   | 1.71                     | 0.88              |
| 2:AB:54:THR:HG21   | 2:AB:201:ILE:HD11  | 1.53                     | 0.88              |
| 10:AJ:88:LEU:HG    | 10:AJ:90:LEU:HD11  | 1.53                     | 0.88              |
| 25:BA:311:A:C1'    | 25:BA:332:A:C8     | 2.56                     | 0.88              |
| 1:CA:1305:G:N2     | 1:CA:1331:G:H2'    | 1.89                     | 0.88              |
| 12:CL:11:VAL:HG13  | 17:CQ:29:HIS:HD2   | 1.01                     | 0.88              |
| 32:DH:37:VAL:HG12  | 32:DH:38:SER:H     | 1.38                     | 0.88              |
| 48:D1:56:GLN:HE21  | 48:D1:56:GLN:HA    | 1.38                     | 0.88              |
| 7:AG:75:VAL:HG11   | 7:AG:144:MET:HB3   | 1.55                     | 0.88              |
| 13:AM:117:VAL:HG12 | 13:AM:118:ALA:H    | 1.37                     | 0.88              |
| 20:AT:37:SER:HB3   | 20:AT:84:LEU:HD21  | 1.55                     | 0.88              |
| 20:AT:44:ALA:HB1   | 20:AT:91:LEU:HB2   | 1.56                     | 0.88              |
| 23:AW:42:C:H2'     | 23:AW:43:C:C6      | 2.08                     | 0.88              |
| 34:BN:14:VAL:CG1   | 34:BN:137:LYS:HG3  | 2.03                     | 0.88              |
| 1:CA:968:A:C4'     | 1:CA:969:A:OP2     | 2.21                     | 0.88              |
| 8:CH:116:LYS:HD2   | 8:CH:129:VAL:HG11  | 1.54                     | 0.88              |
| 36:DP:146:VAL:HG22 | 36:DP:147:LEU:H    | 1.36                     | 0.88              |
| 40:DT:23:ARG:NE    | 40:DT:120:ARG:HD3  | 1.88                     | 0.88              |
| 10:AJ:30:SER:HB2   | 10:AJ:80:LYS:HB3   | 1.53                     | 0.88              |
| 12:AL:41:ARG:HH22  | 12:AL:57:LYS:NZ    | 1.72                     | 0.88              |
| 12:AL:87:GLY:HA2   | 12:AL:98:TYR:HA    | 1.56                     | 0.88              |
| 31:BG:43:LEU:HB2   | 31:BG:88:ILE:HD11  | 0.89                     | 0.88              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 36:BP:85:LEU:HA    | 36:BP:88:LEU:HB3   | 1.53                     | 0.88              |
| 2:CB:16:HIS:HD2    | 2:CB:210:SER:HA    | 1.37                     | 0.88              |
| 4:CD:30:LYS:C      | 4:CD:32:ALA:H      | 1.78                     | 0.88              |
| 7:CG:23:VAL:HG13   | 7:CG:43:PHE:HE2    | 1.38                     | 0.88              |
| 14:AN:15:LYS:HB3   | 14:AN:16:PHE:CE2   | 2.08                     | 0.88              |
| 25:BA:614:U:O2     | 25:BA:614:U:H5'    | 1.72                     | 0.88              |
| 25:BA:2320:A:C5    | 25:BA:2333:A:C6    | 2.62                     | 0.88              |
| 25:BA:2835:A:H4'   | 25:BA:2836:U:OP1   | 1.72                     | 0.88              |
| 27:BC:169:GLY:H    | 27:BC:173:ALA:HA   | 1.36                     | 0.88              |
| 20:CT:72:LEU:HD23  | 20:CT:73:HIS:H     | 1.39                     | 0.88              |
| 32:DH:92:ILE:H     | 32:DH:92:ILE:HD12  | 1.38                     | 0.88              |
| 40:DT:24:PRO:HD3   | 40:DT:52:ILE:CD1   | 2.03                     | 0.88              |
| 40:DT:129:ARG:HD3  | 40:DT:131:ALA:HB2  | 1.56                     | 0.88              |
| 25:BA:2873:A:H1'   | 38:BR:6:SER:HB2    | 1.56                     | 0.88              |
| 13:CM:57:ARG:HH11  | 13:CM:57:ARG:HB2   | 1.37                     | 0.88              |
| 20:CT:48:LYS:HB2   | 20:CT:48:LYS:HZ2   | 1.36                     | 0.88              |
| 9:AI:15:ALA:HB2    | 9:AI:65:VAL:HG23   | 1.54                     | 0.88              |
| 19:AS:9:VAL:HG12   | 19:AS:11:VAL:HG12  | 0.90                     | 0.88              |
| 1:CA:1456:G:N2     | 1:CA:1457:G:C5     | 2.41                     | 0.88              |
| 36:DP:85:LEU:HA    | 36:DP:88:LEU:HB3   | 1.53                     | 0.88              |
| 8:AH:6:ILE:H       | 8:AH:6:ILE:HD12    | 1.38                     | 0.87              |
| 14:AN:13:THR:N     | 14:AN:14:PRO:CD    | 2.37                     | 0.87              |
| 25:BA:1300:U:H5'   | 25:BA:1301:A:C2    | 2.09                     | 0.87              |
| 27:BC:100:ILE:HG22 | 27:BC:101:GLN:HG3  | 1.56                     | 0.87              |
| 40:BT:28:VAL:O     | 40:BT:29:ARG:HB2   | 1.71                     | 0.87              |
| 48:B1:53:VAL:HG23  | 48:B1:74:VAL:HG13  | 1.56                     | 0.87              |
| 1:CA:913:A:H1'     | 1:CA:914:A:O4'     | 1.73                     | 0.87              |
| 5:CE:98:THR:HG22   | 5:CE:99:GLY:O      | 1.75                     | 0.87              |
| 5:CE:104:ALA:C     | 5:CE:106:PRO:HD2   | 1.98                     | 0.87              |
| 25:DA:1819:A:H4'   | 25:DA:1820:U:H5'   | 1.54                     | 0.87              |
| 40:DT:23:ARG:CG    | 40:DT:120:ARG:NH1  | 2.36                     | 0.87              |
| 46:DZ:166:SER:HB2  | 46:DZ:167:PRO:C    | 1.99                     | 0.87              |
| 1:AA:1049:U:O2     | 1:AA:1201:A:C4     | 2.27                     | 0.87              |
| 4:AD:108:LEU:HD11  | 4:AD:174:LEU:HB3   | 1.55                     | 0.87              |
| 25:BA:1826:G:H4'   | 28:BD:242:ARG:HH21 | 1.39                     | 0.87              |
| 1:CA:274:A:O2'     | 1:CA:275:G:H8      | 1.58                     | 0.87              |
| 33:BI:77:LEU:O     | 33:BI:140:LEU:HD12 | 1.73                     | 0.87              |
| 38:BR:37:THR:OG1   | 38:BR:39:PRO:HD2   | 1.74                     | 0.87              |
| 40:BT:3:ARG:HG3    | 40:BT:6:LEU:HB2    | 1.54                     | 0.87              |
| 55:B8:50:LEU:C     | 55:B8:53:PRO:HD2   | 1.99                     | 0.87              |
| 1:CA:533:A:H4'     | 1:CA:534:U:OP1     | 1.73                     | 0.87              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 33:DI:4:ILE:HG12  | 33:DI:18:VAL:HG22  | 1.55                     | 0.87              |
| 28:BD:181:GLU:HA  | 28:BD:272:ALA:HB3  | 1.55                     | 0.87              |
| 38:BR:9:LYS:O     | 38:BR:10:LEU:HD23  | 1.73                     | 0.87              |
| 39:BS:15:ARG:HD3  | 39:BS:15:ARG:N     | 1.89                     | 0.87              |
| 40:BT:30:VAL:HG21 | 40:BT:84:GLN:HG3   | 1.55                     | 0.87              |
| 1:CA:839:U:H2'    | 1:CA:839:U:O2      | 1.75                     | 0.87              |
| 53:D6:19:ARG:HG2  | 53:D6:20:ASN:H     | 1.37                     | 0.87              |
| 1:AA:1049:U:H4'   | 1:AA:1050:G:C5'    | 2.04                     | 0.87              |
| 1:AA:1251:A:H2'   | 1:AA:1252:A:C8     | 2.09                     | 0.87              |
| 11:AK:33:THR:HB   | 11:AK:38:ASN:O     | 1.73                     | 0.87              |
| 36:BP:47:ASP:HB3  | 36:BP:48:PRO:C     | 1.98                     | 0.87              |
| 20:CT:23:ARG:HA   | 20:CT:26:ASN:OD1   | 1.73                     | 0.87              |
| 40:DT:36:GLU:HB3  | 40:DT:38:ASN:HD21  | 1.38                     | 0.87              |
| 50:D3:56:VAL:HG12 | 50:D3:57:GLU:H     | 1.38                     | 0.87              |
| 4:AD:36:ARG:HB3   | 4:AD:38:TYR:CE1    | 2.08                     | 0.87              |
| 1:CA:1054:C:O2    | 1:CA:1054:C:H3'    | 1.75                     | 0.87              |
| 40:DT:117:ASP:OD2 | 40:DT:120:ARG:HG3  | 1.75                     | 0.87              |
| 45:DY:97:ARG:HD3  | 45:DY:97:ARG:H     | 1.36                     | 0.87              |
| 9:AI:70:LYS:O     | 9:AI:74:ILE:HG13   | 1.74                     | 0.87              |
| 25:BA:1494:A:N3   | 25:BA:1494:A:H5'   | 1.88                     | 0.87              |
| 1:CA:668:G:O2'    | 15:CO:46:HIS:HB3   | 1.75                     | 0.87              |
| 4:CD:22:LYS:HG3   | 4:CD:26:CYS:SG     | 2.15                     | 0.87              |
| 6:CF:89:MET:SD    | 18:CR:76:LEU:HD21  | 2.14                     | 0.87              |
| 9:CI:126:SER:O    | 9:CI:127:LYS:HB3   | 1.75                     | 0.87              |
| 16:CP:8:ARG:C     | 16:CP:9:PHE:HD2    | 1.82                     | 0.87              |
| 22:CV:15:G:N1     | 22:CV:49:C:H5      | 1.73                     | 0.87              |
| 1:AA:968:A:C4'    | 1:AA:969:A:OP2     | 2.23                     | 0.87              |
| 12:AL:83:VAL:HG11 | 12:AL:100:ILE:HG12 | 1.53                     | 0.87              |
| 40:BT:80:SER:HB3  | 40:BT:81:PRO:HD3   | 1.54                     | 0.87              |
| 45:BY:14:LEU:CD1  | 45:BY:15:VAL:H     | 1.88                     | 0.87              |
| 45:BY:36:ALA:CB   | 45:BY:67:LEU:O     | 2.22                     | 0.87              |
| 13:CM:94:ARG:HG2  | 19:CS:82:GLY:N     | 1.90                     | 0.87              |
| 20:CT:43:LEU:HD13 | 20:CT:51:GLU:HG2   | 1.57                     | 0.87              |
| 35:DO:49:ARG:HH11 | 35:DO:49:ARG:HG2   | 1.39                     | 0.87              |
| 31:BG:72:ARG:NH1  | 31:BG:86:MET:CB    | 2.36                     | 0.86              |
| 25:DA:676:A:H8    | 25:DA:2069:G:H21   | 1.19                     | 0.86              |
| 19:AS:6:LYS:HG2   | 19:AS:7:LYS:CD     | 2.04                     | 0.86              |
| 25:BA:332:A:H4'   | 25:BA:333:G:OP1    | 1.73                     | 0.86              |
| 25:BA:1452:A:H62  | 25:BA:2703:C:H41   | 1.22                     | 0.86              |
| 25:BA:2745:C:C4   | 25:BA:2746:U:C4    | 2.63                     | 0.86              |
| 44:BX:64:LYS:NZ   | 44:BX:73:ARG:HE    | 1.73                     | 0.86              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 32:DH:150:ALA:C   | 32:DH:152:ARG:H    | 1.77                     | 0.86              |
| 38:DR:8:ARG:HH11  | 38:DR:39:PRO:HB3   | 1.38                     | 0.86              |
| 38:DR:17:ARG:HH11 | 38:DR:17:ARG:HG2   | 1.41                     | 0.86              |
| 25:BA:2458:G:C8   | 25:BA:2490:G:C6    | 2.63                     | 0.86              |
| 40:BT:28:VAL:HG12 | 40:BT:29:ARG:N     | 1.86                     | 0.86              |
| 1:CA:251:G:C1'    | 1:CA:252:U:C6      | 2.58                     | 0.86              |
| 53:D6:46:HIS:HD2  | 53:D6:47:THR:CA    | 1.87                     | 0.86              |
| 3:AC:58:GLU:HB2   | 3:AC:65:ALA:HB2    | 1.56                     | 0.86              |
| 46:BZ:6:LYS:HA    | 46:BZ:60:GLU:HB2   | 1.56                     | 0.86              |
| 10:CJ:51:ARG:HD2  | 10:CJ:59:SER:O     | 1.75                     | 0.86              |
| 19:CS:52:TYR:HD1  | 19:CS:57:HIS:CE1   | 1.93                     | 0.86              |
| 25:DA:2311:A:C8   | 31:DG:88:ILE:HG13  | 2.09                     | 0.86              |
| 31:DG:56:ALA:HB2  | 31:DG:153:ARG:NE   | 1.91                     | 0.86              |
| 1:AA:1226:C:O2'   | 1:AA:1227:A:H5'    | 1.73                     | 0.86              |
| 25:BA:49:A:H1'    | 25:BA:51:G:C5      | 2.11                     | 0.86              |
| 47:B0:26:TYR:H    | 47:B0:29:GLN:NE2   | 1.72                     | 0.86              |
| 22:CV:29:C:C2'    | 22:CV:30:G:C5'     | 2.53                     | 0.86              |
| 36:DP:59:LEU:CA   | 36:DP:61:ARG:NH1   | 2.39                     | 0.86              |
| 45:DY:63:LYS:NZ   | 45:DY:64:GLU:H     | 1.73                     | 0.86              |
| 27:BC:58:VAL:HG21 | 27:BC:166:ASP:N    | 1.89                     | 0.86              |
| 43:BW:51:LEU:HD13 | 43:BW:52:GLU:N     | 1.91                     | 0.86              |
| 45:BY:28:LYS:HE3  | 45:BY:28:LYS:N     | 1.89                     | 0.86              |
| 29:DE:60:ASN:OD1  | 29:DE:62:PRO:HD2   | 1.74                     | 0.86              |
| 44:DX:12:VAL:HG21 | 44:DX:17:ALA:HB2   | 1.56                     | 0.86              |
| 13:AM:65:LYS:CA   | 13:AM:66:LEU:HB2   | 2.05                     | 0.86              |
| 25:BA:243:U:OP1   | 55:B8:6:THR:HG21   | 1.75                     | 0.86              |
| 25:BA:769:G:H5'   | 25:BA:1379:A:H62   | 1.40                     | 0.86              |
| 25:BA:1452:A:H4'  | 25:BA:1453:U:OP2   | 1.76                     | 0.86              |
| 25:BA:2059:A:H5'  | 25:BA:2060:A:OP2   | 1.75                     | 0.86              |
| 5:CE:78:HIS:HD2   | 8:CH:104:ARG:HG3   | 0.71                     | 0.86              |
| 2:AB:187:LEU:HA   | 2:AB:201:ILE:HB    | 1.57                     | 0.86              |
| 25:BA:1493:C:O2   | 25:BA:1493:C:H2'   | 1.74                     | 0.86              |
| 33:BI:5:LEU:HD11  | 33:BI:19:VAL:HG12  | 1.56                     | 0.86              |
| 7:CG:54:THR:OG1   | 7:CG:56:GLN:HG2    | 1.75                     | 0.86              |
| 30:DF:198:ALA:HA  | 30:DF:201:VAL:HG12 | 1.56                     | 0.86              |
| 43:DW:76:VAL:HG23 | 43:DW:103:ILE:HA   | 1.58                     | 0.86              |
| 1:AA:251:G:H4'    | 1:AA:252:U:O5'     | 1.74                     | 0.86              |
| 12:AL:5:PRO:HA    | 12:AL:9:GLN:HE21   | 1.37                     | 0.86              |
| 13:AM:57:ARG:NH2  | 51:B4:60:GLU:HG3   | 1.90                     | 0.86              |
| 1:CA:274:A:H4'    | 1:CA:275:G:O5'     | 1.76                     | 0.86              |
| 1:CA:484:G:O2'    | 1:CA:485:G:H5''    | 1.74                     | 0.86              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:BA:434:U:O2'   | 25:BA:435:C:H5    | 1.58                     | 0.86              |
| 34:BN:62:VAL:HG22 | 34:BN:66:LYS:CG   | 2.05                     | 0.86              |
| 25:DA:1598:C:H5'  | 44:DX:36:LYS:HB2  | 1.58                     | 0.86              |
| 25:DA:1754:C:OP1  | 40:DT:96:ARG:NH1  | 2.08                     | 0.86              |
| 41:DU:108:GLU:CG  | 42:DV:44:LYS:HE3  | 2.02                     | 0.86              |
| 45:DY:81:LYS:HD3  | 45:DY:97:ARG:NE   | 1.91                     | 0.86              |
| 2:AB:25:ASN:ND2   | 2:AB:193:ASP:HB3  | 1.91                     | 0.85              |
| 25:BA:769:G:H5'   | 25:BA:1379:A:N6   | 1.90                     | 0.85              |
| 47:B0:53:MET:HB2  | 47:B0:59:LEU:HD23 | 1.58                     | 0.85              |
| 28:DD:43:ARG:NH1  | 28:DD:44:ASN:ND2  | 2.24                     | 0.85              |
| 36:DP:79:ARG:HD3  | 36:DP:109:GLY:HA2 | 1.57                     | 0.85              |
| 25:BA:2171:A:O2'  | 25:BA:2172:U:H5'  | 1.75                     | 0.85              |
| 32:DH:152:ARG:O   | 32:DH:153:LYS:HB2 | 1.75                     | 0.85              |
| 33:DI:110:ASP:HB2 | 33:DI:111:PRO:C   | 2.01                     | 0.85              |
| 44:DX:12:VAL:HG11 | 44:DX:27:THR:OG1  | 1.76                     | 0.85              |
| 46:DZ:82:ARG:HG3  | 46:DZ:83:PRO:HD2  | 1.57                     | 0.85              |
| 3:AC:79:ARG:HH12  | 11:CK:100:ALA:CB  | 1.88                     | 0.85              |
| 8:AH:95:VAL:HB    | 8:AH:99:GLU:HB2   | 1.59                     | 0.85              |
| 17:AQ:7:THR:HG22  | 17:AQ:58:GLU:HG2  | 1.57                     | 0.85              |
| 28:BD:218:ARG:HB3 | 28:BD:219:PRO:HD2 | 1.58                     | 0.85              |
| 1:CA:251:G:O4'    | 1:CA:252:U:C6     | 2.29                     | 0.85              |
| 4:CD:33:MET:HE2   | 4:CD:37:PRO:HA    | 1.59                     | 0.85              |
| 29:DE:101:ARG:NH2 | 29:DE:171:GLU:HB2 | 1.92                     | 0.85              |
| 45:DY:39:VAL:HG12 | 45:DY:40:GLU:H    | 1.41                     | 0.85              |
| 4:AD:49:ARG:HD3   | 4:AD:50:ARG:N     | 1.91                     | 0.85              |
| 11:AK:21:ILE:HA   | 11:AK:30:VAL:HG12 | 1.57                     | 0.85              |
| 13:AM:25:ILE:HD11 | 13:AM:66:LEU:HD21 | 1.57                     | 0.85              |
| 25:BA:243:U:O4    | 25:BA:254:G:C2    | 2.30                     | 0.85              |
| 42:BV:81:TYR:C    | 42:BV:82:ARG:HD2  | 2.01                     | 0.85              |
| 25:DA:1819:A:H4'  | 25:DA:1820:U:OP2  | 1.77                     | 0.85              |
| 37:DQ:27:VAL:HG23 | 37:DQ:137:TYR:HE1 | 1.40                     | 0.85              |
| 41:DU:95:LEU:HD13 | 42:DV:4:ILE:CG2   | 2.06                     | 0.85              |
| 25:BA:1504:C:O2'  | 25:BA:1505:C:C5'  | 2.24                     | 0.85              |
| 26:BB:14:U:H4'    | 26:BB:15:A:OP2    | 1.74                     | 0.85              |
| 29:BE:73:GLU:HG3  | 29:BE:74:PRO:HD2  | 1.55                     | 0.85              |
| 43:BW:59:VAL:HG12 | 43:BW:60:ASN:OD1  | 1.75                     | 0.85              |
| 2:CB:24:TRP:CH2   | 2:CB:26:PRO:HA    | 2.11                     | 0.85              |
| 13:CM:108:ARG:N   | 13:CM:108:ARG:HD2 | 1.91                     | 0.85              |
| 25:DA:2457:U:H2'  | 25:DA:2458:G:H5'  | 1.56                     | 0.85              |
| 31:DG:67:LYS:HG2  | 51:D4:5:ILE:CG2   | 2.05                     | 0.85              |
| 40:DT:33:LYS:HE2  | 40:DT:43:GLN:CB   | 2.06                     | 0.85              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:531:U:H5''    | 1:AA:532:A:OP1     | 1.75                     | 0.85              |
| 2:AB:91:PRO:HG2    | 2:AB:155:LEU:HD23  | 1.57                     | 0.85              |
| 5:AE:76:ILE:HG12   | 5:AE:77:PRO:HD2    | 1.57                     | 0.85              |
| 9:AI:46:ALA:HA     | 9:AI:78:LYS:HB2    | 1.57                     | 0.85              |
| 12:AL:5:PRO:HA     | 12:AL:9:GLN:NE2    | 1.89                     | 0.85              |
| 31:BG:39:ILE:HD13  | 31:BG:157:ILE:HG23 | 1.58                     | 0.85              |
| 31:BG:144:ILE:HD12 | 31:BG:145:THR:N    | 1.91                     | 0.85              |
| 36:DP:90:ARG:HG2   | 36:DP:91:PHE:HD1   | 1.41                     | 0.85              |
| 46:DZ:145:GLU:HG3  | 46:DZ:146:ILE:HG12 | 1.55                     | 0.85              |
| 1:AA:982:U:H6      | 1:AA:982:U:O5'     | 1.58                     | 0.85              |
| 1:CA:819:A:C5'     | 1:CA:820:U:OP2     | 2.24                     | 0.85              |
| 8:CH:87:SER:HA     | 8:CH:93:VAL:HG23   | 1.59                     | 0.85              |
| 27:DC:68:LEU:HD11  | 27:DC:179:SER:HA   | 1.58                     | 0.85              |
| 34:DN:58:ASP:C     | 34:DN:60:ILE:H     | 1.85                     | 0.85              |
| 1:AA:595:G:C4'     | 1:AA:596:C:OP1     | 2.24                     | 0.85              |
| 8:AH:1:MET:HE2     | 8:AH:2:LEU:H       | 1.42                     | 0.85              |
| 40:BT:26:ASP:OD2   | 40:BT:27:THR:N     | 2.10                     | 0.85              |
| 48:B1:52:ARG:CD    | 48:B1:53:VAL:H     | 1.89                     | 0.85              |
| 24:CX:17:U:C2'     | 24:CX:18:G:H5'     | 2.06                     | 0.85              |
| 25:DA:614(A):U:H4' | 25:DA:614(B):G:OP1 | 1.77                     | 0.85              |
| 40:DT:129:ARG:CD   | 40:DT:131:ALA:HB3  | 2.07                     | 0.85              |
| 6:AF:45:LEU:HD11   | 6:AF:57:GLN:HB3    | 1.58                     | 0.85              |
| 25:BA:1451:C:H5''  | 25:BA:1452:A:OP1   | 1.75                     | 0.85              |
| 34:BN:32:THR:HG23  | 34:BN:37:LYS:HB3   | 1.58                     | 0.85              |
| 38:BR:2:ARG:NH1    | 38:BR:5:LYS:HE2    | 1.91                     | 0.85              |
| 7:CG:10:ARG:HG3    | 7:CG:10:ARG:HH11   | 1.41                     | 0.85              |
| 20:CT:33:ILE:H     | 20:CT:33:ILE:HD13  | 1.42                     | 0.85              |
| 27:DC:59:ARG:HB2   | 27:DC:62:VAL:HG22  | 1.59                     | 0.85              |
| 32:DH:89:ILE:HD13  | 32:DH:90:LYS:N     | 1.92                     | 0.85              |
| 19:AS:11:VAL:HA    | 19:AS:38:SER:HB2   | 1.59                     | 0.85              |
| 35:BO:97:ARG:HH21  | 35:BO:99:PHE:HE1   | 1.23                     | 0.85              |
| 39:BS:12:PHE:CE1   | 39:BS:14:VAL:CG2   | 2.59                     | 0.85              |
| 46:BZ:37:VAL:O     | 46:BZ:38:TYR:HB3   | 1.75                     | 0.85              |
| 49:B2:38:GLN:HA    | 49:B2:41:ILE:HD11  | 1.58                     | 0.85              |
| 20:CT:43:LEU:HD13  | 20:CT:51:GLU:HB2   | 1.58                     | 0.85              |
| 22:AV:15:G:H1      | 22:AV:49:C:H5      | 1.22                     | 0.84              |
| 25:BA:588:U:OP2    | 25:BA:588:U:C5     | 2.30                     | 0.84              |
| 29:BE:3:GLY:HA3    | 29:BE:81:ILE:HG21  | 1.59                     | 0.84              |
| 37:BQ:12:GLN:HG2   | 37:BQ:73:PRO:HD2   | 1.58                     | 0.84              |
| 40:BT:31:SER:OG    | 40:BT:32:TYR:N     | 2.05                     | 0.84              |
| 43:BW:34:ASN:O     | 43:BW:37:ARG:HB3   | 1.76                     | 0.84              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 52:D5:48:GLU:HA   | 52:D5:57:VAL:CG2   | 2.07                     | 0.84              |
| 52:D5:48:GLU:HA   | 52:D5:57:VAL:HG21  | 1.59                     | 0.84              |
| 53:D6:41:PRO:CD   | 53:D6:46:HIS:H     | 1.90                     | 0.84              |
| 1:AA:1049:U:H4'   | 1:AA:1050:G:O5'    | 1.75                     | 0.84              |
| 10:AJ:5:ARG:HA    | 10:AJ:73:ASP:OD1   | 1.77                     | 0.84              |
| 32:BH:148:ILE:O   | 32:BH:151:ILE:HG12 | 1.78                     | 0.84              |
| 48:B1:5:CYS:SG    | 48:B1:8:SER:HB3    | 2.17                     | 0.84              |
| 1:CA:950:U:H1'    | 1:CA:971:G:N7      | 1.93                     | 0.84              |
| 25:DA:1819:A:OP1  | 28:DD:158:ALA:HB3  | 1.77                     | 0.84              |
| 30:DF:128:ALA:O   | 30:DF:129:PHE:CD2  | 2.30                     | 0.84              |
| 32:DH:127:GLU:OE1 | 32:DH:128:PRO:HD2  | 1.78                     | 0.84              |
| 40:DT:23:ARG:HE   | 40:DT:120:ARG:HD3  | 1.40                     | 0.84              |
| 18:AR:74:ARG:HH21 | 18:AR:81:PHE:HA    | 1.42                     | 0.84              |
| 1:CA:1226:C:O2'   | 1:CA:1227:A:H5'    | 1.76                     | 0.84              |
| 28:DD:35:LYS:O    | 28:DD:64:ILE:HG22  | 1.77                     | 0.84              |
| 30:DF:7:TYR:HB3   | 30:DF:21:ALA:HB1   | 1.57                     | 0.84              |
| 13:AM:24:GLY:C    | 13:AM:25:ILE:HD12  | 2.01                     | 0.84              |
| 25:BA:434:U:O2'   | 25:BA:435:C:C5     | 2.30                     | 0.84              |
| 25:BA:1340:U:O2'  | 25:BA:1602:U:H2'   | 1.76                     | 0.84              |
| 30:BF:3:GLU:HG3   | 30:BF:19:GLU:HB2   | 1.59                     | 0.84              |
| 55:B8:30:ARG:O    | 55:B8:30:ARG:HD3   | 1.77                     | 0.84              |
| 25:DA:1693:U:OP2  | 25:DA:1694:C:C5    | 2.30                     | 0.84              |
| 27:BC:196:LEU:C   | 27:BC:198:ALA:H    | 1.86                     | 0.84              |
| 30:BF:17:ARG:HH11 | 30:BF:17:ARG:HG3   | 1.41                     | 0.84              |
| 36:BP:79:ARG:HD3  | 36:BP:109:GLY:HA2  | 1.57                     | 0.84              |
| 12:CL:24:VAL:HG13 | 12:CL:98:TYR:HE2   | 1.41                     | 0.84              |
| 34:DN:4:TYR:HB2   | 41:DU:64:ARG:NH2   | 1.92                     | 0.84              |
| 34:DN:9:VAL:HG12  | 34:DN:10:GLU:H     | 1.43                     | 0.84              |
| 1:AA:1502:A:H2    | 1:AA:1505:G:H22    | 1.26                     | 0.84              |
| 2:AB:236:TYR:HA   | 2:AB:239:VAL:HG23  | 1.60                     | 0.84              |
| 34:BN:24:GLY:O    | 34:BN:28:THR:HB    | 1.76                     | 0.84              |
| 41:BU:66:ASN:HD21 | 41:BU:70:ARG:HE    | 1.22                     | 0.84              |
| 46:BZ:151:HIS:HB2 | 46:BZ:168:GLU:O    | 1.77                     | 0.84              |
| 8:CH:7:ALA:HB2    | 8:CH:85:ARG:HG3    | 1.60                     | 0.84              |
| 19:CS:6:LYS:HG2   | 19:CS:7:LYS:HD3    | 1.58                     | 0.84              |
| 25:DA:2306:C:H3'  | 25:DA:2307:G:H5''  | 1.59                     | 0.84              |
| 32:DH:153:LYS:CG  | 32:DH:162:ILE:H    | 1.90                     | 0.84              |
| 45:DY:47:LYS:HG2  | 45:DY:60:PHE:CE1   | 2.12                     | 0.84              |
| 4:AD:33:MET:HE3   | 4:AD:33:MET:HA     | 1.58                     | 0.84              |
| 9:AI:96:LEU:HG    | 9:AI:102:LEU:HB2   | 1.56                     | 0.84              |
| 13:AM:54:VAL:O    | 13:AM:58:GLU:HG2   | 1.78                     | 0.84              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:BA:2519:U:C4'   | 25:BA:2520:C:OP1   | 2.26                     | 0.84              |
| 28:BD:223:GLY:HA2  | 28:BD:231:HIS:CD2  | 2.12                     | 0.84              |
| 1:CA:136:C:H42     | 1:CA:227:G:H1      | 1.24                     | 0.84              |
| 1:CA:1226:C:N4     | 13:CM:104:ARG:HB2  | 1.92                     | 0.84              |
| 38:DR:8:ARG:NH1    | 38:DR:39:PRO:HB3   | 1.92                     | 0.84              |
| 25:BA:2449:U:C4'   | 25:BA:2450:A:OP1   | 2.26                     | 0.84              |
| 42:BV:19:LYS:HG3   | 42:BV:20:LEU:N     | 1.92                     | 0.84              |
| 7:AG:14:PRO:HG3    | 7:AG:21:VAL:HG12   | 1.60                     | 0.84              |
| 25:BA:2056:G:N2    | 25:BA:2057:A:N9    | 2.26                     | 0.84              |
| 28:BD:31:LYS:O     | 28:BD:35:LYS:HB2   | 1.76                     | 0.84              |
| 34:BN:4:TYR:N      | 34:BN:4:TYR:CD1    | 2.44                     | 0.84              |
| 5:CE:76:ILE:HD11   | 5:CE:142:LEU:HD21  | 1.60                     | 0.84              |
| 32:DH:106:THR:HG22 | 32:DH:112:PRO:HB3  | 1.58                     | 0.84              |
| 35:DO:63:VAL:HG12  | 35:DO:106:LEU:HD11 | 1.58                     | 0.84              |
| 6:AF:76:ALA:O      | 6:AF:80:ARG:HG3    | 1.77                     | 0.84              |
| 28:BD:270:ILE:O    | 28:BD:271:ILE:HG13 | 1.77                     | 0.84              |
| 33:BI:83:ALA:HB2   | 33:BI:88:ILE:HA    | 1.57                     | 0.84              |
| 33:BI:83:ALA:CB    | 33:BI:88:ILE:HA    | 2.08                     | 0.84              |
| 36:BP:90:ARG:HG2   | 36:BP:91:PHE:HD1   | 1.41                     | 0.84              |
| 1:CA:251:G:H1'     | 1:CA:252:U:C6      | 2.12                     | 0.84              |
| 1:CA:251:G:O4'     | 1:CA:252:U:C5      | 2.30                     | 0.84              |
| 13:CM:116:THR:HG22 | 13:CM:117:VAL:N    | 1.92                     | 0.84              |
| 20:CT:81:LYS:O     | 20:CT:85:MET:CG    | 2.25                     | 0.84              |
| 28:DD:24:ILE:HG12  | 28:DD:25:THR:H     | 1.43                     | 0.84              |
| 28:DD:35:LYS:HZ1   | 28:DD:103:ARG:HA   | 1.42                     | 0.84              |
| 32:DH:124:GLU:HB2  | 32:DH:132:ARG:HD2  | 1.60                     | 0.84              |
| 1:AA:1277:C:O2'    | 1:AA:1279:A:C8     | 2.30                     | 0.83              |
| 5:AE:26:PHE:O      | 5:AE:27:ARG:HB2    | 1.77                     | 0.83              |
| 12:AL:6:THR:HG23   | 12:AL:9:GLN:CG     | 2.08                     | 0.83              |
| 25:BA:483:A:H1'    | 45:BY:60:PHE:CZ    | 2.11                     | 0.83              |
| 25:BA:2835:A:C4'   | 25:BA:2836:U:OP1   | 2.26                     | 0.83              |
| 31:BG:86:MET:HG3   | 31:BG:87:PRO:HD2   | 1.59                     | 0.83              |
| 33:DI:93:THR:HG22  | 33:DI:119:PRO:HB3  | 1.60                     | 0.83              |
| 28:BD:231:HIS:ND1  | 28:BD:232:PRO:HD2  | 1.92                     | 0.83              |
| 31:BG:72:ARG:HB3   | 31:BG:86:MET:C     | 2.02                     | 0.83              |
| 33:BI:54:GLN:O     | 33:BI:58:LEU:HB3   | 1.78                     | 0.83              |
| 23:CW:16:U:H3'     | 23:CW:17:C:H5'     | 1.59                     | 0.83              |
| 25:DA:598:G:C4'    | 36:DP:11:GLY:HA3   | 2.08                     | 0.83              |
| 25:DA:1205:U:H4'   | 25:DA:1206:G:OP2   | 1.78                     | 0.83              |
| 25:DA:1819:A:H1'   | 25:DA:1821:A:C6    | 2.13                     | 0.83              |
| 30:DF:95:ARG:NE    | 30:DF:97:TYR:CZ    | 2.44                     | 0.83              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 40:DT:33:LYS:HE3   | 40:DT:43:GLN:CD   | 2.02                     | 0.83              |
| 40:DT:33:LYS:HG2   | 40:DT:43:GLN:CB   | 2.08                     | 0.83              |
| 1:CA:1067:A:O2'    | 1:CA:1068:G:H8    | 1.60                     | 0.83              |
| 3:CC:123:GLN:HB3   | 3:CC:128:PHE:CD2  | 2.13                     | 0.83              |
| 14:CN:13:THR:N     | 14:CN:14:PRO:HD2  | 1.92                     | 0.83              |
| 25:DA:1799:G:O6    | 28:DD:179:SER:HB3 | 1.78                     | 0.83              |
| 36:DP:64:LYS:HB3   | 55:D8:25:MET:HG3  | 1.59                     | 0.83              |
| 5:AE:91:LEU:HD12   | 5:AE:120:THR:HB   | 1.58                     | 0.83              |
| 11:AK:33:THR:HB    | 11:AK:38:ASN:C    | 2.04                     | 0.83              |
| 42:BV:19:LYS:HB3   | 42:BV:94:LEU:O    | 1.78                     | 0.83              |
| 45:BY:37:VAL:CG2   | 45:BY:72:VAL:HG21 | 2.07                     | 0.83              |
| 19:CS:41:VAL:HB    | 19:CS:44:MET:HG2  | 1.60                     | 0.83              |
| 45:DY:63:LYS:HZ2   | 45:DY:64:GLU:N    | 1.76                     | 0.83              |
| 25:BA:2873:A:H1'   | 38:BR:6:SER:CB    | 2.09                     | 0.83              |
| 31:BG:161:THR:HG22 | 31:BG:163:ALA:H   | 1.43                     | 0.83              |
| 53:B6:28:ARG:HA    | 53:B6:32:ASN:HB2  | 1.60                     | 0.83              |
| 25:DA:1455:G:C8    | 38:DR:60:LEU:HD11 | 2.11                     | 0.83              |
| 30:DF:128:ALA:O    | 30:DF:129:PHE:HD2 | 1.61                     | 0.83              |
| 41:DU:69:CYS:SG    | 41:DU:79:PHE:HD1  | 2.01                     | 0.83              |
| 1:AA:1068:G:OP1    | 1:AA:1388:C:H5'   | 1.79                     | 0.83              |
| 25:BA:2012:G:H4'   | 43:BW:96:ILE:HD11 | 1.58                     | 0.83              |
| 30:BF:32:LEU:O     | 30:BF:32:LEU:HD23 | 1.79                     | 0.83              |
| 33:BI:101:LEU:HB3  | 33:BI:109:ILE:CD1 | 2.08                     | 0.83              |
| 48:B1:3:LYS:HG3    | 48:B1:4:VAL:H     | 1.44                     | 0.83              |
| 48:B1:12:PRO:HB3   | 48:B1:43:TYR:HD2  | 1.43                     | 0.83              |
| 24:CX:17:U:H2'     | 24:CX:18:G:H5'    | 1.60                     | 0.83              |
| 29:DE:3:GLY:HA3    | 29:DE:81:ILE:HG21 | 1.57                     | 0.83              |
| 33:DI:13:GLY:HA3   | 33:DI:17:GLN:OE1  | 1.78                     | 0.83              |
| 36:DP:90:ARG:HG2   | 36:DP:91:PHE:CD1  | 2.14                     | 0.83              |
| 1:AA:328:C:O2      | 1:AA:328:C:H2'    | 1.77                     | 0.83              |
| 23:AW:67:C:H2'     | 23:AW:68:C:C6     | 2.13                     | 0.83              |
| 25:BA:242:G:O3'    | 25:BA:243:U:C6    | 2.31                     | 0.83              |
| 25:BA:2614:A:C4'   | 25:BA:2615:U:OP1  | 2.26                     | 0.83              |
| 28:BD:223:GLY:CA   | 28:BD:231:HIS:CD2 | 2.61                     | 0.83              |
| 13:CM:3:ARG:CZ     | 13:CM:7:VAL:HG13  | 2.07                     | 0.83              |
| 1:AA:533:A:H4'     | 1:AA:534:U:OP1    | 1.77                     | 0.83              |
| 9:AI:28:VAL:HG13   | 9:AI:63:ILE:O     | 1.79                     | 0.83              |
| 12:AL:126:LYS:HE2  | 12:AL:127:GLU:H   | 1.42                     | 0.83              |
| 52:B5:41:PRO:HG2   | 52:B5:44:THR:HG21 | 1.61                     | 0.83              |
| 55:B8:31:HIS:CG    | 55:B8:32:LEU:HA   | 2.13                     | 0.83              |
| 2:CB:19:HIS:ND1    | 2:CB:20:GLU:HG2   | 1.93                     | 0.83              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 20:CT:40:ALA:HB2  | 20:CT:55:ILE:HG22 | 1.59                     | 0.83              |
| 22:CV:21:U:H5'    | 22:CV:22:A:OP2    | 1.78                     | 0.83              |
| 42:DV:34:GLU:HG3  | 42:DV:58:VAL:HG22 | 1.61                     | 0.83              |
| 13:AM:3:ARG:HG2   | 13:AM:9:ILE:HG12  | 1.60                     | 0.83              |
| 22:AV:17:C:H3'    | 22:AV:18:U:C5'    | 2.09                     | 0.83              |
| 25:BA:388:G:H5'   | 48:B1:25:LYS:HB3  | 1.58                     | 0.83              |
| 25:BA:2127:G:C6   | 25:BA:2162:G:C2   | 2.67                     | 0.83              |
| 44:BX:55:ASN:HB2  | 44:BX:80:ILE:HD12 | 1.58                     | 0.83              |
| 49:B2:13:ALA:HA   | 49:B2:16:LEU:CD1  | 2.08                     | 0.83              |
| 4:AD:128:VAL:HG12 | 4:AD:129:ASN:ND2  | 1.94                     | 0.83              |
| 9:AI:88:TYR:O     | 9:AI:89:ASN:HB2   | 1.77                     | 0.83              |
| 10:AJ:50:ILE:N    | 10:AJ:50:ILE:HD13 | 1.93                     | 0.83              |
| 22:AV:2:G:H2'     | 22:AV:3:C:C6      | 2.13                     | 0.83              |
| 30:BF:3:GLU:HB2   | 30:BF:24:LEU:HG   | 1.59                     | 0.83              |
| 10:CJ:32:ALA:H    | 10:CJ:76:ASN:HD22 | 1.24                     | 0.83              |
| 25:DA:1139:G:O2'  | 25:DA:1140:C:H5'  | 1.78                     | 0.83              |
| 25:DA:1739:U:H5'' | 25:DA:1739:U:O2   | 1.78                     | 0.83              |
| 25:DA:2701:C:H3'  | 25:DA:2702:U:C5'  | 2.07                     | 0.83              |
| 31:DG:53:LEU:HD23 | 31:DG:54:GLU:N    | 1.94                     | 0.83              |
| 25:BA:1820:U:C4'  | 25:BA:1821:A:OP2  | 2.27                     | 0.82              |
| 25:BA:2835:A:H5'  | 25:BA:2836:U:OP1  | 1.78                     | 0.82              |
| 30:BF:34:TRP:HA   | 36:BP:6:LEU:HD12  | 1.58                     | 0.82              |
| 36:BP:65:ARG:HH12 | 55:B8:15:LYS:HB2  | 1.44                     | 0.82              |
| 36:DP:79:ARG:O    | 36:DP:111:ARG:HB2 | 1.79                     | 0.82              |
| 25:BA:1251:C:H6   | 25:BA:1251:C:C5'  | 1.92                     | 0.82              |
| 1:CA:565:U:H3'    | 1:CA:566:G:H2'    | 1.58                     | 0.82              |
| 25:DA:1819:A:O4'  | 25:DA:1821:A:C5   | 2.32                     | 0.82              |
| 25:BA:32:C:O2'    | 25:BA:33:U:H5'    | 1.79                     | 0.82              |
| 31:BG:111:LEU:HB3 | 31:BG:117:PHE:HE2 | 1.43                     | 0.82              |
| 34:BN:18:ALA:HB1  | 34:BN:21:LYS:HB2  | 1.61                     | 0.82              |
| 41:BU:96:ALA:C    | 41:BU:98:LEU:H    | 1.86                     | 0.82              |
| 45:BY:39:VAL:HG12 | 45:BY:40:GLU:H    | 1.43                     | 0.82              |
| 1:CA:100:C:H2'    | 1:CA:101:A:C8     | 2.14                     | 0.82              |
| 3:CC:58:GLU:H     | 3:CC:65:ALA:HB3   | 1.44                     | 0.82              |
| 9:CI:95:LYS:HD3   | 9:CI:96:LEU:N     | 1.94                     | 0.82              |
| 2:AB:71:VAL:HA    | 2:AB:93:VAL:HG22  | 1.60                     | 0.82              |
| 25:BA:865:C:C4'   | 25:BA:866:A:OP1   | 2.27                     | 0.82              |
| 25:BA:887:A:H1'   | 25:BA:889:C:C4    | 2.13                     | 0.82              |
| 32:BH:102:ALA:HB2 | 32:BH:117:PRO:HD3 | 1.59                     | 0.82              |
| 53:B6:41:PRO:HD2  | 53:B6:46:HIS:H    | 1.45                     | 0.82              |
| 7:CG:113:GLU:HG3  | 7:CG:119:ARG:HG2  | 1.60                     | 0.82              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 19:CS:46:GLY:N     | 19:CS:62:ILE:CG2  | 2.42                     | 0.82              |
| 27:DC:49:ILE:H     | 27:DC:49:ILE:HD12 | 1.44                     | 0.82              |
| 29:DE:36:ARG:NH2   | 29:DE:88:GLY:HA3  | 1.93                     | 0.82              |
| 2:AB:204:ASN:ND2   | 2:AB:206:ASP:H    | 1.76                     | 0.82              |
| 29:BE:132:HIS:CD2  | 29:BE:135:HIS:CE1 | 2.67                     | 0.82              |
| 31:BG:4:ASP:HA     | 31:BG:8:LYS:CD    | 2.09                     | 0.82              |
| 31:BG:22:ARG:HB3   | 31:BG:22:ARG:NH1  | 1.92                     | 0.82              |
| 33:BI:77:LEU:HD12  | 33:BI:104:GLN:NE2 | 1.94                     | 0.82              |
| 47:B0:24:LYS:O     | 47:B0:25:ARG:HD3  | 1.80                     | 0.82              |
| 20:CT:53:LEU:HD13  | 20:CT:53:LEU:N    | 1.92                     | 0.82              |
| 32:DH:55:PRO:HG2   | 32:DH:61:HIS:ND1  | 1.95                     | 0.82              |
| 32:DH:124:GLU:C    | 32:DH:126:PRO:HD3 | 2.05                     | 0.82              |
| 9:AI:95:LYS:HD3    | 9:AI:96:LEU:N     | 1.94                     | 0.82              |
| 4:CD:49:ARG:HD3    | 4:CD:50:ARG:H     | 1.45                     | 0.82              |
| 5:CE:110:LEU:HD21  | 5:CE:139:LEU:HD21 | 1.61                     | 0.82              |
| 10:CJ:78:ASN:HD21  | 10:CJ:80:LYS:CB   | 1.89                     | 0.82              |
| 2:AB:87:ARG:NH2    | 2:AB:233:SER:HB2  | 1.95                     | 0.82              |
| 5:AE:103:GLY:O     | 5:AE:106:PRO:CD   | 2.25                     | 0.82              |
| 29:BE:39:PRO:O     | 29:BE:43:GLY:CA   | 2.27                     | 0.82              |
| 36:BP:79:ARG:O     | 36:BP:111:ARG:HB2 | 1.79                     | 0.82              |
| 39:BS:92:TYR:C     | 39:BS:94:TYR:H    | 1.86                     | 0.82              |
| 9:AI:48:GLU:N      | 9:AI:49:PRO:HD2   | 1.94                     | 0.82              |
| 10:AJ:50:ILE:HG21  | 10:AJ:57:LYS:HD2  | 1.62                     | 0.82              |
| 40:BT:29:ARG:CG    | 40:BT:85:LYS:CA   | 2.33                     | 0.82              |
| 41:BU:95:LEU:HD13  | 42:BV:4:ILE:CD1   | 2.09                     | 0.82              |
| 48:B1:45:ASN:HD21  | 48:B1:47:GLN:HE21 | 1.27                     | 0.82              |
| 48:B1:52:ARG:HD2   | 48:B1:53:VAL:N    | 1.94                     | 0.82              |
| 25:DA:2286:A:H61   | 53:D6:24:GLU:HB3  | 1.44                     | 0.82              |
| 40:DT:129:ARG:NE   | 40:DT:131:ALA:CB  | 2.42                     | 0.82              |
| 52:D5:32:PRO:O     | 52:D5:33:CYS:HB3  | 1.76                     | 0.82              |
| 2:AB:96:ARG:H      | 2:AB:96:ARG:HD2   | 1.45                     | 0.82              |
| 4:AD:22:LYS:HD3    | 4:AD:26:CYS:SG    | 2.20                     | 0.82              |
| 25:BA:2345:G:H1'   | 25:BA:2347:C:C6   | 2.15                     | 0.82              |
| 29:BE:36:ARG:HH22  | 29:BE:88:GLY:HA3  | 0.79                     | 0.82              |
| 12:CL:90:VAL:HG12  | 12:CL:93:LEU:H    | 1.44                     | 0.82              |
| 19:CS:45:VAL:HA    | 19:CS:62:ILE:HG13 | 1.62                     | 0.82              |
| 40:DT:33:LYS:HG2   | 40:DT:43:GLN:HB2  | 1.60                     | 0.82              |
| 31:BG:101:ILE:HG12 | 31:BG:105:LYS:HE3 | 1.60                     | 0.82              |
| 36:BP:90:ARG:HG2   | 36:BP:91:PHE:CD1  | 2.14                     | 0.82              |
| 1:CA:1189:C:OP1    | 10:CJ:51:ARG:NH2  | 2.12                     | 0.82              |
| 18:CR:86:VAL:HG12  | 18:CR:87:ARG:HD2  | 1.61                     | 0.82              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:DA:1558:A:O2'   | 25:DA:1559:G:H5''  | 1.78                     | 0.82              |
| 31:DG:94:LEU:HD23  | 31:DG:94:LEU:H     | 1.45                     | 0.82              |
| 40:DT:74:ARG:HD2   | 40:DT:76:PHE:HE2   | 1.44                     | 0.82              |
| 44:DX:35:THR:HG22  | 44:DX:37:THR:H     | 1.45                     | 0.82              |
| 5:AE:150:ARG:O     | 5:AE:153:LYS:HG2   | 1.80                     | 0.81              |
| 39:BS:89:ARG:HB3   | 39:BS:92:TYR:HB3   | 1.61                     | 0.81              |
| 12:CL:28:LYS:HE2   | 12:CL:33:ARG:HH22  | 1.45                     | 0.81              |
| 25:DA:221:A:H8     | 25:DA:221:A:OP2    | 1.61                     | 0.81              |
| 29:DE:77:ILE:HG22  | 29:DE:78:LEU:N     | 1.94                     | 0.81              |
| 55:D8:52:LYS:N     | 55:D8:53:PRO:HD2   | 1.95                     | 0.81              |
| 4:AD:11:LEU:N      | 4:AD:11:LEU:CD2    | 2.36                     | 0.81              |
| 23:AW:34:G:C5      | 24:AX:14:A:N3      | 2.47                     | 0.81              |
| 41:BU:112:ARG:HH11 | 41:BU:112:ARG:HG2  | 1.45                     | 0.81              |
| 25:DA:2700:C:C2'   | 25:DA:2701:C:H5'   | 2.09                     | 0.81              |
| 28:DD:134:ARG:HG3  | 28:DD:135:PHE:CE2  | 2.14                     | 0.81              |
| 33:DI:3:VAL:HG12   | 33:DI:38:LEU:HA    | 1.62                     | 0.81              |
| 1:AA:1529:G:H4'    | 1:AA:1530:G:OP2    | 1.79                     | 0.81              |
| 3:AC:14:ILE:HG12   | 3:AC:15:THR:H      | 1.45                     | 0.81              |
| 12:AL:47:LYS:HB2   | 12:AL:48:PRO:CD    | 2.04                     | 0.81              |
| 25:BA:2866:U:H4'   | 25:BA:2867:G:OP1   | 1.79                     | 0.81              |
| 31:BG:101:ILE:HD13 | 31:BG:102:PHE:N    | 1.95                     | 0.81              |
| 32:BH:149:ARG:HD3  | 32:BH:164:TYR:CE1  | 2.15                     | 0.81              |
| 36:BP:47:ASP:HB3   | 36:BP:48:PRO:CA    | 2.10                     | 0.81              |
| 36:BP:56:SER:O     | 36:BP:57:THR:HB    | 1.80                     | 0.81              |
| 38:BR:103:ARG:HB2  | 38:BR:109:ALA:O    | 1.80                     | 0.81              |
| 45:BY:90:LEU:HD12  | 45:BY:91:GLU:HB2   | 1.62                     | 0.81              |
| 48:B1:45:ASN:ND2   | 48:B1:47:GLN:HE21  | 1.77                     | 0.81              |
| 1:CA:1067:A:O2'    | 1:CA:1068:G:C8     | 2.31                     | 0.81              |
| 3:CC:20:SER:HB2    | 3:CC:40:ARG:NH2    | 1.93                     | 0.81              |
| 6:CF:18:GLN:O      | 6:CF:21:LEU:HB2    | 1.81                     | 0.81              |
| 20:CT:56:MET:HG2   | 20:CT:84:LEU:HD12  | 1.59                     | 0.81              |
| 30:DF:32:LEU:CD1   | 30:DF:105:VAL:HG13 | 2.10                     | 0.81              |
| 32:DH:98:LEU:HB2   | 32:DH:125:VAL:CG2  | 2.07                     | 0.81              |
| 36:DP:70:GLN:HB3   | 36:DP:72:PRO:CD    | 2.10                     | 0.81              |
| 45:DY:97:ARG:NH2   | 45:DY:98:VAL:HB    | 1.95                     | 0.81              |
| 47:D0:25:ARG:HD2   | 47:D0:29:GLN:NE2   | 1.95                     | 0.81              |
| 25:BA:1342:A:N6    | 25:BA:1397:U:H5    | 1.77                     | 0.81              |
| 5:CE:33:VAL:HG11   | 5:CE:109:ILE:HA    | 1.63                     | 0.81              |
| 10:CJ:34:VAL:HG22  | 10:CJ:74:ILE:HG22  | 1.61                     | 0.81              |
| 12:CL:79:GLU:CD    | 12:CL:79:GLU:H     | 1.88                     | 0.81              |
| 14:CN:4:LYS:HD2    | 14:CN:7:ILE:HD11   | 1.59                     | 0.81              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 29:DE:116:VAL:HG21 | 29:DE:122:PHE:CD2 | 2.15                     | 0.81              |
| 23:AW:17:C:H41     | 25:BA:2181:G:H5'  | 1.45                     | 0.81              |
| 25:BA:1647:G:H4'   | 25:BA:1648:C:O5'  | 1.79                     | 0.81              |
| 25:BA:2286:A:H4'   | 25:BA:2287:A:O4'  | 1.80                     | 0.81              |
| 25:BA:2457:U:C2'   | 25:BA:2458:G:H5'  | 2.10                     | 0.81              |
| 36:DP:47:ASP:HB3   | 36:DP:48:PRO:CA   | 2.10                     | 0.81              |
| 1:AA:815:A:C2      | 1:AA:1529:G:C4    | 2.69                     | 0.81              |
| 1:AA:1279:A:H2'    | 1:AA:1282:C:N4    | 1.94                     | 0.81              |
| 2:AB:21:ARG:O      | 2:AB:22:LYS:HB2   | 1.81                     | 0.81              |
| 25:BA:2171:A:C4'   | 25:BA:2172:U:OP1  | 2.27                     | 0.81              |
| 28:BD:264:LYS:HD3  | 28:BD:266:SER:HB2 | 1.63                     | 0.81              |
| 39:BS:34:HIS:CE1   | 39:BS:54:LEU:CB   | 2.28                     | 0.81              |
| 22:CV:54:G:N3      | 22:CV:55:U:C5     | 2.49                     | 0.81              |
| 1:AA:677:U:H3      | 1:AA:713:G:H22    | 1.25                     | 0.81              |
| 1:AA:1054:C:O2     | 1:AA:1054:C:H2'   | 1.81                     | 0.81              |
| 18:AR:36:ASN:ND2   | 18:AR:39:VAL:HG21 | 1.96                     | 0.81              |
| 25:BA:2317:C:C2'   | 25:BA:2318:G:H5'  | 2.09                     | 0.81              |
| 33:BI:49:ALA:O     | 33:BI:52:ARG:HG3  | 1.80                     | 0.81              |
| 36:BP:112:LEU:HD22 | 36:BP:113:LYS:N   | 1.95                     | 0.81              |
| 37:BQ:60:ARG:HA    | 46:BZ:178:GLU:O   | 1.81                     | 0.81              |
| 30:DF:7:TYR:HB3    | 30:DF:21:ALA:CB   | 2.11                     | 0.81              |
| 30:DF:31:HIS:HB2   | 36:DP:9:ASN:HD21  | 1.45                     | 0.81              |
| 36:DP:52:GLU:OE1   | 36:DP:55:ARG:CD   | 2.29                     | 0.81              |
| 2:AB:61:LEU:CD2    | 2:AB:68:ILE:HD11  | 2.09                     | 0.81              |
| 9:CI:16:ARG:O      | 9:CI:63:ILE:HG23  | 1.80                     | 0.81              |
| 9:CI:78:LYS:HE3    | 9:CI:101:PHE:CE2  | 2.14                     | 0.81              |
| 23:CY:28:G:H2'     | 23:CY:29:G:H8     | 1.45                     | 0.81              |
| 25:DA:806:C:OP2    | 36:DP:41:ARG:NH2  | 2.14                     | 0.81              |
| 28:DD:25:THR:HG22  | 28:DD:26:LYS:H    | 1.45                     | 0.81              |
| 40:DT:129:ARG:CD   | 40:DT:131:ALA:HB2 | 2.09                     | 0.81              |
| 5:AE:76:ILE:CD1    | 5:AE:142:LEU:HD11 | 2.10                     | 0.81              |
| 31:BG:85:GLY:O     | 31:BG:87:PRO:HD2  | 1.79                     | 0.81              |
| 32:BH:109:PHE:CE1  | 32:BH:152:ARG:NH2 | 2.49                     | 0.81              |
| 1:CA:274:A:O2'     | 1:CA:275:G:C8     | 2.31                     | 0.81              |
| 2:CB:69:LEU:HD12   | 2:CB:70:PHE:N     | 1.94                     | 0.81              |
| 9:CI:16:ARG:HB2    | 9:CI:64:THR:HG23  | 1.62                     | 0.81              |
| 16:CP:28:ARG:HG2   | 16:CP:29:ASP:OD2  | 1.80                     | 0.81              |
| 25:DA:1697:G:H3'   | 25:DA:1698:A:H5'' | 1.62                     | 0.81              |
| 40:DT:80:SER:CB    | 40:DT:81:PRO:CD   | 2.59                     | 0.81              |
| 42:DV:98:GLU:C     | 42:DV:99:ILE:HD13 | 2.06                     | 0.81              |
| 45:DY:84:ARG:HH12  | 45:DY:97:ARG:HA   | 1.44                     | 0.81              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:BA:587:C:H4'   | 25:BA:588:U:OP2    | 1.80                     | 0.81              |
| 31:BG:72:ARG:HH11 | 31:BG:86:MET:HB2   | 1.46                     | 0.81              |
| 33:BI:53:ALA:O    | 33:BI:57:ARG:HB2   | 1.81                     | 0.81              |
| 33:BI:77:LEU:HD21 | 33:BI:101:LEU:HD13 | 1.61                     | 0.81              |
| 1:CA:235:C:H5'    | 17:CQ:70:ARG:HG2   | 1.63                     | 0.81              |
| 25:DA:1378:A:H4'  | 25:DA:1379:A:OP1   | 1.81                     | 0.81              |
| 32:DH:4:ILE:HG13  | 32:DH:6:ARG:CZ     | 2.10                     | 0.81              |
| 42:DV:15:GLU:HG3  | 42:DV:16:PRO:HD2   | 1.60                     | 0.81              |
| 42:DV:16:PRO:HB3  | 42:DV:99:ILE:HD11  | 1.63                     | 0.81              |
| 45:DY:47:LYS:HG2  | 45:DY:60:PHE:HE1   | 1.45                     | 0.81              |
| 25:BA:1270:C:N4   | 25:BA:1648:C:H41   | 1.78                     | 0.80              |
| 29:BE:49:LEU:HD13 | 29:BE:81:ILE:HG13  | 1.59                     | 0.80              |
| 32:BH:27:LYS:HG2  | 32:BH:32:GLU:HB2   | 1.60                     | 0.80              |
| 32:BH:123:PHE:HA  | 32:BH:133:VAL:HG22 | 1.60                     | 0.80              |
| 36:BP:19:VAL:HG22 | 36:BP:20:GLY:N     | 1.96                     | 0.80              |
| 38:BR:103:ARG:CB  | 38:BR:109:ALA:O    | 2.28                     | 0.80              |
| 45:BY:36:ALA:HB2  | 45:BY:67:LEU:O     | 1.79                     | 0.80              |
| 2:CB:174:VAL:HG13 | 2:CB:184:VAL:HG11  | 1.62                     | 0.80              |
| 20:CT:43:LEU:HD11 | 20:CT:51:GLU:CG    | 2.10                     | 0.80              |
| 25:DA:530:G:C2    | 25:DA:2021:C:O2'   | 2.34                     | 0.80              |
| 30:DF:128:ALA:O   | 30:DF:129:PHE:HB2  | 1.81                     | 0.80              |
| 39:DS:106:ARG:C   | 39:DS:110:LEU:HD11 | 2.06                     | 0.80              |
| 45:DY:76:CYS:SG   | 45:DY:77:PRO:CD    | 2.66                     | 0.80              |
| 53:D6:46:HIS:HD2  | 53:D6:47:THR:HA    | 1.44                     | 0.80              |
| 1:AA:1157:A:H4'   | 1:AA:1158:C:O5'    | 1.80                     | 0.80              |
| 1:AA:1504:G:OP2   | 1:AA:1507:A:H4'    | 1.80                     | 0.80              |
| 10:AJ:4:ILE:HB    | 10:AJ:74:ILE:HD11  | 1.62                     | 0.80              |
| 25:BA:725:G:H5''  | 25:BA:726:G:OP2    | 1.80                     | 0.80              |
| 31:BG:85:GLY:O    | 31:BG:87:PRO:CD    | 2.30                     | 0.80              |
| 42:BV:34:GLU:O    | 42:BV:36:PRO:HD3   | 1.81                     | 0.80              |
| 10:CJ:30:SER:HB2  | 10:CJ:80:LYS:HB3   | 1.63                     | 0.80              |
| 13:CM:14:ARG:HA   | 13:CM:44:ARG:HA    | 1.61                     | 0.80              |
| 23:CW:57:G:H2'    | 23:CW:58:A:H5'     | 1.62                     | 0.80              |
| 32:DH:152:ARG:HG3 | 32:DH:153:LYS:CE   | 2.10                     | 0.80              |
| 41:DU:102:GLU:OE2 | 42:DV:2:PHE:CE2    | 2.34                     | 0.80              |
| 4:AD:101:LEU:HD23 | 4:AD:121:VAL:HG13  | 1.62                     | 0.80              |
| 25:BA:887:A:C1'   | 25:BA:889:C:N4     | 2.43                     | 0.80              |
| 44:BX:44:GLU:HG3  | 44:BX:51:VAL:HG23  | 1.63                     | 0.80              |
| 3:CC:140:ARG:HH11 | 3:CC:140:ARG:HG3   | 1.46                     | 0.80              |
| 1:AA:1281:U:H4'   | 1:AA:1282:C:OP1    | 1.79                     | 0.80              |
| 3:AC:58:GLU:H     | 3:AC:65:ALA:HB3    | 1.47                     | 0.80              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 16:AP:49:LEU:HD12 | 16:AP:50:LYS:N     | 1.95                     | 0.80              |
| 20:AT:81:LYS:O    | 20:AT:85:MET:CG    | 2.30                     | 0.80              |
| 25:BA:1037:G:H1   | 25:BA:1118:C:H42   | 1.29                     | 0.80              |
| 31:BG:72:ARG:HD3  | 31:BG:86:MET:CB    | 2.10                     | 0.80              |
| 36:BP:71:VAL:N    | 36:BP:72:PRO:CD    | 2.43                     | 0.80              |
| 16:CP:82:GLN:N    | 16:CP:82:GLN:HE21  | 1.78                     | 0.80              |
| 21:CU:6:ARG:HE    | 21:CU:15:ARG:NH2   | 1.78                     | 0.80              |
| 25:DA:752:A:H4'   | 25:DA:753:C:O5'    | 1.81                     | 0.80              |
| 25:DA:753:C:OP2   | 25:DA:753:C:C5     | 2.33                     | 0.80              |
| 25:DA:2849:U:O4   | 40:DT:23:ARG:NH2   | 2.14                     | 0.80              |
| 55:D8:36:LYS:HB3  | 55:D8:40:GLU:HG3   | 1.62                     | 0.80              |
| 29:BE:4:ILE:HG12  | 29:BE:28:ALA:HB1   | 1.62                     | 0.80              |
| 34:BN:62:VAL:O    | 34:BN:62:VAL:CG1   | 2.30                     | 0.80              |
| 1:CA:1226:C:O2'   | 1:CA:1227:A:C5'    | 2.30                     | 0.80              |
| 10:AJ:63:PHE:HA   | 14:AN:59:ALA:HB2   | 1.64                     | 0.80              |
| 13:AM:66:LEU:H    | 13:AM:70:LEU:HB2   | 1.46                     | 0.80              |
| 13:CM:108:ARG:HD2 | 13:CM:108:ARG:H    | 1.46                     | 0.80              |
| 22:CV:53:G:O2'    | 22:CV:54:G:C5'     | 2.30                     | 0.80              |
| 33:DI:64:GLU:HG3  | 33:DI:67:ARG:NH2   | 1.97                     | 0.80              |
| 44:DX:12:VAL:CG2  | 44:DX:17:ALA:HB2   | 2.12                     | 0.80              |
| 7:AG:15:ASP:O     | 7:AG:19:GLY:CA     | 2.29                     | 0.80              |
| 10:AJ:48:THR:HA   | 10:AJ:62:HIS:HB3   | 1.62                     | 0.80              |
| 20:AT:84:LEU:HD12 | 20:AT:84:LEU:C     | 2.07                     | 0.80              |
| 36:BP:124:LYS:NZ  | 36:BP:143:GLY:HA3  | 1.96                     | 0.80              |
| 25:DA:887:A:H1'   | 25:DA:889:C:C4     | 2.16                     | 0.80              |
| 36:DP:75:ILE:H    | 36:DP:75:ILE:CD1   | 1.82                     | 0.80              |
| 1:AA:1300:G:O2'   | 1:AA:1301:U:C5'    | 2.29                     | 0.80              |
| 22:AV:55:U:C2'    | 22:AV:56:U:H5'     | 2.11                     | 0.80              |
| 25:BA:2303:G:O2'  | 31:BG:132:ASN:ND2  | 2.15                     | 0.80              |
| 36:BP:83:VAL:HG12 | 36:BP:112:LEU:HD21 | 1.64                     | 0.80              |
| 37:BQ:56:ARG:HA   | 37:BQ:56:ARG:CZ    | 2.12                     | 0.80              |
| 50:B3:8:LEU:HG    | 50:B3:23:LEU:HD21  | 1.63                     | 0.80              |
| 23:CW:36:A:H2'    | 23:CW:37:A:C5'     | 2.11                     | 0.80              |
| 25:DA:1698:A:H1'  | 25:DA:1700:A:OP2   | 1.82                     | 0.80              |
| 26:DB:42:C:O3'    | 31:DG:67:LYS:HE3   | 1.82                     | 0.80              |
| 32:DH:126:PRO:HG2 | 32:DH:130:ARG:HH11 | 1.46                     | 0.80              |
| 40:DT:28:VAL:HG22 | 40:DT:47:GLY:N     | 1.96                     | 0.80              |
| 53:D6:41:PRO:CD   | 53:D6:46:HIS:N     | 2.44                     | 0.80              |
| 10:AJ:37:PRO:HA   | 10:AJ:72:VAL:CG2   | 2.10                     | 0.80              |
| 25:BA:2171:A:O2'  | 25:BA:2172:U:C5'   | 2.29                     | 0.80              |
| 25:BA:2477:C:N3   | 56:B9:4:ARG:NH1    | 2.29                     | 0.80              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:BG:85:GLY:O     | 31:BG:87:PRO:CG    | 2.30                     | 0.80              |
| 39:BS:89:ARG:O     | 39:BS:90:GLY:O     | 2.00                     | 0.80              |
| 7:CG:14:PRO:HG3    | 7:CG:21:VAL:HG13   | 1.64                     | 0.80              |
| 16:CP:20:VAL:HG21  | 16:CP:32:TYR:CD1   | 2.17                     | 0.80              |
| 20:CT:24:LEU:HD22  | 20:CT:24:LEU:O     | 1.82                     | 0.80              |
| 36:DP:124:LYS:NZ   | 36:DP:143:GLY:HA3  | 1.96                     | 0.80              |
| 37:DQ:34:LEU:HD11  | 37:DQ:129:THR:HB   | 1.64                     | 0.80              |
| 1:AA:1275:A:H2'    | 1:AA:1276:G:C8     | 2.15                     | 0.80              |
| 25:BA:1251:C:O2'   | 25:BA:1252:G:H5''  | 1.81                     | 0.80              |
| 25:BA:2126:A:O2'   | 25:BA:2127:G:C5'   | 2.30                     | 0.80              |
| 34:BN:62:VAL:HG13  | 34:BN:66:LYS:HB2   | 1.64                     | 0.80              |
| 45:BY:50:ARG:HG3   | 45:BY:58:GLY:HA2   | 1.64                     | 0.80              |
| 1:CA:1065:U:H4'    | 1:CA:1066:C:O5'    | 1.79                     | 0.80              |
| 18:CR:76:LEU:HD23  | 18:CR:76:LEU:N     | 1.97                     | 0.80              |
| 33:DI:88:ILE:HG12  | 33:DI:122:GLU:H    | 1.47                     | 0.80              |
| 1:AA:1226:C:N4     | 13:AM:104:ARG:HB2  | 1.96                     | 0.79              |
| 2:AB:76:GLN:O      | 2:AB:208:ILE:HD11  | 1.81                     | 0.79              |
| 25:BA:271(D):G:H1  | 25:BA:271(T):C:H42 | 1.30                     | 0.79              |
| 25:BA:2473:U:O2    | 25:BA:2473:U:H2'   | 1.82                     | 0.79              |
| 29:BE:47:VAL:HG21  | 29:BE:86:PRO:HD3   | 1.61                     | 0.79              |
| 30:BF:51:THR:CG2   | 30:BF:92:PRO:O     | 2.30                     | 0.79              |
| 30:BF:64:ILE:O     | 30:BF:65:TRP:HD1   | 1.65                     | 0.79              |
| 32:BH:151:ILE:N    | 32:BH:151:ILE:HD13 | 1.96                     | 0.79              |
| 38:BR:11:ASN:O     | 38:BR:12:ARG:CG    | 2.30                     | 0.79              |
| 43:BW:51:LEU:C     | 43:BW:51:LEU:CD1   | 2.55                     | 0.79              |
| 1:CA:1065:U:C1'    | 1:CA:1066:C:OP2    | 2.30                     | 0.79              |
| 1:CA:1502:A:H2     | 1:CA:1505:G:H22    | 0.84                     | 0.79              |
| 3:CC:165:THR:O     | 3:CC:165:THR:CG2   | 2.30                     | 0.79              |
| 11:CK:73:MET:SD    | 11:CK:103:LEU:HD23 | 2.23                     | 0.79              |
| 13:CM:84:ILE:HD13  | 19:CS:65:ASN:HB3   | 1.62                     | 0.79              |
| 22:CV:29:C:O2'     | 22:CV:30:G:C5'     | 2.30                     | 0.79              |
| 22:CV:53:G:C2'     | 22:CV:54:G:O5'     | 2.30                     | 0.79              |
| 25:DA:222:A:H4'    | 25:DA:223:A:OP1    | 1.82                     | 0.79              |
| 25:DA:1963:U:H3'   | 25:DA:1963:U:O2    | 1.82                     | 0.79              |
| 31:DG:60:LEU:O     | 31:DG:64:THR:HG22  | 1.82                     | 0.79              |
| 36:DP:112:LEU:HD22 | 36:DP:113:LYS:N    | 1.95                     | 0.79              |
| 37:DQ:30:GLY:HA2   | 37:DQ:107:ALA:HB2  | 1.64                     | 0.79              |
| 38:DR:51:LEU:HD23  | 38:DR:66:VAL:HG13  | 1.64                     | 0.79              |
| 40:DT:89:VAL:HG11  | 40:DT:91:ARG:NE    | 1.96                     | 0.79              |
| 41:DU:104:GLN:NE2  | 41:DU:105:VAL:N    | 2.30                     | 0.79              |
| 1:AA:1226:C:O2'    | 1:AA:1227:A:C5'    | 2.30                     | 0.79              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 25:BA:676:A:H8     | 25:BA:2069:G:H21  | 1.27                     | 0.79              |
| 25:BA:1342:A:C6    | 25:BA:1397:U:C6   | 2.70                     | 0.79              |
| 25:BA:1453:U:C4'   | 25:BA:1455:G:P    | 2.70                     | 0.79              |
| 32:BH:109:PHE:HE1  | 32:BH:152:ARG:CZ  | 1.94                     | 0.79              |
| 41:BU:49:HIS:HA    | 41:BU:52:ARG:HB2  | 1.65                     | 0.79              |
| 2:CB:71:VAL:HA     | 2:CB:93:VAL:HG22  | 1.64                     | 0.79              |
| 3:AC:16:ARG:HB2    | 3:AC:16:ARG:NH1   | 1.97                     | 0.79              |
| 14:AN:27:CYS:SG    | 59:AN:101:ZN:ZN   | 1.70                     | 0.79              |
| 15:AO:16:ALA:HB1   | 15:AO:21:ASP:HB3  | 1.64                     | 0.79              |
| 44:BX:64:LYS:HZ3   | 44:BX:73:ARG:NE   | 1.76                     | 0.79              |
| 2:CB:235:SER:HG    | 2:CB:236:TYR:HD1  | 1.29                     | 0.79              |
| 9:CI:58:HIS:HB3    | 9:CI:59:PHE:CD1   | 2.17                     | 0.79              |
| 28:DD:134:ARG:HG3  | 28:DD:135:PHE:CD2 | 2.16                     | 0.79              |
| 40:DT:81:PRO:O     | 40:DT:82:LEU:CG   | 2.30                     | 0.79              |
| 28:BD:43:ARG:HB3   | 28:BD:54:ARG:HB2  | 1.63                     | 0.79              |
| 28:BD:206:LEU:HD22 | 28:BD:211:ARG:HG2 | 1.65                     | 0.79              |
| 30:BF:64:ILE:HG22  | 30:BF:65:TRP:CD1  | 2.17                     | 0.79              |
| 11:CK:59:TYR:CZ    | 11:CK:63:LEU:HD12 | 2.18                     | 0.79              |
| 28:DD:94:LEU:HD22  | 28:DD:95:LEU:N    | 1.98                     | 0.79              |
| 31:DG:145:THR:O    | 31:DG:146:TYR:HB3 | 1.81                     | 0.79              |
| 33:DI:128:LEU:HD13 | 33:DI:129:THR:N   | 1.97                     | 0.79              |
| 1:AA:792:A:C8      | 1:AA:794:A:N6     | 2.51                     | 0.79              |
| 2:AB:96:ARG:HH11   | 2:AB:148:TYR:HE1  | 1.28                     | 0.79              |
| 22:AV:35:C:C2'     | 22:AV:36:A:O5'    | 2.30                     | 0.79              |
| 25:BA:752:A:C5     | 25:BA:1781:C:O4'  | 2.35                     | 0.79              |
| 29:BE:152:LYS:HB3  | 34:BN:78:TYR:CD2  | 2.17                     | 0.79              |
| 9:CI:58:HIS:CB     | 9:CI:59:PHE:CE1   | 2.64                     | 0.79              |
| 16:CP:5:ARG:HB3    | 16:CP:67:THR:OG1  | 1.81                     | 0.79              |
| 22:CV:53:G:H2'     | 22:CV:54:G:O5'    | 1.82                     | 0.79              |
| 25:DA:1558:A:O2'   | 25:DA:1559:G:C5'  | 2.30                     | 0.79              |
| 40:DT:129:ARG:CD   | 40:DT:129:ARG:O   | 2.30                     | 0.79              |
| 5:AE:91:LEU:HD12   | 5:AE:120:THR:CG2  | 2.13                     | 0.79              |
| 31:BG:44:GLY:H     | 31:BG:88:ILE:CD1  | 1.96                     | 0.79              |
| 34:BN:67:LEU:H     | 34:BN:67:LEU:HD12 | 1.48                     | 0.79              |
| 42:BV:49:THR:HB    | 42:BV:50:PRO:HD2  | 1.65                     | 0.79              |
| 25:BA:2259:G:C8    | 25:BA:2427:C:C5   | 2.70                     | 0.79              |
| 25:BA:2344:U:H4'   | 25:BA:2345:G:OP1  | 1.83                     | 0.79              |
| 1:CA:79:G:C4'      | 1:CA:80:G:OP1     | 2.30                     | 0.79              |
| 1:CA:1456:G:N2     | 1:CA:1457:G:N7    | 2.30                     | 0.79              |
| 7:CG:10:ARG:HH11   | 7:CG:10:ARG:CG    | 1.95                     | 0.79              |
| 25:DA:2850:A:OP2   | 25:DA:2866:U:H5   | 1.66                     | 0.79              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 29:DE:92:THR:O     | 29:DE:95:ILE:HD13  | 1.81                     | 0.79              |
| 32:DH:98:LEU:HD12  | 32:DH:102:ALA:O    | 1.82                     | 0.79              |
| 33:DI:40:THR:HG22  | 33:DI:42:SER:H     | 1.48                     | 0.79              |
| 41:DU:92:ARG:CD    | 42:DV:11:GLN:CD    | 2.52                     | 0.79              |
| 3:AC:175:LEU:HD12  | 3:AC:175:LEU:H     | 1.45                     | 0.79              |
| 8:AH:10:LEU:HD23   | 8:AH:83:ILE:HG12   | 1.64                     | 0.79              |
| 15:AO:82:ILE:HG12  | 15:AO:87:ILE:HB    | 1.65                     | 0.79              |
| 24:AX:13:A:H2      | 24:AX:14:A:H3'     | 1.48                     | 0.79              |
| 14:CN:3:ARG:HG2    | 14:CN:3:ARG:O      | 1.81                     | 0.79              |
| 32:DH:152:ARG:O    | 32:DH:153:LYS:HD2  | 1.83                     | 0.79              |
| 38:DR:24:GLN:OE1   | 38:DR:36:THR:HG21  | 1.83                     | 0.79              |
| 1:AA:1279:A:C2'    | 1:AA:1282:C:H41    | 1.94                     | 0.79              |
| 1:AA:1285:A:C1'    | 1:AA:1286:A:OP2    | 2.30                     | 0.79              |
| 8:AH:64:LYS:HB3    | 8:AH:79:VAL:HG21   | 1.63                     | 0.79              |
| 13:AM:83:ASP:C     | 13:AM:85:GLY:H     | 1.89                     | 0.79              |
| 25:BA:1301:A:C2'   | 25:BA:1302:A:H5''  | 2.13                     | 0.79              |
| 31:BG:172:LEU:O    | 31:BG:176:LEU:HD12 | 1.83                     | 0.79              |
| 33:BI:72:LEU:CD1   | 33:BI:138:ILE:HB   | 2.09                     | 0.79              |
| 11:CK:20:TYR:HB2   | 11:CK:31:THR:CG2   | 2.13                     | 0.79              |
| 25:DA:75:G:H4'     | 49:D2:55:ARG:HH11  | 1.47                     | 0.79              |
| 25:DA:483:A:H4'    | 45:DY:49:VAL:HA    | 1.63                     | 0.79              |
| 39:DS:5:THR:OG1    | 39:DS:8:GLU:HG3    | 1.83                     | 0.79              |
| 47:D0:41:ARG:H     | 47:D0:41:ARG:HD2   | 1.48                     | 0.79              |
| 1:AA:1279:A:H3'    | 1:AA:1279:A:N3     | 1.97                     | 0.79              |
| 9:AI:58:HIS:HB2    | 9:AI:59:PHE:CE1    | 2.18                     | 0.79              |
| 14:AN:45:ARG:HH11  | 14:AN:45:ARG:HG3   | 1.48                     | 0.79              |
| 17:AQ:22:LEU:HD13  | 17:AQ:41:LYS:HG2   | 1.63                     | 0.79              |
| 19:AS:9:VAL:HG11   | 19:AS:11:VAL:HG11  | 1.64                     | 0.79              |
| 25:BA:559:G:H22    | 41:BU:49:HIS:HE1   | 1.31                     | 0.79              |
| 25:BA:1251:C:H5'   | 25:BA:1251:C:C6    | 2.16                     | 0.79              |
| 33:BI:48:GLU:O     | 33:BI:51:ILE:HB    | 1.82                     | 0.79              |
| 39:BS:17:ARG:HA    | 39:BS:20:ARG:HH12  | 1.47                     | 0.79              |
| 40:BT:29:ARG:HA    | 40:BT:29:ARG:CZ    | 2.12                     | 0.79              |
| 2:CB:16:HIS:CE1    | 2:CB:213:LEU:HD13  | 2.17                     | 0.79              |
| 8:CH:91:ARG:HH11   | 8:CH:91:ARG:CG     | 1.95                     | 0.79              |
| 13:CM:57:ARG:HH21  | 51:D4:34:GLU:CG    | 1.91                     | 0.79              |
| 28:DD:131:LEU:HD12 | 28:DD:131:LEU:N    | 1.96                     | 0.79              |
| 36:DP:83:VAL:HG12  | 36:DP:112:LEU:HD21 | 1.64                     | 0.79              |
| 37:DQ:134:ARG:HH21 | 46:DZ:122:ARG:NH2  | 1.79                     | 0.79              |
| 42:DV:35:LEU:HB2   | 42:DV:37:VAL:CG2   | 2.13                     | 0.79              |
| 5:AE:12:LEU:HD22   | 5:AE:13:ILE:H      | 1.48                     | 0.78              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 22:AV:53:G:C2'    | 22:AV:54:G:O5'     | 2.30                     | 0.78              |
| 19:CS:32:LYS:HA   | 19:CS:50:ALA:HB3   | 1.65                     | 0.78              |
| 25:DA:483:A:H4'   | 45:DY:49:VAL:HG13  | 1.64                     | 0.78              |
| 25:DA:767:U:O2'   | 25:DA:768:G:H5'    | 1.83                     | 0.78              |
| 33:DI:61:ARG:HA   | 33:DI:61:ARG:NE    | 1.97                     | 0.78              |
| 33:DI:99:GLU:HG2  | 33:DI:103:ARG:NH2  | 1.98                     | 0.78              |
| 55:D8:4:MET:SD    | 55:D8:61:LEU:HD22  | 2.23                     | 0.78              |
| 12:AL:18:VAL:HG23 | 12:AL:19:ARG:H     | 1.49                     | 0.78              |
| 12:AL:64:TYR:O    | 12:AL:65:GLU:HB2   | 1.82                     | 0.78              |
| 19:AS:6:LYS:HD3   | 19:AS:7:LYS:HE3    | 1.65                     | 0.78              |
| 25:BA:241:A:C4'   | 25:BA:242:G:OP1    | 2.30                     | 0.78              |
| 25:BA:448:U:C1'   | 30:BF:84:VAL:CG1   | 2.61                     | 0.78              |
| 25:BA:2198:A:C4'  | 25:BA:2199:A:OP1   | 2.30                     | 0.78              |
| 27:BC:68:LEU:HD11 | 27:BC:179:SER:HA   | 1.65                     | 0.78              |
| 29:BE:40:GLU:CD   | 29:BE:40:GLU:H     | 1.89                     | 0.78              |
| 31:BG:2:PRO:HG2   | 51:B4:51:TYR:CE2   | 2.17                     | 0.78              |
| 1:CA:376:G:H5''   | 16:CP:5:ARG:HD2    | 1.63                     | 0.78              |
| 1:CA:913:A:O2'    | 1:CA:914:A:C5'     | 2.30                     | 0.78              |
| 22:CV:18:U:C4'    | 22:CV:19:G:OP2     | 2.30                     | 0.78              |
| 6:AF:1:MET:HE1    | 6:AF:68:PRO:HB3    | 1.66                     | 0.78              |
| 20:AT:81:LYS:O    | 20:AT:85:MET:HG3   | 1.83                     | 0.78              |
| 25:BA:240:G:C2    | 25:BA:241:A:N6     | 2.51                     | 0.78              |
| 25:BA:1396:U:O2   | 25:BA:1396:U:H3'   | 1.82                     | 0.78              |
| 25:BA:2172:U:H4'  | 25:BA:2173:A:OP2   | 1.80                     | 0.78              |
| 40:BT:31:SER:CB   | 40:BT:43:GLN:H     | 1.96                     | 0.78              |
| 10:CJ:45:ARG:HH11 | 10:CJ:45:ARG:HG3   | 1.47                     | 0.78              |
| 25:DA:2701:C:C3'  | 25:DA:2702:U:H5''  | 2.10                     | 0.78              |
| 29:DE:77:ILE:CG2  | 29:DE:78:LEU:H     | 1.94                     | 0.78              |
| 29:DE:101:ARG:HD3 | 29:DE:169:ASN:HD21 | 1.47                     | 0.78              |
| 1:AA:407:G:H1     | 1:AA:435:C:H42     | 1.32                     | 0.78              |
| 2:AB:165:VAL:HG23 | 2:AB:166:ASP:H     | 1.49                     | 0.78              |
| 11:AK:32:ILE:HD12 | 11:AK:72:ALA:HB2   | 1.65                     | 0.78              |
| 22:AV:35:C:H2'    | 22:AV:36:A:O5'     | 1.82                     | 0.78              |
| 28:BD:24:ILE:HG23 | 28:BD:25:THR:H     | 1.47                     | 0.78              |
| 39:BS:97:ARG:CZ   | 39:BS:98:VAL:HA    | 2.13                     | 0.78              |
| 40:BT:31:SER:HB3  | 40:BT:43:GLN:O     | 1.83                     | 0.78              |
| 55:B8:6:THR:CG2   | 55:B8:63:PRO:HD3   | 2.13                     | 0.78              |
| 3:CC:70:VAL:HG12  | 3:CC:71:ALA:H      | 1.48                     | 0.78              |
| 5:CE:110:LEU:HD12 | 5:CE:118:ILE:HG21  | 1.65                     | 0.78              |
| 9:CI:96:LEU:HG    | 9:CI:102:LEU:HB2   | 1.66                     | 0.78              |
| 40:DT:106:SER:HA  | 40:DT:110:ILE:HG13 | 1.64                     | 0.78              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 46:DZ:134:PRO:HG2   | 46:DZ:161:VAL:HG21 | 1.65                     | 0.78              |
| 50:D3:48:GLU:O      | 50:D3:51:ALA:HB2   | 1.84                     | 0.78              |
| 10:AJ:50:ILE:HG12   | 14:AN:41:ARG:CD    | 2.13                     | 0.78              |
| 25:BA:242:G:C5      | 55:B8:5:LYS:HG2    | 2.17                     | 0.78              |
| 25:BA:1452:A:C4'    | 25:BA:1453:U:OP2   | 2.30                     | 0.78              |
| 28:BD:130:ALA:C     | 28:BD:131:LEU:HD12 | 2.09                     | 0.78              |
| 41:BU:91:ASP:C      | 41:BU:92:ARG:HD3   | 2.08                     | 0.78              |
| 5:CE:150:ARG:HH11   | 5:CE:150:ARG:HG3   | 1.46                     | 0.78              |
| 8:CH:34:GLU:HB3     | 8:CH:118:VAL:HG21  | 1.66                     | 0.78              |
| 34:DN:23:LEU:HB3    | 34:DN:60:ILE:HG21  | 1.64                     | 0.78              |
| 40:DT:81:PRO:O      | 40:DT:82:LEU:CD1   | 2.30                     | 0.78              |
| 53:D6:47:THR:HB     | 53:D6:49:HIS:HE1   | 1.43                     | 0.78              |
| 1:AA:1299:A:C8      | 1:AA:1301:U:H1'    | 2.19                     | 0.78              |
| 29:BE:30:PRO:O      | 29:BE:32:PRO:HD3   | 1.84                     | 0.78              |
| 29:BE:68:ALA:C      | 29:BE:70:ALA:H     | 1.91                     | 0.78              |
| 5:CE:105:VAL:N      | 5:CE:106:PRO:CD    | 2.46                     | 0.78              |
| 20:CT:40:ALA:HB2    | 20:CT:55:ILE:HG21  | 1.63                     | 0.78              |
| 33:DI:74:ASN:HD22   | 33:DI:74:ASN:H     | 1.31                     | 0.78              |
| 41:DU:112:ARG:HH11  | 41:DU:112:ARG:HG2  | 1.49                     | 0.78              |
| 1:AA:243:A:N6       | 1:AA:281:G:N3      | 2.31                     | 0.78              |
| 1:AA:1158:C:O2      | 1:AA:1158:C:C3'    | 2.31                     | 0.78              |
| 28:BD:24:ILE:HG12   | 28:BD:25:THR:N     | 1.98                     | 0.78              |
| 37:DQ:110:THR:HG23  | 37:DQ:113:GLN:OE1  | 1.83                     | 0.78              |
| 3:AC:6:HIS:ND1      | 14:AN:49:HIS:HB3   | 1.99                     | 0.78              |
| 25:BA:1142(A):A:H4' | 34:BN:25:ARG:HH22  | 1.48                     | 0.78              |
| 25:BA:1452:A:C5'    | 25:BA:1453:U:OP2   | 2.31                     | 0.78              |
| 28:BD:43:ARG:NH1    | 28:BD:44:ASN:HD21  | 1.82                     | 0.78              |
| 43:BW:5:ALA:C       | 43:BW:6:ILE:HG13   | 2.06                     | 0.78              |
| 46:BZ:74:VAL:HG13   | 46:BZ:86:VAL:HG13  | 1.64                     | 0.78              |
| 52:B5:56:LYS:H      | 52:B5:56:LYS:HD2   | 1.47                     | 0.78              |
| 33:DI:11:ASN:O      | 33:DI:12:LEU:HB2   | 1.82                     | 0.78              |
| 33:DI:133:HIS:HB2   | 33:DI:134:PRO:HD2  | 1.66                     | 0.78              |
| 38:DR:56:LYS:HE2    | 38:DR:94:TYR:CE2   | 2.19                     | 0.78              |
| 1:AA:1108:G:H5'     | 3:AC:176:HIS:HD1   | 1.48                     | 0.78              |
| 2:AB:75:LYS:HD3     | 2:AB:75:LYS:C      | 2.07                     | 0.78              |
| 36:BP:70:GLN:HB3    | 36:BP:72:PRO:CD    | 2.14                     | 0.78              |
| 40:BT:29:ARG:HG2    | 40:BT:85:LYS:C     | 2.09                     | 0.78              |
| 41:BU:14:HIS:CD2    | 41:BU:32:PHE:CD1   | 2.71                     | 0.78              |
| 53:B6:19:ARG:H      | 53:B6:19:ARG:HD2   | 1.48                     | 0.78              |
| 1:CA:748:C:H4'      | 1:CA:749:C:O5'     | 1.81                     | 0.78              |
| 2:CB:141:GLU:O      | 2:CB:145:LEU:HB2   | 1.84                     | 0.78              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:CV:30:G:C6      | 22:CV:43:G:C6      | 2.72                     | 0.78              |
| 25:DA:957:A:N1     | 25:DA:2458:G:H4'   | 1.99                     | 0.78              |
| 1:AA:251:G:O2'     | 1:AA:252:U:C5'     | 2.32                     | 0.78              |
| 4:AD:173:TRP:HA    | 4:AD:187:ARG:NH1   | 1.98                     | 0.78              |
| 8:AH:84:ARG:HG3    | 8:AH:85:ARG:N      | 1.97                     | 0.78              |
| 2:CB:34:ALA:O      | 2:CB:41:ILE:HB     | 1.84                     | 0.78              |
| 10:CJ:5:ARG:HG3    | 10:CJ:73:ASP:OD1   | 1.85                     | 0.78              |
| 1:AA:484:G:H4'     | 1:AA:485:G:O5'     | 1.82                     | 0.77              |
| 32:BH:109:PHE:HE1  | 32:BH:152:ARG:NH2  | 1.82                     | 0.77              |
| 36:BP:47:ASP:HB3   | 36:BP:48:PRO:O     | 1.84                     | 0.77              |
| 41:BU:95:LEU:CD1   | 42:BV:4:ILE:HG23   | 2.14                     | 0.77              |
| 52:B5:16:ARG:HH11  | 52:B5:16:ARG:CG    | 1.95                     | 0.77              |
| 3:CC:73:PRO:O      | 3:CC:76:VAL:HG22   | 1.85                     | 0.77              |
| 5:CE:50:GLU:HB3    | 5:CE:53:LEU:HD13   | 1.65                     | 0.77              |
| 19:CS:29:ARG:O     | 19:CS:31:ILE:HG22  | 1.84                     | 0.77              |
| 40:DT:34:VAL:HG13  | 40:DT:39:ARG:HA    | 1.65                     | 0.77              |
| 25:BA:2126:A:O2'   | 25:BA:2127:G:H5''  | 1.84                     | 0.77              |
| 25:BA:2847:U:C5    | 25:BA:2848:G:C6    | 2.71                     | 0.77              |
| 31:BG:128:ARG:C    | 31:BG:130:ASN:H    | 1.92                     | 0.77              |
| 36:BP:106:LEU:HD11 | 36:BP:112:LEU:HD23 | 1.65                     | 0.77              |
| 39:BS:14:VAL:HB    | 39:BS:15:ARG:HD3   | 1.66                     | 0.77              |
| 3:CC:6:HIS:HD2     | 3:CC:7:PRO:HD2     | 1.48                     | 0.77              |
| 16:CP:9:PHE:HE1    | 16:CP:18:ARG:HH21  | 1.31                     | 0.77              |
| 17:CQ:18:THR:HG23  | 17:CQ:69:LYS:HE3   | 1.64                     | 0.77              |
| 25:DA:2032:G:O2'   | 29:DE:145:LYS:NZ   | 2.16                     | 0.77              |
| 25:DA:2681:C:C5    | 25:DA:2725:A:N6    | 2.50                     | 0.77              |
| 41:DU:91:ASP:C     | 41:DU:92:ARG:HD3   | 2.09                     | 0.77              |
| 25:BA:769:G:H4'    | 25:BA:1379:A:N6    | 1.99                     | 0.77              |
| 25:BA:2320:A:C5    | 25:BA:2333:A:C5    | 2.72                     | 0.77              |
| 42:BV:2:PHE:HB3    | 42:BV:42:GLY:N     | 2.00                     | 0.77              |
| 1:CA:129(A):G:O2'  | 1:CA:189(F):U:H3'  | 1.84                     | 0.77              |
| 4:CD:12:CYS:SG     | 4:CD:19:LEU:O      | 2.42                     | 0.77              |
| 4:CD:108:LEU:HB3   | 4:CD:110:PHE:CE1   | 2.18                     | 0.77              |
| 4:CD:108:LEU:CG    | 4:CD:110:PHE:HE1   | 1.89                     | 0.77              |
| 7:CG:113:GLU:CG    | 7:CG:119:ARG:HG2   | 2.14                     | 0.77              |
| 20:CT:73:HIS:HB3   | 20:CT:74:LYS:HG2   | 1.65                     | 0.77              |
| 25:DA:1141:U:OP1   | 34:DN:25:ARG:NH1   | 2.17                     | 0.77              |
| 25:DA:1421:G:N3    | 25:DA:1494:A:N6    | 2.32                     | 0.77              |
| 5:AE:78:HIS:CE1    | 5:AE:142:LEU:HA    | 2.20                     | 0.77              |
| 5:AE:80:ILE:HD12   | 5:AE:138:ALA:HB1   | 1.65                     | 0.77              |
| 16:AP:82:GLN:HG2   | 16:AP:83:GLU:N     | 1.96                     | 0.77              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 23:AY:32:U:H2'    | 23:AY:32:U:O2      | 1.84                     | 0.77              |
| 30:BF:19:GLU:O    | 30:BF:20:LEU:HB2   | 1.84                     | 0.77              |
| 40:BT:28:VAL:CG2  | 40:BT:46:GLU:HG3   | 2.06                     | 0.77              |
| 40:BT:83:ILE:CG1  | 40:BT:84:GLN:H     | 1.96                     | 0.77              |
| 1:CA:710:G:H5''   | 6:CF:54:LYS:HE2    | 1.66                     | 0.77              |
| 1:CA:1456:G:H5''  | 1:CA:1456:G:N3     | 1.99                     | 0.77              |
| 25:DA:84:A:H5''   | 45:DY:8:LYS:HD2    | 1.66                     | 0.77              |
| 25:DA:1340:U:H4'  | 25:DA:1341:U:OP2   | 1.84                     | 0.77              |
| 28:DD:28:GLU:H    | 28:DD:29:PRO:HD2   | 1.50                     | 0.77              |
| 40:DT:24:PRO:HD3  | 40:DT:52:ILE:HD11  | 1.65                     | 0.77              |
| 53:D6:46:HIS:CD2  | 53:D6:47:THR:HA    | 2.20                     | 0.77              |
| 1:AA:1298:C:N4    | 7:AG:114:ARG:HB3   | 1.99                     | 0.77              |
| 8:AH:84:ARG:O     | 8:AH:135:CYS:HB2   | 1.84                     | 0.77              |
| 18:AR:25:THR:O    | 18:AR:26:LEU:HD23  | 1.85                     | 0.77              |
| 22:AV:53:G:H2'    | 22:AV:54:G:O5'     | 1.85                     | 0.77              |
| 28:BD:80:ALA:CB   | 28:BD:96:HIS:CD2   | 2.58                     | 0.77              |
| 47:B0:26:TYR:H    | 47:B0:29:GLN:HE21  | 1.29                     | 0.77              |
| 3:CC:14:ILE:HG12  | 3:CC:15:THR:H      | 1.50                     | 0.77              |
| 3:CC:123:GLN:HB3  | 3:CC:128:PHE:HD2   | 1.48                     | 0.77              |
| 9:CI:2:GLU:N      | 9:CI:88:TYR:HH     | 1.81                     | 0.77              |
| 25:DA:1455:G:N2   | 25:DA:1456:G:H1'   | 2.00                     | 0.77              |
| 35:DO:19:ILE:HG22 | 35:DO:43:VAL:HA    | 1.65                     | 0.77              |
| 41:DU:90:VAL:HG12 | 41:DU:91:ASP:N     | 1.99                     | 0.77              |
| 42:DV:62:LEU:HD11 | 42:DV:95:LEU:HB2   | 1.66                     | 0.77              |
| 45:DY:40:GLU:HA   | 45:DY:64:GLU:OE1   | 1.84                     | 0.77              |
| 1:AA:686:U:O2'    | 11:AK:42:TRP:CZ2   | 2.36                     | 0.77              |
| 5:AE:101:ILE:HG13 | 5:AE:119:LEU:CD2   | 2.15                     | 0.77              |
| 15:AO:63:ARG:O    | 15:AO:67:LEU:HD12  | 1.84                     | 0.77              |
| 28:BD:19:ALA:HB3  | 28:BD:21:PHE:CE2   | 2.20                     | 0.77              |
| 29:BE:77:ILE:HG22 | 29:BE:78:LEU:HG    | 1.67                     | 0.77              |
| 43:BW:5:ALA:HB2   | 43:BW:54:ALA:HB2   | 1.65                     | 0.77              |
| 53:B6:15:GLU:OE2  | 53:B6:41:PRO:HG3   | 1.84                     | 0.77              |
| 1:CA:66:G:C4'     | 1:CA:173:U:O4      | 2.31                     | 0.77              |
| 1:CA:1152:A:H5''  | 10:CJ:13:HIS:HD2   | 1.50                     | 0.77              |
| 5:CE:90:VAL:CG2   | 5:CE:121:LYS:HB3   | 2.15                     | 0.77              |
| 7:CG:26:PHE:O     | 7:CG:30:ILE:HG13   | 1.84                     | 0.77              |
| 25:DA:389:G:H5''  | 48:D1:26:ARG:NH2   | 2.00                     | 0.77              |
| 25:DA:2519:U:H4'  | 25:DA:2520:C:OP1   | 1.84                     | 0.77              |
| 40:DT:23:ARG:HG2  | 40:DT:120:ARG:HH11 | 1.48                     | 0.77              |
| 40:DT:80:SER:CB   | 40:DT:81:PRO:HD3   | 2.14                     | 0.77              |
| 53:D6:41:PRO:CD   | 53:D6:46:HIS:CA    | 2.63                     | 0.77              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 13:AM:10:PRO:HB2   | 13:AM:18:ALA:HB1   | 1.67                     | 0.77              |
| 19:AS:63:THR:HG22  | 19:AS:66:MET:HE2   | 1.66                     | 0.77              |
| 23:AW:72:C:N4      | 23:AW:73:A:N6      | 2.33                     | 0.77              |
| 25:BA:242:G:O3'    | 25:BA:243:U:H6     | 1.67                     | 0.77              |
| 25:BA:1300:U:C4'   | 25:BA:1301:A:O5'   | 2.30                     | 0.77              |
| 25:BA:2056:G:N2    | 25:BA:2057:A:C8    | 2.52                     | 0.77              |
| 25:BA:2787:C:O2    | 29:BE:61:ARG:NH1   | 2.18                     | 0.77              |
| 33:BI:117:GLU:HG3  | 33:BI:118:LYS:H    | 1.49                     | 0.77              |
| 37:BQ:34:LEU:HD11  | 37:BQ:129:THR:HB   | 1.66                     | 0.77              |
| 45:BY:8:LYS:HZ1    | 45:BY:73:ARG:HA    | 1.50                     | 0.77              |
| 1:CA:1305:G:N2     | 1:CA:1331:G:C2'    | 2.48                     | 0.77              |
| 22:CV:60:A:C2'     | 22:CV:61:U:H5'     | 2.15                     | 0.77              |
| 33:DI:76:THR:HG23  | 33:DI:139:GLN:NE2  | 2.00                     | 0.77              |
| 40:DT:129:ARG:O    | 40:DT:129:ARG:CG   | 2.30                     | 0.77              |
| 45:DY:42:VAL:HB    | 45:DY:67:LEU:HD11  | 1.67                     | 0.77              |
| 45:DY:88:LYS:HB3   | 45:DY:90:LEU:HD23  | 1.64                     | 0.77              |
| 51:D4:14:ILE:HG13  | 51:D4:31:ILE:HG21  | 1.67                     | 0.77              |
| 1:AA:981:U:H2'     | 1:AA:982:U:C5      | 2.20                     | 0.77              |
| 1:AA:983:A:C2      | 1:AA:984:C:C4      | 2.71                     | 0.77              |
| 1:AA:1054:C:N4     | 23:AY:34:G:H1'     | 1.98                     | 0.77              |
| 25:BA:1344:G:O2'   | 25:BA:1385:G:H5''  | 1.83                     | 0.77              |
| 25:BA:2171:A:C2    | 25:BA:2172:U:O4    | 2.38                     | 0.77              |
| 28:BD:45:ASN:CG    | 28:BD:46:GLN:H     | 1.91                     | 0.77              |
| 29:BE:37:ARG:O     | 29:BE:38:THR:O     | 2.02                     | 0.77              |
| 43:BW:4:LYS:CE     | 43:BW:6:ILE:CD1    | 2.56                     | 0.77              |
| 45:BY:31:LEU:HD22  | 45:BY:36:ALA:O     | 1.85                     | 0.77              |
| 55:B8:39:LYS:O     | 55:B8:43:GLN:HG3   | 1.85                     | 0.77              |
| 1:CA:1108:G:H5'    | 3:CC:176:HIS:ND1   | 1.99                     | 0.77              |
| 17:CQ:67:LYS:HA    | 17:CQ:70:ARG:NH1   | 1.99                     | 0.77              |
| 23:CW:67:C:H2'     | 23:CW:68:C:H6      | 1.50                     | 0.77              |
| 25:DA:242:G:C5'    | 55:D8:62:LEU:HD13  | 2.14                     | 0.77              |
| 36:DP:106:LEU:HD11 | 36:DP:112:LEU:HD23 | 1.65                     | 0.77              |
| 40:DT:54:ARG:HA    | 40:DT:59:THR:HB    | 1.67                     | 0.77              |
| 40:DT:120:ARG:O    | 40:DT:123:GLN:HG2  | 1.84                     | 0.77              |
| 41:DU:62:ILE:CD1   | 41:DU:93:LYS:HG2   | 2.13                     | 0.77              |
| 2:AB:54:THR:HG21   | 2:AB:201:ILE:CD1   | 2.15                     | 0.77              |
| 3:AC:18:TRP:NE1    | 14:AN:55:GLY:H     | 1.83                     | 0.77              |
| 8:AH:20:TYR:CE2    | 8:AH:75:ARG:HG2    | 2.20                     | 0.77              |
| 13:AM:23:TYR:HB3   | 13:AM:67:GLU:HA    | 1.65                     | 0.77              |
| 20:AT:37:SER:CB    | 20:AT:84:LEU:CD2   | 2.50                     | 0.77              |
| 25:BA:1390:U:H3    | 25:BA:1395:A:H62   | 1.33                     | 0.77              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:BA:2015:A:H1'  | 52:B5:2:ALA:HA     | 1.67                     | 0.77              |
| 29:BE:14:ILE:HD11 | 29:BE:173:VAL:HG11 | 1.67                     | 0.77              |
| 48:B1:44:PRO:O    | 48:B1:46:LEU:HD22  | 1.85                     | 0.77              |
| 55:B8:6:THR:HG22  | 55:B8:63:PRO:HD3   | 1.67                     | 0.77              |
| 1:CA:677:U:H3     | 1:CA:713:G:H22     | 1.31                     | 0.77              |
| 8:CH:119:LEU:HB3  | 8:CH:123:GLU:HB2   | 1.67                     | 0.77              |
| 36:DP:52:GLU:OE1  | 36:DP:55:ARG:HD2   | 1.84                     | 0.77              |
| 46:DZ:144:LEU:O   | 46:DZ:174:VAL:HG21 | 1.83                     | 0.77              |
| 52:D5:56:LYS:HD2  | 52:D5:56:LYS:H     | 1.48                     | 0.77              |
| 1:AA:792:A:N7     | 1:AA:794:A:N6      | 2.32                     | 0.77              |
| 3:AC:29:TYR:OH    | 14:AN:54:PRO:HD2   | 1.84                     | 0.77              |
| 25:BA:1246:A:OP1  | 30:BF:38:ARG:NH1   | 2.18                     | 0.77              |
| 25:BA:1902:C:H1'  | 28:BD:244:ARG:HG3  | 1.66                     | 0.77              |
| 28:BD:13:ARG:HA   | 28:BD:16:MET:HE3   | 1.67                     | 0.77              |
| 35:BO:68:GLU:HB3  | 35:BO:78:ARG:HH11  | 1.50                     | 0.77              |
| 36:BP:97:PRO:HD3  | 36:BP:126:VAL:O    | 1.85                     | 0.77              |
| 42:BV:65:GLY:HA3  | 42:BV:91:TYR:HE1   | 1.50                     | 0.77              |
| 55:B8:50:LEU:HD12 | 55:B8:51:ALA:N     | 1.98                     | 0.77              |
| 19:CS:22:LEU:O    | 19:CS:26:GLY:HA2   | 1.83                     | 0.77              |
| 33:DI:72:LEU:HD11 | 33:DI:101:LEU:HD11 | 1.66                     | 0.77              |
| 12:AL:25:PRO:C    | 12:AL:27:LEU:H     | 1.91                     | 0.76              |
| 25:BA:2318:G:O2'  | 25:BA:2319:G:P     | 2.42                     | 0.76              |
| 28:BD:261:LYS:HZ1 | 28:BD:263:ARG:CZ   | 1.98                     | 0.76              |
| 30:BF:157:VAL:HB  | 30:BF:194:MET:HB3  | 1.64                     | 0.76              |
| 31:BG:16:ARG:HH11 | 31:BG:16:ARG:HG3   | 1.50                     | 0.76              |
| 31:BG:43:LEU:N    | 31:BG:43:LEU:CD1   | 2.47                     | 0.76              |
| 31:DG:101:ILE:CD1 | 51:D4:9:LEU:HD11   | 2.15                     | 0.76              |
| 32:DH:21:PRO:HG2  | 32:DH:22:GLY:H     | 1.48                     | 0.76              |
| 36:DP:71:VAL:N    | 36:DP:72:PRO:CD    | 2.47                     | 0.76              |
| 36:DP:97:PRO:HD3  | 36:DP:126:VAL:O    | 1.85                     | 0.76              |
| 40:DT:36:GLU:CB   | 40:DT:38:ASN:HD21  | 1.97                     | 0.76              |
| 1:AA:1267:C:O2    | 1:AA:1267:C:C2'    | 2.33                     | 0.76              |
| 25:BA:1721:G:H5'' | 25:BA:1721:G:N3    | 2.00                     | 0.76              |
| 13:CM:14:ARG:HG2  | 13:CM:16:ASP:OD2   | 1.84                     | 0.76              |
| 23:CW:68:C:H2'    | 23:CW:69:G:C8      | 2.18                     | 0.76              |
| 40:DT:24:PRO:CD   | 40:DT:52:ILE:HD12  | 2.15                     | 0.76              |
| 2:AB:42:ILE:HD13  | 2:AB:203:GLY:HA2   | 1.68                     | 0.76              |
| 2:AB:111:ARG:HH11 | 2:AB:111:ARG:HG2   | 1.49                     | 0.76              |
| 7:AG:115:ARG:O    | 7:AG:118:VAL:HG22  | 1.85                     | 0.76              |
| 10:AJ:24:VAL:HG11 | 10:AJ:37:PRO:HD3   | 1.64                     | 0.76              |
| 25:BA:1451:C:C5'  | 25:BA:1452:A:OP1   | 2.33                     | 0.76              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 25:BA:2127:G:O6    | 25:BA:2162:G:C6   | 2.38                     | 0.76              |
| 31:BG:125:PHE:O    | 31:BG:128:ARG:HG2 | 1.85                     | 0.76              |
| 39:BS:12:PHE:C     | 39:BS:12:PHE:CD1  | 2.64                     | 0.76              |
| 43:BW:59:VAL:HG12  | 43:BW:60:ASN:N    | 2.00                     | 0.76              |
| 45:BY:75:ILE:CG1   | 45:BY:79:CYS:HA   | 2.13                     | 0.76              |
| 4:CD:62:GLN:O      | 4:CD:66:ARG:HG3   | 1.86                     | 0.76              |
| 10:CJ:45:ARG:NH1   | 14:CN:36:PHE:CE2  | 2.53                     | 0.76              |
| 20:CT:48:LYS:HZ3   | 20:CT:48:LYS:HB3  | 1.49                     | 0.76              |
| 29:DE:111:ARG:HB3  | 38:DR:1:MET:SD    | 2.25                     | 0.76              |
| 32:DH:152:ARG:NE   | 32:DH:153:LYS:HE3 | 1.99                     | 0.76              |
| 40:DT:38:ASN:O     | 40:DT:39:ARG:CG   | 2.30                     | 0.76              |
| 53:D6:30:THR:HB    | 53:D6:31:PRO:HD2  | 1.67                     | 0.76              |
| 2:AB:68:ILE:HD12   | 2:AB:161:ALA:HB3  | 1.66                     | 0.76              |
| 22:AV:15:G:N1      | 22:AV:49:C:H5     | 1.81                     | 0.76              |
| 32:BH:126:PRO:HG2  | 32:BH:130:ARG:HD2 | 1.66                     | 0.76              |
| 39:BS:20:ARG:HG2   | 39:BS:20:ARG:NH1  | 1.91                     | 0.76              |
| 40:BT:28:VAL:HG13  | 40:BT:45:PHE:O    | 1.85                     | 0.76              |
| 46:BZ:53:ILE:CG2   | 46:BZ:71:VAL:HB   | 2.14                     | 0.76              |
| 9:CI:55:ALA:HB1    | 9:CI:58:HIS:CB    | 2.15                     | 0.76              |
| 10:CJ:34:VAL:CG2   | 10:CJ:74:ILE:HG22 | 2.15                     | 0.76              |
| 19:CS:4:SER:O      | 19:CS:5:LEU:HB2   | 1.85                     | 0.76              |
| 23:CY:28:G:H2'     | 23:CY:29:G:C8     | 2.21                     | 0.76              |
| 32:DH:153:LYS:HG2  | 32:DH:162:ILE:H   | 1.49                     | 0.76              |
| 2:AB:59:GLU:HB2    | 2:AB:221:LEU:HD12 | 1.68                     | 0.76              |
| 25:BA:311:A:H1'    | 25:BA:332:A:C8    | 2.20                     | 0.76              |
| 30:BF:28:ILE:HD12  | 30:BF:28:ILE:O    | 1.85                     | 0.76              |
| 32:BH:107:VAL:HG23 | 32:BH:107:VAL:O   | 1.86                     | 0.76              |
| 40:BT:28:VAL:HG12  | 40:BT:29:ARG:H    | 1.47                     | 0.76              |
| 40:BT:92:GLY:HA2   | 40:BT:114:LEU:HB3 | 1.65                     | 0.76              |
| 42:BV:98:GLU:OE1   | 42:BV:100:ARG:HD3 | 1.86                     | 0.76              |
| 55:B8:23:VAL:HG11  | 55:B8:46:ARG:HD3  | 1.67                     | 0.76              |
| 25:DA:631:A:OP1    | 36:DP:64:LYS:HE2  | 1.85                     | 0.76              |
| 25:DA:1204:A:H1'   | 25:DA:1206:G:C5   | 2.20                     | 0.76              |
| 25:DA:2090:G:H21   | 48:D1:45:ASN:HD21 | 1.31                     | 0.76              |
| 25:DA:2879:C:C5'   | 25:DA:2880:C:OP1  | 2.33                     | 0.76              |
| 29:DE:49:LEU:H     | 29:DE:49:LEU:CD1  | 1.96                     | 0.76              |
| 44:DX:60:ARG:HH22  | 54:D7:47:ARG:NH2  | 1.84                     | 0.76              |
| 1:AA:189(E):U:O2'  | 1:AA:189(F):U:H5' | 1.86                     | 0.76              |
| 25:BA:242:G:N2     | 25:BA:254:G:C8    | 2.54                     | 0.76              |
| 25:BA:614(C):A:C4' | 25:BA:615:G:OP1   | 2.31                     | 0.76              |
| 25:BA:2238:G:C5'   | 25:BA:2239:G:OP1  | 2.33                     | 0.76              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 48:B1:12:PRO:HB3  | 48:B1:43:TYR:CD2   | 2.20                     | 0.76              |
| 4:CD:108:LEU:HB3  | 4:CD:110:PHE:HD1   | 0.97                     | 0.76              |
| 16:CP:43:LYS:HG2  | 16:CP:48:TRP:CD2   | 2.20                     | 0.76              |
| 25:DA:1497:U:O2   | 25:DA:1497:U:C3'   | 2.34                     | 0.76              |
| 36:DP:57:THR:CG2  | 36:DP:59:LEU:HB3   | 2.15                     | 0.76              |
| 6:AF:72:VAL:HG13  | 6:AF:73:ASN:N      | 2.00                     | 0.76              |
| 20:AT:50:GLU:CA   | 20:AT:100:ILE:HG12 | 2.16                     | 0.76              |
| 25:BA:34:C:C4     | 25:BA:454:A:O2'    | 2.39                     | 0.76              |
| 31:BG:60:LEU:O    | 31:BG:64:THR:HG22  | 1.86                     | 0.76              |
| 37:BQ:85:LYS:HG3  | 47:B0:7:LEU:HB3    | 1.66                     | 0.76              |
| 38:BR:72:ASP:HB3  | 38:BR:75:LEU:HB2   | 1.68                     | 0.76              |
| 45:BY:67:LEU:HD12 | 45:BY:68:HIS:H     | 1.49                     | 0.76              |
| 7:CG:10:ARG:HG3   | 7:CG:10:ARG:NH1    | 1.99                     | 0.76              |
| 10:CJ:9:ARG:HB2   | 10:CJ:95:GLU:HB3   | 1.65                     | 0.76              |
| 22:CV:24:C:O2'    | 22:CV:25:U:H5'     | 1.85                     | 0.76              |
| 22:CV:60:A:H2'    | 22:CV:61:U:H5'     | 1.68                     | 0.76              |
| 25:DA:84:A:H5''   | 45:DY:8:LYS:CD     | 2.16                     | 0.76              |
| 28:DD:79:VAL:HG21 | 28:DD:111:LEU:HD11 | 1.68                     | 0.76              |
| 34:DN:40:PRO:HB3  | 41:DU:68:ALA:HB2   | 1.67                     | 0.76              |
| 35:DO:7:TYR:C     | 35:DO:8:LEU:HD22   | 2.11                     | 0.76              |
| 36:DP:47:ASP:HB3  | 36:DP:48:PRO:O     | 1.84                     | 0.76              |
| 36:DP:63:PRO:CB   | 55:D8:13:ARG:HB3   | 2.12                     | 0.76              |
| 36:DP:78:PRO:HB3  | 36:DP:111:ARG:NH2  | 2.01                     | 0.76              |
| 38:DR:33:ARG:HG3  | 38:DR:115:GLU:HB2  | 1.67                     | 0.76              |
| 41:DU:88:ILE:HD12 | 41:DU:109:LEU:HD22 | 1.67                     | 0.76              |
| 1:AA:792:A:C5     | 1:AA:794:A:C6      | 2.73                     | 0.76              |
| 1:AA:1392:G:H21   | 1:AA:1502:A:H8     | 1.30                     | 0.76              |
| 7:AG:22:LEU:HD23  | 7:AG:62:PHE:HE2    | 1.50                     | 0.76              |
| 25:BA:769:G:C4'   | 25:BA:1379:A:N6    | 2.49                     | 0.76              |
| 25:BA:2259:G:C5   | 25:BA:2427:C:N4    | 2.54                     | 0.76              |
| 28:BD:26:LYS:HZ3  | 28:BD:81:ALA:HB1   | 1.50                     | 0.76              |
| 30:BF:2:LYS:O     | 30:BF:25:PRO:HD2   | 1.84                     | 0.76              |
| 30:BF:64:ILE:CG2  | 30:BF:65:TRP:NE1   | 2.43                     | 0.76              |
| 43:BW:29:LEU:HG   | 43:BW:33:ARG:HD2   | 1.68                     | 0.76              |
| 45:BY:37:VAL:HG21 | 45:BY:72:VAL:HG21  | 1.65                     | 0.76              |
| 10:CJ:78:ASN:HD22 | 10:CJ:80:LYS:H     | 1.29                     | 0.76              |
| 22:CV:15:G:H22    | 22:CV:49:C:N4      | 1.84                     | 0.76              |
| 22:CV:53:G:H2'    | 22:CV:54:G:C5'     | 2.16                     | 0.76              |
| 33:DI:64:GLU:O    | 33:DI:67:ARG:HB3   | 1.85                     | 0.76              |
| 38:DR:67:LEU:HD13 | 38:DR:76:VAL:HG21  | 1.68                     | 0.76              |
| 39:DS:106:ARG:HA  | 39:DS:110:LEU:CD2  | 2.16                     | 0.76              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 3:AC:15:THR:HG21   | 3:AC:181:ASN:HA   | 1.66                     | 0.76              |
| 7:AG:24:THR:HA     | 7:AG:27:ILE:HG13  | 1.66                     | 0.76              |
| 25:BA:1453:U:C3'   | 25:BA:1455:G:P    | 2.74                     | 0.76              |
| 25:BA:1790:C:H5''  | 25:BA:1791:A:OP1  | 1.85                     | 0.76              |
| 29:BE:29:GLY:HA3   | 29:BE:51:PHE:HE2  | 1.51                     | 0.76              |
| 37:BQ:62:GLY:O     | 46:BZ:178:GLU:HG3 | 1.86                     | 0.76              |
| 39:BS:85:VAL:H     | 39:BS:106:ARG:HB2 | 1.49                     | 0.76              |
| 40:BT:83:ILE:CG1   | 40:BT:84:GLN:HG3  | 2.14                     | 0.76              |
| 48:B1:51:VAL:HG21  | 48:B1:74:VAL:HG21 | 1.68                     | 0.76              |
| 41:DU:95:LEU:HD13  | 42:DV:4:ILE:HG21  | 1.68                     | 0.76              |
| 46:DZ:141:VAL:HG21 | 46:DZ:144:LEU:HB2 | 1.65                     | 0.76              |
| 3:AC:18:TRP:H      | 3:AC:18:TRP:HE3   | 1.34                     | 0.76              |
| 19:AS:49:ILE:H     | 19:AS:49:ILE:HD12 | 1.51                     | 0.76              |
| 25:BA:769:G:C5'    | 25:BA:1379:A:N6   | 2.49                     | 0.76              |
| 25:BA:1493:C:O2    | 25:BA:1493:C:C2'  | 2.33                     | 0.76              |
| 29:BE:60:ASN:OD1   | 29:BE:62:PRO:HD2  | 1.86                     | 0.76              |
| 30:BF:51:THR:HG23  | 30:BF:92:PRO:O    | 1.84                     | 0.76              |
| 37:BQ:79:LEU:HD22  | 37:BQ:80:GLU:HG3  | 1.66                     | 0.76              |
| 42:BV:15:GLU:HB3   | 42:BV:16:PRO:HD2  | 1.67                     | 0.76              |
| 47:B0:68:GLU:HG2   | 47:B0:80:HIS:HB2  | 1.68                     | 0.76              |
| 55:B8:51:ALA:HA    | 55:B8:54:GLU:OE1  | 1.86                     | 0.76              |
| 3:CC:58:GLU:HB2    | 3:CC:65:ALA:HB2   | 1.67                     | 0.76              |
| 12:CL:84:LEU:HG    | 12:CL:105:TYR:HE1 | 1.51                     | 0.76              |
| 22:CV:24:C:H2'     | 22:CV:25:U:H6     | 1.51                     | 0.76              |
| 25:DA:598:G:H5'    | 36:DP:11:GLY:HA3  | 1.68                     | 0.76              |
| 25:DA:2835:A:H5'   | 25:DA:2836:U:OP1  | 1.86                     | 0.76              |
| 31:DG:180:PHE:C    | 31:DG:182:LYS:H   | 1.90                     | 0.76              |
| 32:DH:10:PRO:O     | 32:DH:11:VAL:HG13 | 1.86                     | 0.76              |
| 39:DS:71:ARG:HA    | 39:DS:104:GLY:O   | 1.86                     | 0.76              |
| 14:AN:12:ARG:C     | 14:AN:14:PRO:CD   | 2.46                     | 0.75              |
| 19:AS:18:LYS:O     | 19:AS:22:LEU:HD23 | 1.86                     | 0.75              |
| 24:AX:14:A:H2'     | 24:AX:15:A:C8     | 2.21                     | 0.75              |
| 30:BF:125:LEU:HD11 | 30:BF:199:TRP:CD1 | 2.20                     | 0.75              |
| 35:BO:1:MET:HG3    | 35:BO:32:TYR:CD1  | 2.20                     | 0.75              |
| 45:BY:8:LYS:HE3    | 45:BY:72:VAL:C    | 2.12                     | 0.75              |
| 1:CA:189(E):U:O2'  | 1:CA:189(F):U:H5' | 1.85                     | 0.75              |
| 1:CA:342:C:O2'     | 1:CA:343:U:H5'    | 1.84                     | 0.75              |
| 1:CA:484:G:O2'     | 1:CA:485:G:C5'    | 2.33                     | 0.75              |
| 16:CP:5:ARG:HB3    | 16:CP:67:THR:HG1  | 1.49                     | 0.75              |
| 16:CP:19:ILE:HG22  | 16:CP:36:ILE:HG12 | 1.66                     | 0.75              |
| 20:CT:73:HIS:O     | 20:CT:76:ALA:HB3  | 1.86                     | 0.75              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:DA:753:C:OP2    | 25:DA:753:C:C6     | 2.39                     | 0.75              |
| 25:DA:1128:A:N7    | 25:DA:2518:A:N6    | 2.34                     | 0.75              |
| 25:DA:2847:U:C3'   | 25:DA:2848:G:H5'   | 2.17                     | 0.75              |
| 28:DD:45:ASN:CG    | 28:DD:46:GLN:H     | 1.93                     | 0.75              |
| 32:DH:153:LYS:HG2  | 32:DH:162:ILE:HG13 | 1.68                     | 0.75              |
| 43:DW:84:ARG:HB2   | 43:DW:96:ILE:HG22  | 1.68                     | 0.75              |
| 44:DX:80:ILE:HD13  | 44:DX:80:ILE:O     | 1.87                     | 0.75              |
| 1:AA:992:U:O2'     | 1:AA:993:G:C5'     | 2.35                     | 0.75              |
| 20:AT:26:ASN:HB3   | 20:AT:71:THR:HG1   | 1.47                     | 0.75              |
| 20:AT:43:LEU:HB2   | 20:AT:52:ALA:HB2   | 1.67                     | 0.75              |
| 25:BA:588:U:OP2    | 25:BA:588:U:C6     | 2.39                     | 0.75              |
| 33:BI:79:ILE:HG12  | 33:BI:140:LEU:HD11 | 1.68                     | 0.75              |
| 34:BN:45:ASN:ND2   | 34:BN:46:VAL:N     | 2.35                     | 0.75              |
| 36:BP:78:PRO:HB3   | 36:BP:111:ARG:NH2  | 2.01                     | 0.75              |
| 39:BS:106:ARG:NH1  | 39:BS:108:GLY:HA3  | 2.00                     | 0.75              |
| 1:CA:243:A:N1      | 1:CA:246:A:N7      | 2.35                     | 0.75              |
| 1:CA:748:C:H1'     | 1:CA:749:C:C4      | 2.21                     | 0.75              |
| 8:CH:68:ARG:HH11   | 8:CH:68:ARG:HG2    | 1.50                     | 0.75              |
| 18:CR:85:LEU:HD12  | 18:CR:86:VAL:H     | 1.51                     | 0.75              |
| 25:DA:1205:U:C4'   | 25:DA:1206:G:OP2   | 2.33                     | 0.75              |
| 26:DB:14:U:O2'     | 26:DB:108:U:H4'    | 1.84                     | 0.75              |
| 28:DD:43:ARG:HH11  | 28:DD:44:ASN:ND2   | 1.84                     | 0.75              |
| 31:DG:113:ARG:HH12 | 31:DG:142:PRO:HA   | 1.51                     | 0.75              |
| 39:DS:3:ARG:HG2    | 39:DS:4:LEU:N      | 1.99                     | 0.75              |
| 53:D6:41:PRO:HD3   | 53:D6:46:HIS:C     | 2.11                     | 0.75              |
| 12:AL:26:ALA:O     | 12:AL:27:LEU:HB2   | 1.85                     | 0.75              |
| 19:AS:29:ARG:O     | 19:AS:31:ILE:HG22  | 1.84                     | 0.75              |
| 25:BA:2259:G:N7    | 25:BA:2427:C:N4    | 2.35                     | 0.75              |
| 25:BA:2712:U:H2'   | 25:BA:2713:A:H5''  | 1.67                     | 0.75              |
| 28:BD:33:LEU:HD12  | 28:BD:33:LEU:H     | 1.50                     | 0.75              |
| 30:BF:33:LEU:O     | 30:BF:36:VAL:HG23  | 1.86                     | 0.75              |
| 36:BP:34:GLY:O     | 36:BP:35:HIS:C     | 2.28                     | 0.75              |
| 37:BQ:10:ARG:HH11  | 37:BQ:10:ARG:CG    | 1.99                     | 0.75              |
| 2:CB:48:MET:HA     | 2:CB:51:LEU:HD12   | 1.67                     | 0.75              |
| 2:CB:90:MET:HE2    | 2:CB:90:MET:HA     | 1.66                     | 0.75              |
| 19:CS:63:THR:HG23  | 19:CS:66:MET:CG    | 2.15                     | 0.75              |
| 25:DA:572:A:OP2    | 42:DV:78:LYS:NZ    | 2.19                     | 0.75              |
| 36:DP:57:THR:HG23  | 36:DP:59:LEU:H     | 1.51                     | 0.75              |
| 39:DS:39:ILE:HD11  | 39:DS:73:LEU:HD11  | 1.68                     | 0.75              |
| 46:DZ:19:ARG:HH12  | 46:DZ:84:GLU:CA    | 1.99                     | 0.75              |
| 19:AS:29:ARG:HH11  | 19:AS:30:LEU:N     | 1.84                     | 0.75              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 44:BX:12:VAL:HG13 | 44:BX:27:THR:O     | 1.86                     | 0.75              |
| 2:CB:16:HIS:CD2   | 2:CB:210:SER:HA    | 2.21                     | 0.75              |
| 2:CB:183:PRO:HA   | 2:CB:198:ASP:OD1   | 1.86                     | 0.75              |
| 19:CS:46:GLY:N    | 19:CS:62:ILE:HG23  | 2.01                     | 0.75              |
| 1:AA:1238:A:H62   | 1:AA:1301:U:H3     | 1.32                     | 0.75              |
| 4:AD:30:LYS:C     | 4:AD:32:ALA:H      | 1.90                     | 0.75              |
| 12:AL:7:ILE:HA    | 12:AL:10:LEU:HD12  | 1.67                     | 0.75              |
| 29:BE:137:HIS:HB3 | 29:BE:138:PRO:HD2  | 1.67                     | 0.75              |
| 40:BT:28:VAL:HG22 | 40:BT:47:GLY:H     | 1.49                     | 0.75              |
| 4:CD:92:VAL:O     | 4:CD:96:LEU:HD12   | 1.87                     | 0.75              |
| 6:CF:82:ARG:HB2   | 6:CF:85:VAL:HG23   | 1.68                     | 0.75              |
| 19:CS:6:LYS:HG2   | 19:CS:7:LYS:CD     | 2.15                     | 0.75              |
| 36:DP:79:ARG:CG   | 36:DP:109:GLY:O    | 2.35                     | 0.75              |
| 38:DR:97:VAL:HG22 | 38:DR:114:VAL:HG22 | 1.68                     | 0.75              |
| 53:D6:41:PRO:HD2  | 53:D6:46:HIS:CA    | 2.17                     | 0.75              |
| 19:AS:63:THR:H    | 19:AS:66:MET:HE3   | 1.51                     | 0.75              |
| 25:BA:662:G:H5'   | 36:BP:15:ARG:HA    | 1.68                     | 0.75              |
| 25:BA:1275:A:C4   | 38:BR:16:HIS:CD2   | 2.74                     | 0.75              |
| 25:BA:1452:A:H62  | 25:BA:2703:C:N4    | 1.85                     | 0.75              |
| 28:BD:75:ILE:HD13 | 28:BD:99:ASP:OD1   | 1.87                     | 0.75              |
| 36:BP:63:PRO:CB   | 55:B8:13:ARG:HB3   | 2.11                     | 0.75              |
| 46:BZ:23:LYS:HG2  | 46:BZ:38:TYR:HE1   | 1.52                     | 0.75              |
| 1:CA:484:G:O4'    | 1:CA:486:U:C6      | 2.39                     | 0.75              |
| 23:CW:20:U:H2'    | 23:CW:21:A:H4'     | 1.68                     | 0.75              |
| 25:DA:2879:C:H4'  | 25:DA:2880:C:OP1   | 1.86                     | 0.75              |
| 32:DH:135:GLY:HA3 | 32:DH:141:VAL:HG22 | 1.69                     | 0.75              |
| 33:DI:115:ALA:HB3 | 33:DI:128:LEU:CD1  | 2.06                     | 0.75              |
| 42:DV:39:LEU:O    | 42:DV:40:LEU:HD23  | 1.85                     | 0.75              |
| 43:DW:50:VAL:HG13 | 43:DW:51:LEU:H     | 1.51                     | 0.75              |
| 5:AE:91:LEU:HD12  | 5:AE:120:THR:CB    | 2.16                     | 0.75              |
| 30:BF:53:THR:HG23 | 30:BF:56:GLU:HG3   | 1.69                     | 0.75              |
| 36:BP:57:THR:HG23 | 36:BP:59:LEU:HB3   | 1.69                     | 0.75              |
| 38:BR:11:ASN:O    | 38:BR:12:ARG:CB    | 2.34                     | 0.75              |
| 41:BU:66:ASN:ND2  | 41:BU:70:ARG:HE    | 1.85                     | 0.75              |
| 10:CJ:40:LEU:HG   | 10:CJ:69:ASN:HB3   | 1.69                     | 0.75              |
| 22:CV:15:G:N2     | 22:CV:49:C:H41     | 1.83                     | 0.75              |
| 23:CW:26:A:H61    | 23:CW:44:G:H1      | 1.32                     | 0.75              |
| 25:DA:221:A:C4'   | 25:DA:222:A:O5'    | 2.30                     | 0.75              |
| 25:DA:2298:A:H62  | 25:DA:2318:G:H8    | 1.35                     | 0.75              |
| 25:DA:2850:A:OP2  | 25:DA:2866:U:C5    | 2.39                     | 0.75              |
| 32:DH:86:GLU:HG3  | 32:DH:165:ALA:HB3  | 1.69                     | 0.75              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 33:DI:114:LEU:HD12 | 33:DI:128:LEU:HD12 | 1.68                     | 0.75              |
| 45:DY:81:LYS:HB2   | 45:DY:96:ILE:HG22  | 1.66                     | 0.75              |
| 4:AD:33:MET:HE2    | 4:AD:37:PRO:HA     | 1.68                     | 0.75              |
| 4:AD:72:GLU:OE2    | 4:AD:72:GLU:HA     | 1.86                     | 0.75              |
| 19:AS:6:LYS:CD     | 19:AS:7:LYS:HD3    | 2.17                     | 0.75              |
| 25:BA:2198:A:H1'   | 33:BI:28:ASN:O     | 1.86                     | 0.75              |
| 25:BA:2287:A:H2    | 25:BA:2346:A:C2    | 2.04                     | 0.75              |
| 28:BD:26:LYS:NZ    | 28:BD:82:ILE:H     | 1.85                     | 0.75              |
| 31:BG:141:PHE:O    | 31:BG:144:ILE:HG22 | 1.87                     | 0.75              |
| 32:BH:85:LYS:O     | 32:BH:132:ARG:HA   | 1.87                     | 0.75              |
| 40:BT:29:ARG:HD2   | 40:BT:86:ILE:N     | 2.02                     | 0.75              |
| 46:BZ:103:ARG:HD3  | 46:BZ:136:PHE:CE1  | 2.22                     | 0.75              |
| 22:CV:29:C:H2'     | 22:CV:30:G:C5'     | 2.10                     | 0.75              |
| 30:DF:63:LYS:CE    | 30:DF:67:GLN:HB3   | 2.17                     | 0.75              |
| 50:D3:4:LEU:HB2    | 50:D3:39:ASP:HB2   | 1.69                     | 0.75              |
| 2:AB:69:LEU:HB3    | 2:AB:162:ILE:HG22  | 1.67                     | 0.75              |
| 6:AF:45:LEU:HD12   | 6:AF:46:ARG:H      | 1.51                     | 0.75              |
| 1:CA:429:U:O4'     | 1:CA:430:A:C8      | 2.40                     | 0.75              |
| 25:DA:1247:A:OP1   | 30:DF:95:ARG:NH2   | 2.19                     | 0.75              |
| 25:DA:1653:G:C4'   | 25:DA:1654:A:OP1   | 2.30                     | 0.75              |
| 29:DE:81:ILE:HG22  | 29:DE:81:ILE:O     | 1.85                     | 0.75              |
| 29:DE:111:ARG:HA   | 38:DR:1:MET:SD     | 2.27                     | 0.75              |
| 32:DH:150:ALA:C    | 32:DH:152:ARG:N    | 2.42                     | 0.75              |
| 36:DP:70:GLN:CB    | 36:DP:72:PRO:HD2   | 2.16                     | 0.75              |
| 42:DV:38:LEU:HD12  | 42:DV:56:SER:CA    | 2.16                     | 0.75              |
| 1:AA:983:A:H3'     | 1:AA:983:A:N3      | 2.02                     | 0.74              |
| 17:AQ:21:VAL:HG21  | 17:AQ:59:ILE:HD11  | 1.67                     | 0.74              |
| 33:BI:29:TYR:HD2   | 33:BI:30:LEU:HD23  | 1.51                     | 0.74              |
| 36:BP:79:ARG:CG    | 36:BP:109:GLY:O    | 2.35                     | 0.74              |
| 49:B2:69:ARG:HH11  | 49:B2:69:ARG:HG2   | 1.52                     | 0.74              |
| 1:CA:79:G:H4'      | 1:CA:80:G:OP1      | 1.86                     | 0.74              |
| 32:DH:153:LYS:HG3  | 32:DH:161:GLY:CA   | 2.17                     | 0.74              |
| 1:AA:327:A:C4      | 1:AA:329:A:C8      | 2.75                     | 0.74              |
| 25:BA:859:G:N2     | 25:BA:917:A:OP2    | 2.20                     | 0.74              |
| 34:BN:14:VAL:HG22  | 34:BN:137:LYS:HE3  | 1.69                     | 0.74              |
| 50:B3:26:LEU:HD21  | 50:B3:46:ASN:HB3   | 1.67                     | 0.74              |
| 52:B5:49:CYS:O     | 52:B5:56:LYS:HB3   | 1.87                     | 0.74              |
| 1:CA:250:A:C4'     | 1:CA:251:G:O5'     | 2.34                     | 0.74              |
| 1:CA:342:C:H2'     | 1:CA:343:U:H5'     | 1.69                     | 0.74              |
| 12:CL:101:VAL:HG12 | 12:CL:104:VAL:HG23 | 1.67                     | 0.74              |
| 25:DA:975(A):G:C2' | 25:DA:976:C:H5'    | 2.17                     | 0.74              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 32:DH:143:GLN:HE22 | 32:DH:147:ASN:HD21 | 1.32                     | 0.74              |
| 33:DI:101:LEU:HD21 | 33:DI:107:VAL:HB   | 1.67                     | 0.74              |
| 35:DO:35:VAL:HG21  | 35:DO:69:ILE:HD13  | 1.68                     | 0.74              |
| 36:DP:34:GLY:O     | 36:DP:35:HIS:C     | 2.28                     | 0.74              |
| 45:DY:63:LYS:HZ2   | 45:DY:63:LYS:HA    | 1.52                     | 0.74              |
| 15:AO:78:TYR:O     | 15:AO:82:ILE:HG22  | 1.88                     | 0.74              |
| 16:AP:39:TYR:O     | 16:AP:41:PRO:HD3   | 1.87                     | 0.74              |
| 25:BA:2689:U:H4'   | 25:BA:2690:C:C5'   | 2.17                     | 0.74              |
| 32:BH:107:VAL:HG23 | 32:BH:109:PHE:CE1  | 2.21                     | 0.74              |
| 41:BU:61:TRP:CH2   | 41:BU:94:ASN:HB2   | 2.22                     | 0.74              |
| 51:B4:48:ILE:H     | 51:B4:48:ILE:HD12  | 1.50                     | 0.74              |
| 22:CV:54:G:C4      | 22:CV:55:U:C5      | 2.74                     | 0.74              |
| 36:DP:61:ARG:HH11  | 55:D8:13:ARG:HD2   | 1.49                     | 0.74              |
| 39:DS:106:ARG:HA   | 39:DS:110:LEU:HD21 | 1.69                     | 0.74              |
| 1:AA:974:A:H1'     | 14:AN:31:ARG:HE    | 1.51                     | 0.74              |
| 1:AA:992:U:C4'     | 1:AA:993:G:O5'     | 2.30                     | 0.74              |
| 1:AA:1054:C:O2     | 1:AA:1054:C:C2'    | 2.33                     | 0.74              |
| 3:AC:22:TRP:CZ3    | 3:AC:32:LEU:HB3    | 2.21                     | 0.74              |
| 13:AM:3:ARG:NH1    | 31:BG:113:ARG:HE   | 1.86                     | 0.74              |
| 25:BA:581:C:OP1    | 41:BU:33:ARG:HG3   | 1.87                     | 0.74              |
| 29:BE:50:GLY:HA2   | 29:BE:78:LEU:HB3   | 1.69                     | 0.74              |
| 40:BT:78:LEU:O     | 40:BT:78:LEU:HD23  | 1.87                     | 0.74              |
| 25:DA:9271:G:C2    | 25:DA:9272:G:H1'   | 2.22                     | 0.74              |
| 31:DG:13:GLU:O     | 31:DG:14:GLU:HB2   | 1.85                     | 0.74              |
| 32:DH:30:LYS:HD2   | 32:DH:81:GLU:H     | 1.52                     | 0.74              |
| 38:DR:38:VAL:HB    | 38:DR:39:PRO:HD3   | 1.70                     | 0.74              |
| 39:DS:83:LYS:O     | 39:DS:109:GLY:HA3  | 1.87                     | 0.74              |
| 45:DY:50:ARG:HD3   | 45:DY:53:PRO:HG2   | 1.69                     | 0.74              |
| 51:D4:10:VAL:HB    | 51:D4:11:PRO:HD2   | 1.69                     | 0.74              |
| 8:AH:88:LYS:HB3    | 8:AH:89:PRO:HD2    | 1.70                     | 0.74              |
| 24:AX:13:A:C2      | 24:AX:14:A:H3'     | 2.21                     | 0.74              |
| 25:BA:1340:U:H4'   | 25:BA:1341:U:OP2   | 1.88                     | 0.74              |
| 30:BF:1:MET:HE2    | 30:BF:26:ALA:C     | 2.13                     | 0.74              |
| 30:BF:40:GLN:NE2   | 30:BF:182:ASN:HB2  | 2.03                     | 0.74              |
| 38:BR:79:LEU:O     | 38:BR:79:LEU:HD22  | 1.87                     | 0.74              |
| 2:CB:15:VAL:HG21   | 2:CB:209:ARG:HE    | 1.51                     | 0.74              |
| 2:CB:18:GLY:H      | 2:CB:42:ILE:HG22   | 1.51                     | 0.74              |
| 25:DA:389:G:H5''   | 48:D1:26:ARG:HH22  | 1.53                     | 0.74              |
| 45:DY:42:VAL:CG1   | 45:DY:65:ALA:HB3   | 2.17                     | 0.74              |
| 13:AM:83:ASP:OD1   | 19:AS:74:PHE:CE1   | 2.41                     | 0.74              |
| 20:AT:25:ARG:HH11  | 20:AT:25:ARG:HG3   | 1.52                     | 0.74              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:BA:752:A:H4'    | 25:BA:753:C:O5'    | 1.87                     | 0.74              |
| 36:BP:56:SER:O     | 36:BP:57:THR:CB    | 2.35                     | 0.74              |
| 47:B0:68:GLU:CG    | 47:B0:80:HIS:HB2   | 2.18                     | 0.74              |
| 53:B6:17:LYS:C     | 53:B6:18:ARG:HD3   | 2.13                     | 0.74              |
| 13:CM:68:GLY:HA3   | 31:DG:116:ASP:OD2  | 1.88                     | 0.74              |
| 13:CM:124:PRO:CB   | 13:CM:125:ARG:CG   | 2.44                     | 0.74              |
| 25:DA:995:C:H6     | 41:DU:57:PHE:CE1   | 1.99                     | 0.74              |
| 25:DA:2751:G:H8    | 25:DA:2751:G:O5'   | 1.69                     | 0.74              |
| 28:DD:154:LYS:C    | 28:DD:155:LEU:HD12 | 2.12                     | 0.74              |
| 46:DZ:23:LYS:HG3   | 46:DZ:38:TYR:CE1   | 2.22                     | 0.74              |
| 12:AL:86:ARG:HB2   | 12:AL:101:VAL:HG23 | 1.68                     | 0.74              |
| 25:BA:2835:A:C5'   | 25:BA:2836:U:OP1   | 2.36                     | 0.74              |
| 41:BU:14:HIS:CD2   | 41:BU:32:PHE:CG    | 2.75                     | 0.74              |
| 46:BZ:5:LEU:HD12   | 46:BZ:6:LYS:H      | 1.53                     | 0.74              |
| 4:CD:100:ARG:NH1   | 4:CD:137:SER:HA    | 2.02                     | 0.74              |
| 5:CE:34:VAL:O      | 5:CE:41:VAL:HG12   | 1.87                     | 0.74              |
| 9:CI:58:HIS:CB     | 9:CI:59:PHE:CD1    | 2.71                     | 0.74              |
| 10:CJ:38:ILE:CD1   | 10:CJ:71:LEU:HD23  | 2.17                     | 0.74              |
| 18:CR:40:LEU:O     | 18:CR:42:ARG:N     | 2.21                     | 0.74              |
| 20:CT:64:ASP:HA    | 20:CT:67:ALA:HB3   | 1.69                     | 0.74              |
| 22:CV:3:C:H2'      | 22:CV:4:G:H5'      | 1.69                     | 0.74              |
| 24:CX:16:A:N3      | 24:CX:17:U:C6      | 2.55                     | 0.74              |
| 37:DQ:141:GLN:HE22 | 46:DZ:72:ARG:HA    | 1.52                     | 0.74              |
| 39:DS:83:LYS:HG2   | 39:DS:109:GLY:H    | 1.53                     | 0.74              |
| 40:DT:33:LYS:CG    | 40:DT:43:GLN:HB2   | 2.17                     | 0.74              |
| 40:DT:74:ARG:HD2   | 40:DT:76:PHE:CE2   | 2.22                     | 0.74              |
| 45:DY:84:ARG:HH12  | 45:DY:97:ARG:CA    | 2.01                     | 0.74              |
| 7:AG:120:ILE:O     | 7:AG:124:LEU:HB2   | 1.88                     | 0.74              |
| 9:AI:43:ALA:HA     | 9:AI:74:ILE:HD13   | 1.68                     | 0.74              |
| 9:AI:58:HIS:O      | 9:AI:59:PHE:CD1    | 2.41                     | 0.74              |
| 11:AK:124:LYS:HD2  | 11:AK:125:PHE:HE1  | 1.52                     | 0.74              |
| 16:AP:18:ARG:HA    | 16:AP:38:TYR:HA    | 1.68                     | 0.74              |
| 21:AU:2:GLY:C      | 21:AU:4:GLY:H      | 1.96                     | 0.74              |
| 25:BA:2127:G:C5    | 25:BA:2162:G:C2    | 2.75                     | 0.74              |
| 25:BA:2172:U:H1'   | 25:BA:2173:A:OP1   | 1.87                     | 0.74              |
| 30:BF:24:LEU:O     | 30:BF:26:ALA:N     | 2.21                     | 0.74              |
| 38:BR:92:GLY:O     | 38:BR:94:TYR:CE2   | 2.41                     | 0.74              |
| 55:B8:46:ARG:O     | 55:B8:47:LYS:HB3   | 1.87                     | 0.74              |
| 3:CC:113:ALA:HB3   | 3:CC:114:PRO:HD3   | 1.70                     | 0.74              |
| 15:CO:7:GLU:O      | 15:CO:11:VAL:HG23  | 1.88                     | 0.74              |
| 20:CT:49:ALA:HB1   | 20:CT:100:ILE:HD13 | 1.67                     | 0.74              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:CW:36:A:C2      | 23:CW:37:A:C4      | 2.75                     | 0.74              |
| 25:DA:2879:C:C4'   | 25:DA:2880:C:OP1   | 2.35                     | 0.74              |
| 39:DS:5:THR:OG1    | 39:DS:7:TYR:HB3    | 1.88                     | 0.74              |
| 40:DT:24:PRO:HD3   | 40:DT:52:ILE:HD12  | 1.70                     | 0.74              |
| 41:DU:92:ARG:CG    | 42:DV:11:GLN:OE1   | 2.36                     | 0.74              |
| 1:AA:1255:G:H5''   | 3:AC:26:LYS:HZ2    | 1.53                     | 0.74              |
| 12:AL:24:VAL:HG12  | 12:AL:24:VAL:O     | 1.87                     | 0.74              |
| 15:AO:39:LEU:HD12  | 15:AO:56:LEU:HB2   | 1.70                     | 0.74              |
| 16:AP:49:LEU:HD12  | 16:AP:50:LYS:H     | 1.52                     | 0.74              |
| 25:BA:2287:A:O2'   | 25:BA:2288:A:H2'   | 1.88                     | 0.74              |
| 28:BD:11:PRO:C     | 28:BD:13:ARG:H     | 1.93                     | 0.74              |
| 30:BF:64:ILE:HG22  | 30:BF:65:TRP:CG    | 2.23                     | 0.74              |
| 31:BG:64:THR:HG23  | 31:BG:66:GLN:H     | 1.53                     | 0.74              |
| 42:BV:47:VAL:HB    | 42:BV:50:PRO:O     | 1.88                     | 0.74              |
| 49:B2:13:ALA:HA    | 49:B2:16:LEU:HD12  | 1.68                     | 0.74              |
| 9:CI:19:LEU:CD2    | 9:CI:59:PHE:HB3    | 2.18                     | 0.74              |
| 20:CT:89:ARG:NH2   | 20:CT:104:LEU:HD21 | 2.02                     | 0.74              |
| 25:DA:1494:A:H2'   | 25:DA:1495:A:C8    | 2.22                     | 0.74              |
| 29:DE:1:MET:HB2    | 29:DE:83:ASP:O     | 1.87                     | 0.74              |
| 35:DO:35:VAL:HG11  | 35:DO:103:ALA:HB3  | 1.70                     | 0.74              |
| 4:AD:31:CYS:C      | 4:AD:33:MET:H      | 1.94                     | 0.74              |
| 19:AS:45:VAL:C     | 19:AS:47:HIS:H     | 1.95                     | 0.74              |
| 25:BA:311:A:C8     | 25:BA:332:A:N7     | 2.56                     | 0.74              |
| 42:BV:18:LEU:CD1   | 42:BV:19:LYS:H     | 2.00                     | 0.74              |
| 45:BY:39:VAL:HG12  | 45:BY:40:GLU:N     | 2.00                     | 0.74              |
| 47:B0:27:GLU:HB2   | 47:B0:69:PHE:HD1   | 1.52                     | 0.74              |
| 2:CB:163:PHE:HA    | 2:CB:185:ILE:O     | 1.87                     | 0.74              |
| 9:CI:8:GLY:HA3     | 9:CI:76:ALA:O      | 1.88                     | 0.74              |
| 9:CI:46:ALA:HA     | 9:CI:78:LYS:HB2    | 1.70                     | 0.74              |
| 9:CI:83:ARG:HE     | 9:CI:102:LEU:HD11  | 1.52                     | 0.74              |
| 16:CP:4:ILE:HB     | 16:CP:66:PRO:HB3   | 1.69                     | 0.74              |
| 19:CS:44:MET:HA    | 19:CS:44:MET:HE3   | 1.69                     | 0.74              |
| 30:DF:20:LEU:HD12  | 30:DF:21:ALA:H     | 1.51                     | 0.74              |
| 33:DI:64:GLU:HG3   | 33:DI:67:ARG:CZ    | 2.18                     | 0.74              |
| 40:DT:88:ILE:HG22  | 40:DT:89:VAL:CG2   | 2.15                     | 0.74              |
| 46:DZ:144:LEU:HD12 | 46:DZ:174:VAL:HG23 | 1.70                     | 0.74              |
| 7:AG:32:ARG:O      | 7:AG:33:ASP:HB2    | 1.87                     | 0.73              |
| 8:AH:17:THR:HG22   | 8:AH:63:LEU:HG     | 1.70                     | 0.73              |
| 9:AI:17:VAL:HG11   | 9:AI:81:ILE:HD13   | 1.70                     | 0.73              |
| 20:AT:50:GLU:HA    | 20:AT:100:ILE:HG21 | 1.70                     | 0.73              |
| 20:AT:56:MET:CE    | 20:AT:85:MET:HE2   | 2.18                     | 0.73              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:AW:33:U:C2'    | 23:AW:35:A:OP2    | 2.35                     | 0.73              |
| 23:AW:66:U:H2'    | 23:AW:67:C:C6     | 2.23                     | 0.73              |
| 28:BD:72:LYS:HB3  | 28:BD:75:ILE:HD12 | 1.68                     | 0.73              |
| 39:BS:69:VAL:O    | 39:BS:72:ALA:HB3  | 1.88                     | 0.73              |
| 2:CB:88:ALA:HB2   | 2:CB:219:VAL:CG1  | 2.18                     | 0.73              |
| 3:CC:23:TYR:C     | 3:CC:23:TYR:CD2   | 2.66                     | 0.73              |
| 5:CE:115:VAL:HG12 | 5:CE:116:THR:H    | 1.52                     | 0.73              |
| 14:CN:27:CYS:SG   | 59:CN:101:ZN:ZN   | 1.76                     | 0.73              |
| 25:DA:1287:A:C6   | 25:DA:1288:U:C4   | 2.76                     | 0.73              |
| 25:DA:1799:G:C4'  | 25:DA:1800:C:O5'  | 2.30                     | 0.73              |
| 28:DD:43:ARG:HB3  | 28:DD:54:ARG:HB2  | 1.70                     | 0.73              |
| 33:DI:60:GLU:HG3  | 33:DI:61:ARG:HH22 | 1.53                     | 0.73              |
| 1:AA:1300:G:C2'   | 1:AA:1301:U:OP2   | 2.35                     | 0.73              |
| 25:BA:727:A:N6    | 25:BA:728:G:C6    | 2.57                     | 0.73              |
| 25:BA:2126:A:C1'  | 25:BA:2127:G:O4'  | 2.35                     | 0.73              |
| 39:BS:53:SER:OG   | 39:BS:54:LEU:HD22 | 1.88                     | 0.73              |
| 39:BS:66:ALA:O    | 39:BS:69:VAL:HG12 | 1.86                     | 0.73              |
| 41:BU:27:LEU:HB2  | 41:BU:34:LYS:CG   | 2.18                     | 0.73              |
| 45:BY:66:PRO:O    | 45:BY:67:LEU:HG   | 1.88                     | 0.73              |
| 1:CA:243:A:C6     | 1:CA:246:A:N7     | 2.55                     | 0.73              |
| 1:CA:1456:G:N2    | 1:CA:1457:G:C8    | 2.57                     | 0.73              |
| 20:CT:53:LEU:CD2  | 20:CT:100:ILE:CG2 | 2.62                     | 0.73              |
| 25:DA:242:G:C8    | 55:D8:3:LYS:HD3   | 2.23                     | 0.73              |
| 25:DA:1819:A:C1'  | 25:DA:1821:A:C6   | 2.71                     | 0.73              |
| 28:DD:62:TYR:HA   | 28:DD:87:ASN:HD21 | 1.53                     | 0.73              |
| 32:DH:152:ARG:O   | 32:DH:153:LYS:CB  | 2.36                     | 0.73              |
| 36:DP:20:GLY:O    | 36:DP:21:ARG:HD2  | 1.88                     | 0.73              |
| 42:DV:11:GLN:HE21 | 42:DV:39:LEU:HD23 | 1.53                     | 0.73              |
| 45:DY:76:CYS:HB3  | 45:DY:96:ILE:HD13 | 1.69                     | 0.73              |
| 1:AA:1067:A:H4'   | 1:AA:1068:G:O5'   | 1.89                     | 0.73              |
| 4:AD:134:ASP:O    | 4:AD:136:PRO:HD3  | 1.88                     | 0.73              |
| 25:BA:2820:A:O2'  | 38:BR:2:ARG:NH2   | 2.21                     | 0.73              |
| 36:BP:64:LYS:CB   | 55:B8:25:MET:HG3  | 2.16                     | 0.73              |
| 37:BQ:35:VAL:HG23 | 37:BQ:101:ARG:O   | 1.88                     | 0.73              |
| 45:BY:28:LYS:O    | 45:BY:29:GLU:C    | 2.31                     | 0.73              |
| 1:CA:1201:A:H5'   | 1:CA:1203:C:OP2   | 1.88                     | 0.73              |
| 19:CS:19:VAL:O    | 19:CS:23:ASN:HB2  | 1.88                     | 0.73              |
| 29:DE:51:PHE:CE1  | 29:DE:52:LEU:HD13 | 2.23                     | 0.73              |
| 13:AM:40:ASN:HB3  | 13:AM:43:THR:HG23 | 1.70                     | 0.73              |
| 25:BA:2259:G:C8   | 25:BA:2427:C:C4   | 2.76                     | 0.73              |
| 47:B0:43:THR:HG23 | 47:B0:43:THR:O    | 1.89                     | 0.73              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:327:A:N3      | 1:CA:329:A:H1'     | 2.03                     | 0.73              |
| 12:CL:21:LYS:N     | 12:CL:21:LYS:HD2   | 2.03                     | 0.73              |
| 18:CR:61:LYS:O     | 18:CR:65:ILE:HD12  | 1.87                     | 0.73              |
| 22:CV:21:U:C5'     | 22:CV:22:A:OP2     | 2.36                     | 0.73              |
| 22:CV:29:C:C2      | 22:CV:30:G:C8      | 2.75                     | 0.73              |
| 23:CW:38:A:H3'     | 23:CW:39:U:H5''    | 1.71                     | 0.73              |
| 46:DZ:58:VAL:HA    | 46:DZ:67:LEU:O     | 1.88                     | 0.73              |
| 46:DZ:151:HIS:HB3  | 46:DZ:170:THR:HA   | 1.70                     | 0.73              |
| 1:AA:686:U:H1'     | 11:AK:42:TRP:NE1   | 2.03                     | 0.73              |
| 5:AE:121:LYS:CG    | 5:AE:122:GLU:N     | 2.21                     | 0.73              |
| 10:AJ:89:ASP:C     | 10:AJ:91:PRO:HD3   | 2.13                     | 0.73              |
| 25:BA:2168:G:N2    | 25:BA:2171:A:C8    | 2.55                     | 0.73              |
| 29:BE:152:LYS:HG2  | 34:BN:78:TYR:CE1   | 2.23                     | 0.73              |
| 31:BG:125:PHE:CE2  | 31:BG:131:TYR:HB2  | 2.23                     | 0.73              |
| 38:BR:9:LYS:O      | 38:BR:10:LEU:CD2   | 2.36                     | 0.73              |
| 7:CG:145:ALA:O     | 7:CG:147:ALA:N     | 2.20                     | 0.73              |
| 13:CM:49:THR:HG22  | 13:CM:51:ALA:H     | 1.53                     | 0.73              |
| 19:CS:19:VAL:HG12  | 19:CS:20:LEU:HG    | 1.71                     | 0.73              |
| 29:DE:49:LEU:HD12  | 29:DE:49:LEU:N     | 2.00                     | 0.73              |
| 29:DE:101:ARG:HD3  | 29:DE:169:ASN:ND2  | 2.02                     | 0.73              |
| 39:DS:105:ALA:C    | 39:DS:110:LEU:HD21 | 2.14                     | 0.73              |
| 40:DT:92:GLY:C     | 40:DT:94:ALA:H     | 1.96                     | 0.73              |
| 46:DZ:61:LEU:HD12  | 46:DZ:65:GLN:HE21  | 1.52                     | 0.73              |
| 2:AB:36:ARG:HE     | 2:AB:36:ARG:N      | 1.86                     | 0.73              |
| 6:AF:7:ASN:ND2     | 18:AR:34:TYR:HE1   | 1.84                     | 0.73              |
| 23:AW:45:U:O2'     | 23:AW:46:G:H5'     | 1.89                     | 0.73              |
| 25:BA:7:G:H1       | 25:BA:2896:C:H42   | 1.36                     | 0.73              |
| 25:BA:2124:G:H1    | 25:BA:2174:C:H42   | 1.36                     | 0.73              |
| 25:BA:2679:A:H5'   | 29:BE:165:VAL:HG21 | 1.69                     | 0.73              |
| 26:BB:22:U:H3      | 26:BB:61:G:H1      | 1.37                     | 0.73              |
| 29:BE:134:ILE:HD13 | 29:BE:134:ILE:N    | 1.99                     | 0.73              |
| 31:BG:16:ARG:O     | 31:BG:20:ILE:HG13  | 1.87                     | 0.73              |
| 31:BG:37:VAL:CG1   | 31:BG:94:LEU:HD12  | 2.17                     | 0.73              |
| 33:BI:97:ILE:HD12  | 33:BI:114:LEU:HD11 | 1.68                     | 0.73              |
| 37:BQ:69:PHE:CD1   | 37:BQ:70:PRO:HD2   | 2.22                     | 0.73              |
| 40:BT:28:VAL:CG1   | 40:BT:29:ARG:H     | 2.01                     | 0.73              |
| 49:B2:29:LYS:HD2   | 49:B2:57:ILE:HD13  | 1.69                     | 0.73              |
| 53:B6:32:ASN:CG    | 53:B6:33:LYS:H     | 1.97                     | 0.73              |
| 1:CA:511:C:H1'     | 4:CD:43:HIS:NE2    | 2.03                     | 0.73              |
| 1:CA:1125:U:OP2    | 1:CA:1145:C:N4     | 2.21                     | 0.73              |
| 21:CU:25:LYS:HG2   | 21:CU:26:LYS:N     | 2.04                     | 0.73              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 28:DD:43:ARG:HD2   | 28:DD:44:ASN:OD1  | 1.89                     | 0.73              |
| 28:DD:102:LYS:C    | 28:DD:103:ARG:HG2 | 2.13                     | 0.73              |
| 29:DE:143:ASN:HB2  | 29:DE:147:PRO:HD2 | 1.69                     | 0.73              |
| 30:DF:95:ARG:CZ    | 30:DF:97:TYR:CE1  | 2.72                     | 0.73              |
| 30:DF:128:ALA:O    | 30:DF:129:PHE:CB  | 2.37                     | 0.73              |
| 31:DG:126:ASP:CG   | 31:DG:130:ASN:HB2 | 2.13                     | 0.73              |
| 1:AA:817:C:H1'     | 1:AA:819:A:H5'    | 1.70                     | 0.73              |
| 1:AA:1266:G:N2     | 1:AA:1269:A:OP2   | 2.20                     | 0.73              |
| 5:AE:10:MET:HA     | 5:AE:32:VAL:HG22  | 1.71                     | 0.73              |
| 6:AF:91:VAL:CG1    | 18:AR:72:ARG:NH1  | 2.51                     | 0.73              |
| 13:AM:7:VAL:HG22   | 31:BG:115:ARG:HA  | 1.70                     | 0.73              |
| 14:AN:41:ARG:HG3   | 14:AN:42:ILE:N    | 2.03                     | 0.73              |
| 15:AO:17:ARG:HD3   | 15:AO:26:GLU:HG3  | 1.69                     | 0.73              |
| 22:AV:15:G:H22     | 22:AV:49:C:H41    | 1.36                     | 0.73              |
| 25:BA:995:C:O2'    | 41:BU:61:TRP:CH2  | 2.42                     | 0.73              |
| 30:BF:164:ARG:HH11 | 30:BF:164:ARG:HG2 | 1.54                     | 0.73              |
| 34:BN:2:LYS:O      | 34:BN:4:TYR:CE1   | 2.42                     | 0.73              |
| 36:BP:70:GLN:CB    | 36:BP:72:PRO:HD2  | 2.17                     | 0.73              |
| 39:BS:74:ALA:HB1   | 39:BS:103:GLU:HG3 | 1.70                     | 0.73              |
| 40:BT:28:VAL:CG1   | 40:BT:29:ARG:N    | 2.51                     | 0.73              |
| 40:BT:31:SER:O     | 40:BT:32:TYR:HD2  | 1.71                     | 0.73              |
| 53:B6:16:CYS:O     | 53:B6:17:LYS:HB2  | 1.88                     | 0.73              |
| 22:CV:29:C:N3      | 22:CV:30:G:N7     | 2.36                     | 0.73              |
| 32:DH:9:ILE:HG22   | 32:DH:51:ARG:HG2  | 1.69                     | 0.73              |
| 34:DN:4:TYR:CB     | 41:DU:64:ARG:HH22 | 1.97                     | 0.73              |
| 40:DT:80:SER:HB3   | 40:DT:81:PRO:HD2  | 1.68                     | 0.73              |
| 25:BA:1826:G:H2'   | 25:BA:1827:C:C6   | 2.24                     | 0.73              |
| 30:BF:51:THR:CG2   | 30:BF:92:PRO:CD   | 2.67                     | 0.73              |
| 38:BR:4:LEU:O      | 38:BR:4:LEU:CD1   | 2.30                     | 0.73              |
| 22:CV:53:G:O2'     | 22:CV:54:G:H5'    | 1.88                     | 0.73              |
| 25:DA:1140:C:H4'   | 25:DA:1143:A:C6   | 2.24                     | 0.73              |
| 3:AC:155:GLY:O     | 3:AC:156:ARG:HB2  | 1.88                     | 0.73              |
| 5:AE:78:HIS:HE1    | 5:AE:143:ARG:H    | 1.37                     | 0.73              |
| 6:AF:62:TRP:CG     | 18:AR:35:ARG:NH1  | 2.57                     | 0.73              |
| 13:AM:25:ILE:HD11  | 13:AM:66:LEU:CD2  | 2.18                     | 0.73              |
| 25:BA:2238:G:H5'   | 25:BA:2239:G:OP1  | 1.87                     | 0.73              |
| 28:BD:31:LYS:HG3   | 28:BD:33:LEU:CD1  | 2.15                     | 0.73              |
| 33:BI:77:LEU:CD1   | 33:BI:104:GLN:NE2 | 2.51                     | 0.73              |
| 38:BR:51:LEU:HD23  | 38:BR:66:VAL:HG22 | 1.70                     | 0.73              |
| 40:BT:31:SER:O     | 40:BT:32:TYR:CD2  | 2.42                     | 0.73              |
| 1:CA:49:U:C5       | 1:CA:364:A:N6     | 2.55                     | 0.73              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 14:CN:43:CYS:SG   | 59:CN:101:ZN:ZN    | 1.78                     | 0.73              |
| 32:DH:154:PRO:HD3 | 32:DH:161:GLY:HA3  | 1.71                     | 0.73              |
| 36:DP:48:PRO:O    | 36:DP:49:ARG:C     | 2.30                     | 0.73              |
| 41:DU:83:LEU:HG   | 41:DU:88:ILE:HD11  | 1.69                     | 0.73              |
| 1:AA:1152:A:H5''  | 10:AJ:13:HIS:CD2   | 2.21                     | 0.73              |
| 19:AS:9:VAL:HG11  | 19:AS:11:VAL:CG1   | 2.18                     | 0.73              |
| 25:BA:995:C:O2'   | 41:BU:61:TRP:HZ2   | 1.67                     | 0.73              |
| 25:BA:1453:U:O4   | 38:BR:73:VAL:CG1   | 2.36                     | 0.73              |
| 36:BP:80:TYR:HA   | 36:BP:111:ARG:O    | 1.89                     | 0.73              |
| 40:BT:35:LYS:H    | 40:BT:39:ARG:HA    | 1.52                     | 0.73              |
| 41:BU:62:ILE:HG13 | 41:BU:76:TYR:CZ    | 2.24                     | 0.73              |
| 1:CA:764:C:H5''   | 15:CO:50:HIS:CE1   | 2.23                     | 0.73              |
| 1:CA:1054:C:O2    | 1:CA:1054:C:C3'    | 2.37                     | 0.73              |
| 9:CI:99:LEU:HD13  | 9:CI:99:LEU:O      | 1.89                     | 0.73              |
| 19:CS:63:THR:CG2  | 19:CS:66:MET:HG3   | 2.19                     | 0.73              |
| 20:CT:82:SER:O    | 20:CT:85:MET:HG3   | 1.89                     | 0.73              |
| 30:DF:62:ARG:HH11 | 30:DF:62:ARG:CG    | 1.90                     | 0.73              |
| 31:DG:58:GLN:HE22 | 31:DG:148:MET:HE1  | 1.54                     | 0.73              |
| 39:DS:10:ARG:O    | 39:DS:12:PHE:N     | 2.22                     | 0.73              |
| 1:AA:250:A:C4'    | 1:AA:251:G:O5'     | 2.30                     | 0.72              |
| 6:AF:91:VAL:HG11  | 18:AR:72:ARG:NH1   | 2.04                     | 0.72              |
| 6:AF:91:VAL:HG11  | 18:AR:72:ARG:HH11  | 1.53                     | 0.72              |
| 8:AH:36:LEU:HA    | 8:AH:39:LEU:HD23   | 1.71                     | 0.72              |
| 13:AM:19:LEU:O    | 13:AM:22:ILE:HG13  | 1.89                     | 0.72              |
| 20:AT:49:ALA:CB   | 20:AT:100:ILE:HD11 | 2.18                     | 0.72              |
| 25:BA:887:A:N3    | 25:BA:889:C:C5     | 2.58                     | 0.72              |
| 25:BA:2745:C:C5   | 25:BA:2746:U:O4    | 2.42                     | 0.72              |
| 28:BD:3:VAL:CG1   | 28:BD:17:THR:HB    | 2.19                     | 0.72              |
| 35:BO:97:ARG:NH2  | 35:BO:99:PHE:HE1   | 1.87                     | 0.72              |
| 55:B8:51:ALA:N    | 55:B8:53:PRO:HD2   | 2.02                     | 0.72              |
| 22:CV:29:C:C2     | 22:CV:30:G:N7      | 2.57                     | 0.72              |
| 25:DA:749:C:C4    | 25:DA:1618:A:C2    | 2.77                     | 0.72              |
| 25:DA:995:C:N3    | 34:DN:1:MET:HG3    | 2.03                     | 0.72              |
| 25:DA:2519:U:C4'  | 25:DA:2520:C:OP1   | 2.37                     | 0.72              |
| 34:DN:24:GLY:HA2  | 34:DN:106:MET:HE1  | 1.71                     | 0.72              |
| 46:DZ:68:PRO:HB2  | 46:DZ:91:LEU:HB2   | 1.69                     | 0.72              |
| 51:D4:20:ASN:HD22 | 51:D4:21:VAL:N     | 1.87                     | 0.72              |
| 53:D6:46:HIS:HD2  | 53:D6:46:HIS:C     | 1.86                     | 0.72              |
| 1:AA:413:G:N2     | 1:AA:428:G:O2'     | 2.21                     | 0.72              |
| 19:AS:63:THR:N    | 19:AS:66:MET:HE3   | 2.04                     | 0.72              |
| 25:BA:530:G:N3    | 25:BA:2021:C:O2'   | 2.21                     | 0.72              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 33:BI:14:ASP:HB2  | 33:BI:17:GLN:HE21  | 1.53                     | 0.72              |
| 33:BI:113:ARG:O   | 33:BI:130:TYR:HD1  | 1.71                     | 0.72              |
| 41:BU:27:LEU:CB   | 41:BU:31:SER:HB3   | 2.19                     | 0.72              |
| 49:B2:65:ASN:HB3  | 49:B2:69:ARG:NH2   | 2.04                     | 0.72              |
| 1:CA:1256:A:N6    | 1:CA:1278:U:O2'    | 2.22                     | 0.72              |
| 1:CA:1456:G:O2'   | 20:CT:39:LYS:NZ    | 2.23                     | 0.72              |
| 2:CB:14:GLY:O     | 2:CB:15:VAL:HG13   | 1.88                     | 0.72              |
| 6:CF:23:LYS:O     | 6:CF:27:GLN:HG2    | 1.89                     | 0.72              |
| 16:CP:12:LYS:O    | 16:CP:13:HIS:HB2   | 1.87                     | 0.72              |
| 17:CQ:45:HIS:O    | 17:CQ:73:VAL:HG23  | 1.88                     | 0.72              |
| 22:CV:24:C:C2'    | 22:CV:25:U:H5'     | 2.19                     | 0.72              |
| 40:DT:13:ARG:CZ   | 40:DT:13:ARG:HA    | 2.19                     | 0.72              |
| 40:DT:23:ARG:CD   | 40:DT:120:ARG:HD3  | 2.19                     | 0.72              |
| 42:DV:52:VAL:CG2  | 42:DV:55:ALA:HB3   | 2.20                     | 0.72              |
| 48:D1:23:LYS:HE2  | 48:D1:28:GLY:H     | 1.53                     | 0.72              |
| 9:AI:58:HIS:HB2   | 9:AI:59:PHE:HE1    | 1.51                     | 0.72              |
| 19:AS:15:LEU:O    | 19:AS:19:VAL:HG23  | 1.88                     | 0.72              |
| 25:BA:601:C:H4'   | 30:BF:104:LYS:NZ   | 2.05                     | 0.72              |
| 25:BA:2357:U:OP1  | 47:B0:20:ARG:NH1   | 2.22                     | 0.72              |
| 30:BF:51:THR:OG1  | 30:BF:88:VAL:CG1   | 2.38                     | 0.72              |
| 32:BH:85:LYS:HD3  | 32:BH:133:VAL:HB   | 1.70                     | 0.72              |
| 33:BI:27:ARG:HA   | 33:BI:31:LEU:HD22  | 1.70                     | 0.72              |
| 37:BQ:141:GLN:HB2 | 46:BZ:98:MET:HA    | 1.71                     | 0.72              |
| 38:BR:24:GLN:NE2  | 38:BR:36:THR:HG21  | 2.04                     | 0.72              |
| 41:BU:95:LEU:CD1  | 42:BV:4:ILE:CG2    | 2.67                     | 0.72              |
| 1:CA:992:U:C4'    | 1:CA:993:G:O5'     | 2.37                     | 0.72              |
| 5:CE:148:VAL:HG21 | 8:CH:107:LEU:HD22  | 1.70                     | 0.72              |
| 20:CT:89:ARG:HH22 | 20:CT:104:LEU:HD21 | 1.54                     | 0.72              |
| 25:DA:221:A:OP2   | 25:DA:221:A:C8     | 2.42                     | 0.72              |
| 25:DA:1022:G:H22  | 25:DA:1142(A):A:H2 | 1.35                     | 0.72              |
| 25:DA:1791:A:N6   | 25:DA:1828:G:O2'   | 2.23                     | 0.72              |
| 28:DD:71:ASP:HB2  | 28:DD:103:ARG:HH22 | 1.54                     | 0.72              |
| 28:DD:76:PRO:O    | 28:DD:98:VAL:HG23  | 1.88                     | 0.72              |
| 33:DI:94:ALA:HA   | 33:DI:97:ILE:HG12  | 1.70                     | 0.72              |
| 40:DT:80:SER:HB3  | 40:DT:81:PRO:HD3   | 1.71                     | 0.72              |
| 52:D5:4:HIS:HB3   | 52:D5:5:PRO:CD     | 2.17                     | 0.72              |
| 55:D8:8:LYS:O     | 55:D8:12:LYS:HG3   | 1.89                     | 0.72              |
| 2:AB:87:ARG:HH22  | 2:AB:233:SER:HB2   | 1.54                     | 0.72              |
| 8:AH:129:VAL:HG23 | 8:AH:130:GLY:N     | 2.03                     | 0.72              |
| 10:AJ:62:HIS:O    | 14:AN:59:ALA:HB3   | 1.89                     | 0.72              |
| 25:BA:1287:A:C6   | 25:BA:1288:U:C4    | 2.77                     | 0.72              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 28:BD:223:GLY:HA3  | 28:BD:231:HIS:CD2  | 2.24                     | 0.72              |
| 28:BD:261:LYS:HZ1  | 28:BD:263:ARG:NH2  | 1.88                     | 0.72              |
| 42:BV:19:LYS:HG2   | 42:BV:94:LEU:HB2   | 1.72                     | 0.72              |
| 1:CA:251:G:O2'     | 1:CA:252:U:C5'     | 2.33                     | 0.72              |
| 3:CC:70:VAL:HG12   | 3:CC:72:LYS:H      | 1.54                     | 0.72              |
| 25:DA:995:C:C6     | 41:DU:57:PHE:HE1   | 2.06                     | 0.72              |
| 28:DD:108:PRO:HB3  | 28:DD:143:HIS:HE1  | 1.54                     | 0.72              |
| 33:DI:124:GLY:O    | 33:DI:142:VAL:HG22 | 1.88                     | 0.72              |
| 36:DP:63:PRO:O     | 36:DP:65:ARG:N     | 2.22                     | 0.72              |
| 41:DU:95:LEU:CD1   | 42:DV:4:ILE:CG2    | 2.67                     | 0.72              |
| 42:DV:49:THR:CB    | 42:DV:50:PRO:HD2   | 2.19                     | 0.72              |
| 6:AF:69:GLU:O      | 6:AF:72:VAL:HG12   | 1.87                     | 0.72              |
| 12:AL:81:SER:HA    | 12:AL:106:ASP:OD2  | 1.89                     | 0.72              |
| 28:BD:85:ASP:HB2   | 28:BD:92:ILE:HD12  | 1.71                     | 0.72              |
| 40:BT:50:ILE:HD11  | 40:BT:102:ILE:HG12 | 1.72                     | 0.72              |
| 1:CA:251:G:HO2'    | 1:CA:252:U:H5''    | 1.54                     | 0.72              |
| 3:CC:166:GLU:HA    | 3:CC:166:GLU:OE1   | 1.90                     | 0.72              |
| 19:CS:62:ILE:HD12  | 19:CS:63:THR:N     | 2.05                     | 0.72              |
| 25:DA:1272:A:N9    | 25:DA:1618:A:C8    | 2.58                     | 0.72              |
| 25:DA:1902:C:H5'   | 28:DD:246:PRO:HD3  | 1.70                     | 0.72              |
| 27:DC:41:VAL:HA    | 27:DC:213:TYR:HA   | 1.71                     | 0.72              |
| 33:DI:72:LEU:HD13  | 33:DI:107:VAL:HG11 | 1.69                     | 0.72              |
| 42:DV:95:LEU:HD13  | 42:DV:97:LYS:HE3   | 1.69                     | 0.72              |
| 55:D8:43:GLN:C     | 55:D8:44:LYS:HD2   | 2.15                     | 0.72              |
| 1:AA:689:C:OP1     | 11:AK:27:ASN:ND2   | 2.22                     | 0.72              |
| 13:AM:28:ALA:C     | 13:AM:30:ALA:H     | 1.96                     | 0.72              |
| 16:AP:13:HIS:C     | 16:AP:15:PRO:HD3   | 2.14                     | 0.72              |
| 16:AP:28:ARG:HH11  | 16:AP:28:ARG:HG2   | 1.55                     | 0.72              |
| 17:AQ:85:VAL:HG12  | 17:AQ:89:LEU:HD12  | 1.72                     | 0.72              |
| 18:AR:82:THR:HG22  | 18:AR:83:GLU:N     | 2.04                     | 0.72              |
| 25:BA:1301:A:O2'   | 25:BA:1302:A:H5''  | 1.90                     | 0.72              |
| 30:BF:63:LYS:HE2   | 30:BF:67:GLN:HB3   | 1.71                     | 0.72              |
| 30:BF:132:VAL:HG13 | 30:BF:133:ASN:H    | 1.53                     | 0.72              |
| 40:BT:30:VAL:HG21  | 40:BT:84:GLN:CG    | 2.18                     | 0.72              |
| 1:CA:872:A:C2      | 1:CA:874:G:C6      | 2.77                     | 0.72              |
| 7:CG:60:LYS:HA     | 7:CG:60:LYS:NZ     | 2.05                     | 0.72              |
| 23:CW:67:C:H2'     | 23:CW:68:C:C6      | 2.24                     | 0.72              |
| 29:DE:36:ARG:HH12  | 29:DE:86:PRO:HD2   | 1.53                     | 0.72              |
| 36:DP:63:PRO:C     | 36:DP:65:ARG:H     | 1.96                     | 0.72              |
| 36:DP:80:TYR:HA    | 36:DP:111:ARG:O    | 1.89                     | 0.72              |
| 39:DS:10:ARG:O     | 39:DS:14:VAL:HG12  | 1.89                     | 0.72              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:676:A:H1'     | 11:AK:115:PRO:HB3  | 1.72                     | 0.72              |
| 6:AF:91:VAL:HG12   | 6:AF:92:LYS:O      | 1.89                     | 0.72              |
| 8:AH:40:ALA:C      | 8:AH:42:GLU:H      | 1.98                     | 0.72              |
| 13:AM:8:GLU:OE1    | 13:AM:22:ILE:HG23  | 1.90                     | 0.72              |
| 19:AS:10:PHE:O     | 19:AS:38:SER:HA    | 1.89                     | 0.72              |
| 25:BA:587:C:O2     | 36:BP:33:ARG:NH1   | 2.21                     | 0.72              |
| 25:BA:2056:G:C2    | 25:BA:2057:A:C8    | 2.77                     | 0.72              |
| 25:BA:2745:C:C4    | 25:BA:2746:U:O4    | 2.43                     | 0.72              |
| 36:BP:63:PRO:C     | 36:BP:65:ARG:H     | 1.96                     | 0.72              |
| 36:BP:63:PRO:O     | 36:BP:65:ARG:N     | 2.22                     | 0.72              |
| 49:B2:33:MET:HE3   | 49:B2:37:PHE:CE1   | 2.23                     | 0.72              |
| 6:CF:17:SER:O      | 6:CF:21:LEU:HD23   | 1.90                     | 0.72              |
| 23:CW:18:G:H1      | 23:CW:55:U:H1'     | 1.55                     | 0.72              |
| 3:AC:11:ARG:HH21   | 3:AC:180:ALA:HB3   | 1.53                     | 0.72              |
| 20:AT:63:ILE:HD13  | 20:AT:80:ARG:HB2   | 1.71                     | 0.72              |
| 25:BA:242:G:C6     | 55:B8:5:LYS:CE     | 2.71                     | 0.72              |
| 25:BA:2848:G:C4'   | 25:BA:2849:U:OP1   | 2.37                     | 0.72              |
| 36:BP:48:PRO:O     | 36:BP:49:ARG:C     | 2.30                     | 0.72              |
| 20:CT:104:LEU:HD23 | 20:CT:105:SER:N    | 2.05                     | 0.72              |
| 26:DB:3:C:H42      | 26:DB:118:G:H1     | 1.37                     | 0.72              |
| 30:DF:63:LYS:HA    | 30:DF:76:GLY:O     | 1.90                     | 0.72              |
| 32:DH:101:ARG:HG2  | 32:DH:117:PRO:HG3  | 1.71                     | 0.72              |
| 2:AB:167:PRO:HG2   | 2:AB:192:SER:OG    | 1.89                     | 0.72              |
| 3:AC:90:GLU:OE1    | 3:AC:93:LYS:HD2    | 1.90                     | 0.72              |
| 8:AH:40:ALA:O      | 8:AH:42:GLU:N      | 2.22                     | 0.72              |
| 12:AL:46:LYS:HG2   | 12:AL:47:LYS:N     | 2.05                     | 0.72              |
| 25:BA:13:A:O2'     | 25:BA:15:G:N7      | 2.22                     | 0.72              |
| 25:BA:321:G:OP2    | 30:BF:136:THR:HG22 | 1.90                     | 0.72              |
| 30:BF:152:GLU:OE1  | 30:BF:191:ARG:HD2  | 1.90                     | 0.72              |
| 31:BG:72:ARG:HB3   | 31:BG:86:MET:O     | 1.88                     | 0.72              |
| 40:BT:92:GLY:C     | 40:BT:94:ALA:H     | 1.95                     | 0.72              |
| 1:CA:186:C:O2'     | 20:CT:85:MET:SD    | 2.47                     | 0.72              |
| 1:CA:872:A:C2      | 1:CA:874:G:O6      | 2.43                     | 0.72              |
| 1:CA:1300:G:O2'    | 1:CA:1301:U:H6     | 1.72                     | 0.72              |
| 20:CT:53:LEU:O     | 20:CT:57:ARG:HB2   | 1.90                     | 0.72              |
| 25:DA:27:G:N2      | 25:DA:512:G:H2'    | 2.05                     | 0.72              |
| 25:DA:72:U:H1'     | 49:D2:58:ALA:HA    | 1.71                     | 0.72              |
| 25:DA:2285:C:H5    | 53:D6:27:LYS:HE3   | 1.53                     | 0.72              |
| 30:DF:31:HIS:HB2   | 36:DP:9:ASN:ND2    | 2.04                     | 0.72              |
| 33:DI:92:VAL:HG13  | 33:DI:120:ILE:CG2  | 2.17                     | 0.72              |
| 37:DQ:137:TYR:OH   | 46:DZ:81:ARG:NH2   | 2.23                     | 0.72              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 38:DR:12:ARG:HG3  | 38:DR:12:ARG:HH11  | 1.53                     | 0.72              |
| 39:DS:106:ARG:N   | 39:DS:110:LEU:HD21 | 2.05                     | 0.72              |
| 41:DU:104:GLN:NE2 | 41:DU:105:VAL:HG23 | 2.02                     | 0.72              |
| 46:DZ:19:ARG:HH12 | 46:DZ:84:GLU:HA    | 1.53                     | 0.72              |
| 48:D1:52:ARG:HG3  | 48:D1:53:VAL:H     | 1.53                     | 0.72              |
| 1:AA:839:U:O2     | 1:AA:839:U:C3'     | 2.38                     | 0.72              |
| 1:AA:1118:C:H5''  | 9:AI:104:ARG:HG3   | 1.72                     | 0.72              |
| 3:AC:11:ARG:HB3   | 3:AC:15:THR:HB     | 1.70                     | 0.72              |
| 3:AC:113:ALA:HA   | 3:AC:116:VAL:HG23  | 1.72                     | 0.72              |
| 13:AM:96:LEU:HD23 | 13:AM:97:PRO:HD2   | 1.71                     | 0.72              |
| 16:AP:44:THR:C    | 16:AP:45:THR:HG22  | 2.14                     | 0.72              |
| 23:AW:63:G:O2'    | 27:BC:53:ARG:HG2   | 1.89                     | 0.72              |
| 25:BA:196:A:N3    | 25:BA:196:A:H2'    | 2.03                     | 0.72              |
| 27:BC:51:PRO:HG3  | 27:BC:204:ALA:HB2  | 1.72                     | 0.72              |
| 31:BG:46:ALA:C    | 31:BG:82:LEU:HD11  | 2.15                     | 0.72              |
| 40:BT:28:VAL:HG11 | 40:BT:46:GLU:CA    | 2.13                     | 0.72              |
| 2:CB:98:LEU:HG    | 2:CB:101:MET:HE3   | 1.70                     | 0.72              |
| 13:CM:3:ARG:NH1   | 13:CM:7:VAL:HG22   | 2.04                     | 0.72              |
| 34:DN:4:TYR:N     | 34:DN:4:TYR:CD1    | 2.53                     | 0.72              |
| 41:DU:62:ILE:HD12 | 41:DU:76:TYR:CZ    | 2.24                     | 0.72              |
| 41:DU:91:ASP:OD2  | 41:DU:96:ALA:HB2   | 1.90                     | 0.72              |
| 5:AE:148:VAL:HG21 | 8:AH:107:LEU:HD13  | 1.71                     | 0.71              |
| 36:BP:52:GLU:OE1  | 36:BP:55:ARG:CD    | 2.38                     | 0.71              |
| 1:CA:791:G:H2'    | 1:CA:792:A:H5'     | 1.70                     | 0.71              |
| 9:CI:19:LEU:CD2   | 9:CI:59:PHE:CB     | 2.65                     | 0.71              |
| 11:CK:20:TYR:HB2  | 11:CK:31:THR:HG23  | 1.72                     | 0.71              |
| 19:CS:40:ILE:HG12 | 19:CS:71:LEU:HD23  | 1.72                     | 0.71              |
| 20:CT:50:GLU:OE2  | 20:CT:50:GLU:CA    | 2.33                     | 0.71              |
| 25:DA:84:A:C5'    | 45:DY:8:LYS:HG2    | 2.14                     | 0.71              |
| 25:DA:529:A:H62   | 25:DA:2041:U:H3    | 1.37                     | 0.71              |
| 25:DA:1558:A:C4'  | 25:DA:1559:G:O5'   | 2.37                     | 0.71              |
| 33:DI:60:GLU:HG3  | 33:DI:61:ARG:NH2   | 2.05                     | 0.71              |
| 47:D0:73:GLY:C    | 47:D0:75:LEU:H     | 1.98                     | 0.71              |
| 20:AT:50:GLU:HA   | 20:AT:100:ILE:HG12 | 1.72                     | 0.71              |
| 25:BA:1646:C:C2'  | 25:BA:1647:G:OP1   | 2.39                     | 0.71              |
| 25:BA:1788:C:OP1  | 28:BD:222:ARG:NH2  | 2.23                     | 0.71              |
| 35:BO:2:ILE:HD12  | 35:BO:6:THR:HG21   | 1.70                     | 0.71              |
| 43:BW:6:ILE:HG12  | 43:BW:104:THR:HG23 | 1.71                     | 0.71              |
| 1:CA:243:A:C2     | 1:CA:246:A:N7      | 2.58                     | 0.71              |
| 1:CA:484:G:H1'    | 1:CA:486:U:C5      | 2.24                     | 0.71              |
| 5:CE:48:ALA:HB3   | 5:CE:54:ALA:N      | 2.05                     | 0.71              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 9:CI:50:LEU:HA    | 9:CI:53:VAL:HG22   | 1.72                     | 0.71              |
| 25:DA:645:C:H2'   | 25:DA:645:C:O2     | 1.89                     | 0.71              |
| 27:DC:58:VAL:HG21 | 27:DC:166:ASP:N    | 1.97                     | 0.71              |
| 28:DD:26:LYS:O    | 28:DD:27:THR:HB    | 1.89                     | 0.71              |
| 30:DF:24:LEU:HD23 | 30:DF:115:ALA:HA   | 1.70                     | 0.71              |
| 30:DF:95:ARG:CZ   | 30:DF:97:TYR:HE1   | 2.03                     | 0.71              |
| 46:DZ:5:LEU:HD21  | 46:DZ:39:VAL:HB    | 1.71                     | 0.71              |
| 7:AG:69:VAL:HG12  | 7:AG:100:ALA:HA    | 1.71                     | 0.71              |
| 30:BF:7:TYR:HB2   | 30:BF:17:ARG:N     | 2.06                     | 0.71              |
| 31:BG:142:PRO:CG  | 31:BG:143:GLU:OE1  | 2.30                     | 0.71              |
| 33:BI:77:LEU:O    | 33:BI:140:LEU:CD1  | 2.36                     | 0.71              |
| 45:BY:31:LEU:HB2  | 45:BY:32:PRO:HA    | 1.72                     | 0.71              |
| 45:BY:67:LEU:CD1  | 45:BY:71:LYS:HG3   | 2.20                     | 0.71              |
| 55:B8:53:PRO:HA   | 55:B8:56:GLU:HB3   | 1.71                     | 0.71              |
| 2:CB:155:LEU:HD13 | 2:CB:157:ARG:H     | 1.54                     | 0.71              |
| 2:CB:171:ALA:HA   | 2:CB:174:VAL:HG23  | 1.72                     | 0.71              |
| 2:CB:219:VAL:O    | 2:CB:222:ILE:HB    | 1.90                     | 0.71              |
| 20:CT:29:LYS:CD   | 20:CT:66:ALA:HB2   | 2.19                     | 0.71              |
| 25:DA:1694:C:H4'  | 25:DA:1695:G:C4    | 2.25                     | 0.71              |
| 30:DF:180:GLY:O   | 30:DF:181:LEU:C    | 2.32                     | 0.71              |
| 32:DH:87:LEU:HD13 | 32:DH:148:ILE:HG21 | 1.72                     | 0.71              |
| 33:DI:77:LEU:O    | 33:DI:78:THR:HG23  | 1.91                     | 0.71              |
| 40:DT:102:ILE:O   | 40:DT:106:SER:HB3  | 1.91                     | 0.71              |
| 41:DU:66:ASN:HB2  | 41:DU:76:TYR:HB2   | 1.72                     | 0.71              |
| 47:D0:40:GLN:NE2  | 47:D0:43:THR:HA    | 2.05                     | 0.71              |
| 22:AV:63:C:H2'    | 22:AV:64:G:C8      | 2.26                     | 0.71              |
| 41:BU:27:LEU:HB2  | 41:BU:34:LYS:HG3   | 1.72                     | 0.71              |
| 1:CA:687:A:C2     | 1:CA:704:A:C5      | 2.78                     | 0.71              |
| 22:CV:3:C:H42     | 22:CV:71:G:H1      | 1.38                     | 0.71              |
| 25:DA:942:G:O2'   | 25:DA:1189:A:N3    | 2.22                     | 0.71              |
| 28:DD:264:LYS:HD3 | 28:DD:266:SER:HB3  | 1.71                     | 0.71              |
| 32:DH:154:PRO:HG2 | 32:DH:162:ILE:O    | 1.91                     | 0.71              |
| 36:DP:11:GLY:O    | 36:DP:12:ALA:HB3   | 1.90                     | 0.71              |
| 40:DT:36:GLU:CB   | 40:DT:38:ASN:ND2   | 2.49                     | 0.71              |
| 1:AA:971:G:OP1    | 1:AA:971:G:H3'     | 1.89                     | 0.71              |
| 25:BA:1270:C:N4   | 25:BA:1648:C:N4    | 2.38                     | 0.71              |
| 30:BF:65:TRP:CH2  | 30:BF:72:ARG:NH2   | 2.58                     | 0.71              |
| 32:BH:86:GLU:HA   | 32:BH:132:ARG:HA   | 1.72                     | 0.71              |
| 4:CD:31:CYS:C     | 4:CD:33:MET:H      | 1.97                     | 0.71              |
| 9:CI:59:PHE:CD1   | 9:CI:59:PHE:N      | 2.56                     | 0.71              |
| 35:DO:113:LYS:O   | 35:DO:117:LEU:HB2  | 1.91                     | 0.71              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 40:DT:125:ARG:O   | 40:DT:128:GLU:CG   | 2.36                     | 0.71              |
| 46:DZ:59:LEU:HG   | 46:DZ:69:THR:HG21  | 1.72                     | 0.71              |
| 1:AA:1047:G:H2'   | 1:AA:1048:G:H5'    | 1.71                     | 0.71              |
| 17:AQ:56:VAL:HB   | 17:AQ:78:GLU:HG2   | 1.71                     | 0.71              |
| 23:AY:35:A:C2'    | 23:AY:36:A:O5'     | 2.39                     | 0.71              |
| 25:BA:395:U:O2'   | 25:BA:396:G:N7     | 2.21                     | 0.71              |
| 25:BA:2681:C:H5   | 25:BA:2725:A:H62   | 1.36                     | 0.71              |
| 30:BF:205:ARG:HG2 | 30:BF:205:ARG:O    | 1.90                     | 0.71              |
| 33:BI:83:ALA:HA   | 33:BI:89:TYR:CD1   | 2.25                     | 0.71              |
| 40:BT:36:GLU:HG3  | 40:BT:38:ASN:HB3   | 1.72                     | 0.71              |
| 1:CA:411:A:C8     | 1:CA:429:U:O4      | 2.43                     | 0.71              |
| 1:CA:538:G:H5''   | 12:CL:114:LYS:HB2  | 1.72                     | 0.71              |
| 1:CA:820:U:H6     | 1:CA:820:U:O5'     | 1.72                     | 0.71              |
| 10:CJ:63:PHE:HB3  | 14:CN:58:LYS:CA    | 2.18                     | 0.71              |
| 20:CT:83:ARG:C    | 20:CT:85:MET:H     | 1.99                     | 0.71              |
| 22:CV:48:U:C6     | 22:CV:51:U:OP1     | 2.44                     | 0.71              |
| 25:DA:2015:A:H1'  | 52:D5:2:ALA:HA     | 1.72                     | 0.71              |
| 31:DG:146:TYR:O   | 31:DG:149:VAL:HG22 | 1.90                     | 0.71              |
| 33:DI:60:GLU:HG3  | 33:DI:61:ARG:HH12  | 1.56                     | 0.71              |
| 40:DT:66:VAL:HA   | 40:DT:71:GLY:HA2   | 1.72                     | 0.71              |
| 1:AA:1524:C:OP1   | 11:AK:120:ARG:NH1  | 2.22                     | 0.71              |
| 2:AB:95:GLN:HG3   | 2:AB:148:TYR:HA    | 1.72                     | 0.71              |
| 19:AS:29:ARG:HH11 | 19:AS:30:LEU:H     | 1.35                     | 0.71              |
| 21:AU:2:GLY:O     | 21:AU:4:GLY:N      | 2.22                     | 0.71              |
| 25:BA:240:G:N1    | 25:BA:241:A:N6     | 2.39                     | 0.71              |
| 29:BE:11:MET:HB2  | 29:BE:23:VAL:O     | 1.91                     | 0.71              |
| 43:BW:4:LYS:HE3   | 43:BW:6:ILE:HD12   | 1.70                     | 0.71              |
| 43:BW:82:LEU:HB3  | 43:BW:84:ARG:HH12  | 1.55                     | 0.71              |
| 19:CS:58:VAL:HG11 | 19:CS:75:ALA:HB1   | 1.71                     | 0.71              |
| 25:DA:2725:A:O2'  | 25:DA:2726:U:C2    | 2.44                     | 0.71              |
| 41:DU:79:PHE:HE2  | 41:DU:83:LEU:CD2   | 2.04                     | 0.71              |
| 45:DY:20:TYR:CE1  | 45:DY:42:VAL:HA    | 2.26                     | 0.71              |
| 45:DY:84:ARG:HH12 | 45:DY:97:ARG:CB    | 2.04                     | 0.71              |
| 46:DZ:14:LYS:HZ2  | 46:DZ:14:LYS:H     | 1.36                     | 0.71              |
| 6:AF:91:VAL:HG21  | 18:AR:72:ARG:HD3   | 1.71                     | 0.71              |
| 23:AW:8:U:O2      | 23:AW:21:A:H2      | 1.72                     | 0.71              |
| 25:BA:1653:G:C4'  | 25:BA:1654:A:O5'   | 2.37                     | 0.71              |
| 25:BA:2238:G:C4'  | 25:BA:2239:G:OP1   | 2.39                     | 0.71              |
| 31:BG:111:LEU:HB3 | 31:BG:117:PHE:CE2  | 2.26                     | 0.71              |
| 35:BO:98:VAL:HG12 | 35:BO:117:LEU:HD22 | 1.72                     | 0.71              |
| 36:BP:124:LYS:HZ2 | 36:BP:143:GLY:HA3  | 1.56                     | 0.71              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 41:BU:90:VAL:HG12  | 41:BU:91:ASP:H    | 1.56                     | 0.71              |
| 43:BW:100:THR:HG22 | 43:BW:100:THR:O   | 1.91                     | 0.71              |
| 2:CB:21:ARG:CB     | 2:CB:39:ILE:HA    | 2.15                     | 0.71              |
| 8:CH:104:ARG:C     | 8:CH:106:GLY:H    | 1.98                     | 0.71              |
| 11:CK:54:ARG:HH12  | 23:CW:40:C:H5''   | 1.55                     | 0.71              |
| 23:CW:33:U:O2'     | 23:CW:34:G:H5''   | 1.91                     | 0.71              |
| 23:CW:60:U:H2'     | 23:CW:61:C:H5     | 1.55                     | 0.71              |
| 25:DA:1694:C:H6    | 25:DA:1694:C:OP2  | 1.74                     | 0.71              |
| 28:DD:80:ALA:CB    | 28:DD:94:LEU:HD13 | 2.19                     | 0.71              |
| 31:DG:151:ALA:HB3  | 31:DG:153:ARG:NH1 | 2.05                     | 0.71              |
| 39:DS:106:ARG:HA   | 39:DS:110:LEU:CG  | 2.21                     | 0.71              |
| 40:DT:40:THR:O     | 40:DT:41:ARG:HB2  | 1.91                     | 0.71              |
| 5:AE:100:VAL:HG13  | 5:AE:118:ILE:CG2  | 2.21                     | 0.71              |
| 12:AL:5:PRO:CA     | 12:AL:9:GLN:HE21  | 2.02                     | 0.71              |
| 13:AM:57:ARG:HH22  | 51:B4:60:GLU:HG3  | 1.53                     | 0.71              |
| 25:BA:2126:A:C4'   | 25:BA:2127:G:O5'  | 2.32                     | 0.71              |
| 45:BY:13:VAL:HG22  | 45:BY:28:LYS:HE2  | 1.71                     | 0.71              |
| 13:CM:3:ARG:HB3    | 51:D4:34:GLU:HG2  | 1.72                     | 0.71              |
| 16:CP:49:LEU:HD12  | 16:CP:50:LYS:N    | 2.06                     | 0.71              |
| 25:DA:1204:A:H1'   | 25:DA:1206:G:C8   | 2.25                     | 0.71              |
| 25:DA:1645:G:C5'   | 25:DA:1646:C:H5'  | 2.16                     | 0.71              |
| 35:DO:2:ILE:HD12   | 35:DO:6:THR:HG21  | 1.73                     | 0.71              |
| 53:D6:36:LEU:HD13  | 53:D6:50:ARG:NH1  | 2.05                     | 0.71              |
| 10:AJ:37:PRO:HA    | 10:AJ:72:VAL:HG22 | 1.73                     | 0.71              |
| 25:BA:1342:A:C5    | 25:BA:1397:U:C5   | 2.77                     | 0.71              |
| 25:BA:1966:A:C1'   | 25:BA:2593:U:H5'  | 2.16                     | 0.71              |
| 25:BA:2222:G:H5''  | 28:BD:186:HIS:HE2 | 1.55                     | 0.71              |
| 28:BD:97:TYR:HE1   | 28:BD:103:ARG:HG3 | 1.56                     | 0.71              |
| 38:BR:38:VAL:O     | 38:BR:42:LYS:HG3  | 1.91                     | 0.71              |
| 40:BT:30:VAL:CG1   | 40:BT:31:SER:N    | 2.54                     | 0.71              |
| 1:CA:66:G:H4'      | 1:CA:173:U:O4     | 1.91                     | 0.71              |
| 5:CE:126:ARG:HH11  | 5:CE:126:ARG:CG   | 2.01                     | 0.71              |
| 22:CV:62:C:O2'     | 22:CV:63:C:H5'    | 1.91                     | 0.71              |
| 25:DA:1689:A:H62   | 25:DA:1698:A:H2   | 1.39                     | 0.71              |
| 37:DQ:27:VAL:HG23  | 37:DQ:137:TYR:CE1 | 2.26                     | 0.71              |
| 42:DV:49:THR:OG1   | 42:DV:50:PRO:HD2  | 1.91                     | 0.71              |
| 53:D6:35:GLU:HB3   | 53:D6:51:GLU:HG3  | 1.71                     | 0.71              |
| 1:AA:979:C:OP1     | 1:AA:1223:C:N4    | 2.23                     | 0.70              |
| 7:AG:145:ALA:O     | 7:AG:146:GLU:HB2  | 1.88                     | 0.70              |
| 9:AI:8:GLY:HA2     | 9:AI:79:LEU:HD12  | 1.73                     | 0.70              |
| 34:BN:58:ASP:C     | 34:BN:60:ILE:H    | 1.98                     | 0.70              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 35:BO:3:GLN:HB2    | 35:BO:4:PRO:HD2   | 1.72                     | 0.70              |
| 40:BT:31:SER:HB3   | 40:BT:43:GLN:H    | 1.54                     | 0.70              |
| 52:B5:36:CYS:HB2   | 52:B5:49:CYS:SG   | 2.31                     | 0.70              |
| 1:CA:1067:A:HO2'   | 1:CA:1068:G:H8    | 1.22                     | 0.70              |
| 1:CA:1432:G:OP1    | 40:DT:107:ASP:HB2 | 1.91                     | 0.70              |
| 25:DA:83:G:H21     | 25:DA:84:A:N6     | 1.89                     | 0.70              |
| 25:DA:2713:A:H5'   | 25:DA:2714:G:OP2  | 1.91                     | 0.70              |
| 33:DI:25:TYR:HE2   | 33:DI:29:TYR:HD2  | 1.37                     | 0.70              |
| 40:DT:31:SER:HB3   | 40:DT:43:GLN:O    | 1.90                     | 0.70              |
| 40:DT:89:VAL:CG1   | 40:DT:91:ARG:HE   | 2.04                     | 0.70              |
| 46:DZ:24:LEU:HD21  | 46:DZ:86:VAL:HG23 | 1.72                     | 0.70              |
| 55:D8:30:ARG:HE    | 55:D8:30:ARG:HA   | 1.56                     | 0.70              |
| 1:AA:390:C:O3'     | 16:AP:28:ARG:NH2  | 2.24                     | 0.70              |
| 6:AF:61:LEU:O      | 6:AF:62:TRP:HB2   | 1.89                     | 0.70              |
| 9:AI:28:VAL:HG22   | 9:AI:63:ILE:HB    | 1.74                     | 0.70              |
| 13:AM:15:VAL:O     | 13:AM:19:LEU:HD23 | 1.90                     | 0.70              |
| 18:AR:43:PHE:O     | 18:AR:51:LEU:HD12 | 1.91                     | 0.70              |
| 25:BA:2745:C:H2'   | 25:BA:2746:U:C6   | 2.27                     | 0.70              |
| 28:BD:33:LEU:O     | 28:BD:35:LYS:N    | 2.24                     | 0.70              |
| 30:BF:51:THR:CG2   | 30:BF:92:PRO:HD2  | 2.16                     | 0.70              |
| 1:CA:429:U:O4'     | 1:CA:430:A:H8     | 1.72                     | 0.70              |
| 1:CA:1442(B):A:N1  | 40:DT:118:ARG:NH1 | 2.39                     | 0.70              |
| 3:CC:103:VAL:O     | 3:CC:103:VAL:HG12 | 1.92                     | 0.70              |
| 8:CH:103:VAL:HG12  | 8:CH:108:GLY:HA3  | 1.73                     | 0.70              |
| 19:CS:63:THR:HG22  | 19:CS:66:MET:SD   | 2.31                     | 0.70              |
| 25:DA:84:A:H5'     | 45:DY:8:LYS:CG    | 2.16                     | 0.70              |
| 25:DA:750:A:H2'    | 25:DA:752:A:OP1   | 1.91                     | 0.70              |
| 28:DD:24:ILE:CG1   | 28:DD:25:THR:N    | 2.53                     | 0.70              |
| 29:DE:203:LYS:HE2  | 29:DE:204:ALA:HB2 | 1.73                     | 0.70              |
| 33:DI:60:GLU:HG3   | 33:DI:61:ARG:NH1  | 2.07                     | 0.70              |
| 1:AA:971:G:OP1     | 1:AA:972:C:H5''   | 1.92                     | 0.70              |
| 2:AB:32:ILE:HD11   | 2:AB:190:THR:CG2  | 2.21                     | 0.70              |
| 20:AT:12:ALA:O     | 20:AT:15:ARG:HB2  | 1.91                     | 0.70              |
| 25:BA:673:C:H5'    | 30:BF:54:ARG:HH12 | 1.57                     | 0.70              |
| 29:BE:116:VAL:HG21 | 29:BE:122:PHE:CD2 | 2.26                     | 0.70              |
| 36:BP:15:ARG:O     | 36:BP:16:ARG:C    | 2.34                     | 0.70              |
| 36:BP:19:VAL:CG2   | 36:BP:20:GLY:H    | 2.02                     | 0.70              |
| 40:BT:28:VAL:O     | 40:BT:29:ARG:CB   | 2.39                     | 0.70              |
| 40:BT:29:ARG:HD2   | 40:BT:86:ILE:O    | 1.91                     | 0.70              |
| 1:CA:913:A:C1'     | 1:CA:914:A:O4'    | 2.38                     | 0.70              |
| 23:CW:60:U:H2'     | 23:CW:61:C:C5     | 2.26                     | 0.70              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:DA:913:U:C4'    | 25:DA:914:C:OP1    | 2.34                     | 0.70              |
| 29:DE:33:VAL:HG13  | 29:DE:69:LYS:HE3   | 1.72                     | 0.70              |
| 31:DG:21:ARG:HH11  | 31:DG:21:ARG:HG2   | 1.55                     | 0.70              |
| 32:DH:109:PHE:C    | 32:DH:111:HIS:H    | 1.98                     | 0.70              |
| 40:DT:32:TYR:OH    | 40:DT:76:PHE:CE2   | 2.44                     | 0.70              |
| 53:D6:9:LEU:HD23   | 53:D6:10:LEU:N     | 2.07                     | 0.70              |
| 12:AL:28:LYS:O     | 12:AL:28:LYS:CG    | 2.32                     | 0.70              |
| 23:AY:31:A:C5      | 23:AY:32:U:C5      | 2.80                     | 0.70              |
| 25:BA:651:G:H5''   | 55:B8:18:ALA:HB3   | 1.73                     | 0.70              |
| 25:BA:769:G:C5'    | 25:BA:1379:A:H62   | 2.04                     | 0.70              |
| 25:BA:2392:A:H2    | 25:BA:2424:C:H42   | 1.35                     | 0.70              |
| 28:BD:200:ASP:O    | 28:BD:203:ASN:HB2  | 1.90                     | 0.70              |
| 28:BD:270:ILE:H    | 28:BD:270:ILE:HD12 | 1.56                     | 0.70              |
| 40:BT:31:SER:OG    | 40:BT:43:GLN:N     | 2.25                     | 0.70              |
| 48:B1:3:LYS:CG     | 48:B1:4:VAL:H      | 2.05                     | 0.70              |
| 2:CB:61:LEU:CD2    | 2:CB:68:ILE:HD11   | 2.21                     | 0.70              |
| 2:CB:167:PRO:HG2   | 2:CB:192:SER:OG    | 1.91                     | 0.70              |
| 2:CB:236:TYR:HA    | 2:CB:239:VAL:HG21  | 1.73                     | 0.70              |
| 8:CH:82:HIS:CD2    | 8:CH:138:TRP:CE2   | 2.78                     | 0.70              |
| 20:CT:33:ILE:H     | 20:CT:33:ILE:CD1   | 2.04                     | 0.70              |
| 25:DA:598:G:C5'    | 36:DP:11:GLY:HA3   | 2.22                     | 0.70              |
| 25:DA:1272:A:C1'   | 25:DA:1618:A:C8    | 2.74                     | 0.70              |
| 28:DD:121:PRO:HB3  | 28:DD:135:PHE:CE1  | 2.26                     | 0.70              |
| 32:DH:20:ALA:HB3   | 32:DH:21:PRO:HD2   | 1.73                     | 0.70              |
| 39:DS:60:GLY:O     | 39:DS:61:ASN:HB2   | 1.90                     | 0.70              |
| 39:DS:106:ARG:CA   | 39:DS:110:LEU:HD21 | 2.21                     | 0.70              |
| 47:D0:24:LYS:O     | 47:D0:25:ARG:HD3   | 1.90                     | 0.70              |
| 1:AA:1300:G:H2'    | 1:AA:1301:U:OP2    | 1.91                     | 0.70              |
| 3:AC:131:ARG:HH11  | 5:AE:50:GLU:HG2    | 1.56                     | 0.70              |
| 4:AD:49:ARG:CD     | 4:AD:50:ARG:H      | 2.02                     | 0.70              |
| 25:BA:181:A:C2     | 25:BA:435:C:C5     | 2.79                     | 0.70              |
| 25:BA:804:A:H5''   | 25:BA:805:G:OP1    | 1.91                     | 0.70              |
| 28:BD:221:VAL:HG22 | 28:BD:226:MET:HE2  | 1.73                     | 0.70              |
| 36:BP:64:LYS:HB3   | 55:B8:25:MET:CG    | 2.18                     | 0.70              |
| 41:BU:96:ALA:C     | 41:BU:98:LEU:N     | 2.46                     | 0.70              |
| 42:BV:15:GLU:HB3   | 42:BV:16:PRO:CD    | 2.22                     | 0.70              |
| 1:CA:1049:U:H1'    | 1:CA:1201:A:C8     | 2.27                     | 0.70              |
| 2:CB:224:GLN:HA    | 2:CB:229:VAL:HG22  | 1.72                     | 0.70              |
| 8:CH:87:SER:HA     | 8:CH:93:VAL:CG2    | 2.20                     | 0.70              |
| 19:CS:63:THR:HG23  | 19:CS:66:MET:HG2   | 1.74                     | 0.70              |
| 25:DA:1918:A:O2'   | 25:DA:1919:A:N7    | 2.22                     | 0.70              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 28:DD:8:PRO:HB3    | 28:DD:14:ARG:HB2   | 1.72                     | 0.70              |
| 28:DD:172:TYR:CD1  | 28:DD:186:HIS:HA   | 2.27                     | 0.70              |
| 31:DG:6:ALA:HB3    | 31:DG:104:GLU:OE2  | 1.91                     | 0.70              |
| 32:DH:4:ILE:HG13   | 32:DH:6:ARG:CD     | 2.22                     | 0.70              |
| 32:DH:117:PRO:HB3  | 32:DH:123:PHE:CE1  | 2.26                     | 0.70              |
| 40:DT:32:TYR:HD2   | 40:DT:81:PRO:O     | 1.74                     | 0.70              |
| 43:DW:55:ALA:HA    | 43:DW:107:LEU:HD23 | 1.72                     | 0.70              |
| 5:AE:135:THR:O     | 5:AE:138:ALA:HB3   | 1.91                     | 0.70              |
| 10:AJ:35:SER:O     | 10:AJ:72:VAL:HG13  | 1.90                     | 0.70              |
| 22:AV:19:G:N2      | 22:AV:59:A:C8      | 2.60                     | 0.70              |
| 22:AV:41:C:O2'     | 22:AV:42:C:H5'     | 1.91                     | 0.70              |
| 23:AY:35:A:H2'     | 23:AY:36:A:O5'     | 1.90                     | 0.70              |
| 25:BA:2578:G:OP2   | 25:BA:2578:G:H4'   | 1.89                     | 0.70              |
| 30:BF:47:GLY:HA3   | 30:BF:95:ARG:O     | 1.92                     | 0.70              |
| 33:BI:4:ILE:HG12   | 33:BI:18:VAL:HG22  | 1.71                     | 0.70              |
| 36:BP:63:PRO:C     | 36:BP:65:ARG:N     | 2.49                     | 0.70              |
| 39:BS:97:ARG:NH1   | 39:BS:98:VAL:HA    | 2.06                     | 0.70              |
| 1:CA:397:A:N7      | 1:CA:547:A:O2'     | 2.24                     | 0.70              |
| 4:CD:49:ARG:HD3    | 4:CD:50:ARG:N      | 2.05                     | 0.70              |
| 7:CG:41:ARG:O      | 7:CG:45:ASP:HB2    | 1.91                     | 0.70              |
| 33:DI:25:TYR:HE2   | 33:DI:29:TYR:CD2   | 2.09                     | 0.70              |
| 1:AA:686:U:O2'     | 11:AK:42:TRP:HZ2   | 1.74                     | 0.70              |
| 5:AE:70:PRO:HB2    | 5:AE:144:THR:CG2   | 2.22                     | 0.70              |
| 25:BA:2222:G:H5''  | 28:BD:186:HIS:NE2  | 2.07                     | 0.70              |
| 29:BE:116:VAL:HG22 | 29:BE:117:MET:N    | 2.06                     | 0.70              |
| 1:CA:839:U:O2      | 1:CA:839:U:C2'     | 2.39                     | 0.70              |
| 11:CK:125:PHE:HD1  | 11:CK:125:PHE:N    | 1.88                     | 0.70              |
| 20:CT:48:LYS:CB    | 20:CT:48:LYS:HZ3   | 2.02                     | 0.70              |
| 28:DD:95:LEU:O     | 28:DD:95:LEU:HD12  | 1.92                     | 0.70              |
| 38:DR:56:LYS:HE2   | 38:DR:94:TYR:HE2   | 1.56                     | 0.70              |
| 45:DY:63:LYS:NZ    | 45:DY:63:LYS:HA    | 2.07                     | 0.70              |
| 1:AA:366:C:O2'     | 1:AA:367:U:P       | 2.49                     | 0.70              |
| 1:AA:1067:A:HO2'   | 1:AA:1068:G:H8     | 0.74                     | 0.70              |
| 1:AA:1226:C:HO2'   | 1:AA:1227:A:C5'    | 2.05                     | 0.70              |
| 4:AD:8:VAL:O       | 4:AD:11:LEU:CD2    | 2.39                     | 0.70              |
| 5:AE:75:THR:OG1    | 5:AE:76:ILE:N      | 2.22                     | 0.70              |
| 9:AI:5:TYR:CG      | 9:AI:6:GLY:N       | 2.59                     | 0.70              |
| 25:BA:974:G:N2     | 25:BA:989:G:H1'    | 2.07                     | 0.70              |
| 37:BQ:56:ARG:HA    | 37:BQ:56:ARG:NH1   | 2.06                     | 0.70              |
| 45:BY:46:LYS:HB3   | 45:BY:47:LYS:HD2   | 1.72                     | 0.70              |
| 49:B2:63:VAL:O     | 49:B2:66:GLU:HG2   | 1.92                     | 0.70              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:376:G:P       | 16:CP:67:THR:HG21  | 2.32                     | 0.70              |
| 11:CK:20:TYR:O     | 11:CK:30:VAL:HA    | 1.92                     | 0.70              |
| 20:CT:49:ALA:HB3   | 20:CT:100:ILE:HD11 | 1.71                     | 0.70              |
| 20:CT:56:MET:O     | 20:CT:60:GLU:HB2   | 1.91                     | 0.70              |
| 22:CV:24:C:H2'     | 22:CV:25:U:C6      | 2.26                     | 0.70              |
| 25:DA:395:U:O2'    | 25:DA:396:G:N7     | 2.23                     | 0.70              |
| 25:DA:975(A):G:O2' | 25:DA:976:C:H5'    | 1.91                     | 0.70              |
| 39:DS:27:SER:HA    | 39:DS:88:ASP:HB3   | 1.73                     | 0.70              |
| 9:AI:59:PHE:CD1    | 9:AI:59:PHE:N      | 2.57                     | 0.70              |
| 11:AK:85:ARG:HD3   | 11:AK:113:PRO:HD3  | 1.72                     | 0.70              |
| 25:BA:1341:U:O4    | 44:BX:16:LYS:HE2   | 1.91                     | 0.70              |
| 25:BA:1646:C:H2'   | 25:BA:1647:G:OP1   | 1.92                     | 0.70              |
| 29:BE:64:LYS:C     | 29:BE:66:HIS:H     | 1.98                     | 0.70              |
| 33:BI:83:ALA:HA    | 33:BI:89:TYR:HD1   | 1.54                     | 0.70              |
| 39:BS:17:ARG:O     | 39:BS:19:LYS:N     | 2.25                     | 0.70              |
| 39:BS:97:ARG:HH22  | 39:BS:98:VAL:HG23  | 1.57                     | 0.70              |
| 40:BT:32:TYR:CD2   | 40:BT:81:PRO:O     | 2.45                     | 0.70              |
| 45:BY:36:ALA:HB1   | 45:BY:67:LEU:O     | 1.91                     | 0.70              |
| 4:CD:119:GLN:O     | 4:CD:123:HIS:HB2   | 1.92                     | 0.70              |
| 23:CY:27:G:H2'     | 23:CY:28:G:C8      | 2.26                     | 0.70              |
| 25:DA:973:A:H5''   | 25:DA:974:G:OP2    | 1.92                     | 0.70              |
| 33:DI:49:ALA:O     | 33:DI:52:ARG:HG2   | 1.91                     | 0.70              |
| 41:DU:62:ILE:HD12  | 41:DU:76:TYR:CE1   | 2.26                     | 0.70              |
| 45:DY:81:LYS:HB2   | 45:DY:96:ILE:CG2   | 2.21                     | 0.70              |
| 5:AE:91:LEU:CD1    | 5:AE:120:THR:HB    | 2.22                     | 0.70              |
| 9:AI:47:LEU:C      | 9:AI:49:PRO:HD2    | 2.17                     | 0.70              |
| 13:AM:94:ARG:HG2   | 19:AS:82:GLY:N     | 2.07                     | 0.70              |
| 15:AO:65:ARG:HH11  | 15:AO:65:ARG:HG2   | 1.55                     | 0.70              |
| 23:AW:16:U:H3'     | 23:AW:17:C:H5'     | 1.71                     | 0.70              |
| 29:BE:91:VAL:HG13  | 29:BE:95:ILE:HG12  | 1.74                     | 0.70              |
| 31:BG:54:GLU:HA    | 31:BG:57:ALA:HB3   | 1.74                     | 0.70              |
| 43:BW:12:ILE:HG12  | 43:BW:17:VAL:HG12  | 1.73                     | 0.70              |
| 45:BY:8:LYS:HD2    | 45:BY:8:LYS:N      | 2.04                     | 0.70              |
| 1:CA:1054:C:O2     | 1:CA:1054:C:C2'    | 2.40                     | 0.70              |
| 1:CA:1504:G:H3'    | 1:CA:1504:G:P      | 2.32                     | 0.70              |
| 10:CJ:90:LEU:N     | 10:CJ:91:PRO:HD3   | 2.07                     | 0.70              |
| 16:CP:17:TYR:HE1   | 16:CP:41:PRO:HG3   | 1.56                     | 0.70              |
| 17:CQ:12:SER:HB3   | 17:CQ:20:THR:HB    | 1.74                     | 0.70              |
| 22:CV:48:U:H3'     | 22:CV:49:C:C5'     | 2.22                     | 0.70              |
| 32:DH:8:PRO:HG2    | 32:DH:69:ARG:NE    | 2.07                     | 0.70              |
| 33:DI:23:PRO:HB2   | 33:DI:27:ARG:HH12  | 1.56                     | 0.70              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 38:DR:33:ARG:HG3   | 38:DR:115:GLU:CB   | 2.21                     | 0.70              |
| 41:DU:95:LEU:HD13  | 42:DV:4:ILE:HG23   | 1.71                     | 0.70              |
| 1:AA:1528:U:O2'    | 1:AA:1530:G:H5'    | 1.92                     | 0.69              |
| 2:AB:215:LEU:O     | 2:AB:219:VAL:HG23  | 1.92                     | 0.69              |
| 8:AH:111:ILE:O     | 8:AH:112:LEU:HD23  | 1.92                     | 0.69              |
| 25:BA:2134:A:N6    | 25:BA:2157:G:O2'   | 2.25                     | 0.69              |
| 30:BF:123:LEU:HD12 | 30:BF:124:LEU:N    | 2.04                     | 0.69              |
| 32:BH:102:ALA:HB1  | 32:BH:115:VAL:O    | 1.92                     | 0.69              |
| 39:BS:85:VAL:HG23  | 39:BS:106:ARG:HG3  | 1.73                     | 0.69              |
| 40:BT:27:THR:CG2   | 40:BT:49:VAL:CG2   | 2.70                     | 0.69              |
| 55:B8:22:VAL:HG11  | 55:B8:56:GLU:HG2   | 1.72                     | 0.69              |
| 1:CA:407:G:H1      | 1:CA:435:C:H42     | 1.40                     | 0.69              |
| 1:CA:429:U:H4'     | 1:CA:430:A:O5'     | 1.91                     | 0.69              |
| 5:CE:78:HIS:CD2    | 8:CH:104:ARG:HG2   | 2.27                     | 0.69              |
| 13:CM:125:ARG:CD   | 13:CM:126:LYS:H    | 1.92                     | 0.69              |
| 25:DA:2835:A:C5'   | 25:DA:2836:U:OP1   | 2.39                     | 0.69              |
| 30:DF:136:THR:O    | 30:DF:140:LEU:HB2  | 1.92                     | 0.69              |
| 33:DI:2:LYS:HA     | 33:DI:20:ASP:HA    | 1.72                     | 0.69              |
| 37:DQ:59:ARG:O     | 37:DQ:60:ARG:HB2   | 1.91                     | 0.69              |
| 43:DW:68:ARG:HD2   | 43:DW:110:LYS:CB   | 2.22                     | 0.69              |
| 45:DY:86:ARG:HB2   | 45:DY:95:LYS:HD2   | 1.72                     | 0.69              |
| 53:D6:19:ARG:HG2   | 53:D6:20:ASN:N     | 2.05                     | 0.69              |
| 25:BA:2689:U:H5'   | 25:BA:2689:U:C6    | 2.27                     | 0.69              |
| 28:BD:172:TYR:HD1  | 28:BD:186:HIS:HA   | 1.57                     | 0.69              |
| 30:BF:2:LYS:HD3    | 30:BF:2:LYS:N      | 2.06                     | 0.69              |
| 35:BO:35:VAL:HG11  | 35:BO:103:ALA:HB3  | 1.74                     | 0.69              |
| 1:CA:1348:U:H4'    | 9:CI:120:ARG:CD    | 2.20                     | 0.69              |
| 3:CC:105:GLU:HG2   | 3:CC:106:VAL:H     | 1.56                     | 0.69              |
| 10:CJ:58:ASP:O     | 10:CJ:60:ARG:N     | 2.24                     | 0.69              |
| 14:CN:44:LEU:C     | 14:CN:44:LEU:HD12  | 2.18                     | 0.69              |
| 19:CS:63:THR:CG2   | 19:CS:66:MET:HE3   | 2.21                     | 0.69              |
| 29:DE:110:GLY:HA2  | 29:DE:161:GLY:HA3  | 1.72                     | 0.69              |
| 32:DH:30:LYS:HE3   | 32:DH:81:GLU:HA    | 1.74                     | 0.69              |
| 32:DH:46:GLU:OE2   | 32:DH:51:ARG:HD2   | 1.91                     | 0.69              |
| 32:DH:168:PRO:O    | 32:DH:169:VAL:HG12 | 1.91                     | 0.69              |
| 33:DI:32:PRO:C     | 33:DI:34:GLY:H     | 1.98                     | 0.69              |
| 41:DU:33:ARG:O     | 41:DU:37:GLU:HG3   | 1.91                     | 0.69              |
| 41:DU:83:LEU:HD12  | 41:DU:113:ALA:HB2  | 1.74                     | 0.69              |
| 1:AA:1216:G:H5''   | 14:AN:5:ALA:HB2    | 1.73                     | 0.69              |
| 2:AB:54:THR:HG22   | 2:AB:58:ILE:HD11   | 1.73                     | 0.69              |
| 2:AB:81:VAL:O      | 2:AB:85:ALA:HB2    | 1.93                     | 0.69              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 5:AE:68:GLU:O       | 5:AE:68:GLU:CD     | 2.35                     | 0.69              |
| 13:AM:25:ILE:HD12   | 13:AM:25:ILE:N     | 2.05                     | 0.69              |
| 25:BA:221:A:N7      | 25:BA:266:G:C6     | 2.59                     | 0.69              |
| 25:BA:517:C:OP1     | 52:B5:16:ARG:NH2   | 2.25                     | 0.69              |
| 25:BA:1747(A):G:H2' | 25:BA:1748:G:H5''  | 1.74                     | 0.69              |
| 29:BE:116:VAL:O     | 29:BE:117:MET:HB3  | 1.90                     | 0.69              |
| 36:BP:85:LEU:HA     | 36:BP:88:LEU:CB    | 2.22                     | 0.69              |
| 40:BT:27:THR:HG22   | 40:BT:49:VAL:HG23  | 1.75                     | 0.69              |
| 41:BU:102:GLU:O     | 41:BU:105:VAL:HG23 | 1.92                     | 0.69              |
| 4:CD:161:ASN:O      | 4:CD:165:MET:HG2   | 1.92                     | 0.69              |
| 12:CL:90:VAL:HG11   | 12:CL:93:LEU:HG    | 1.73                     | 0.69              |
| 25:DA:958:U:O2      | 26:DB:90:A:H4'     | 1.92                     | 0.69              |
| 25:DA:1171:G:H3'    | 25:DA:1173:G:H4'   | 1.72                     | 0.69              |
| 25:DA:1817:G:H2'    | 25:DA:1818:U:H5'   | 1.74                     | 0.69              |
| 28:DD:11:PRO:C      | 28:DD:13:ARG:H     | 1.97                     | 0.69              |
| 30:DF:198:ALA:CA    | 30:DF:201:VAL:HG12 | 2.23                     | 0.69              |
| 31:DG:130:ASN:OD1   | 31:DG:160:VAL:HA   | 1.92                     | 0.69              |
| 33:DI:38:LEU:HD12   | 33:DI:38:LEU:N     | 2.07                     | 0.69              |
| 48:D1:19:GLN:HB2    | 48:D1:35:THR:HG22  | 1.74                     | 0.69              |
| 6:AF:45:LEU:CD1     | 6:AF:57:GLN:HB3    | 2.22                     | 0.69              |
| 8:AH:6:ILE:HD12     | 8:AH:6:ILE:N       | 2.06                     | 0.69              |
| 13:AM:81:LEU:HD22   | 13:AM:86:CYS:SG    | 2.33                     | 0.69              |
| 25:BA:1966:A:C4'    | 25:BA:1967:C:OP1   | 2.37                     | 0.69              |
| 25:BA:2056:G:N2     | 25:BA:2057:A:C4    | 2.61                     | 0.69              |
| 29:BE:81:ILE:HG22   | 29:BE:81:ILE:O     | 1.92                     | 0.69              |
| 30:BF:51:THR:HG21   | 30:BF:92:PRO:N     | 2.07                     | 0.69              |
| 35:BO:115:VAL:O     | 35:BO:118:ALA:N    | 2.25                     | 0.69              |
| 39:BS:106:ARG:HD2   | 39:BS:107:GLU:O    | 1.91                     | 0.69              |
| 46:BZ:33:LEU:HD23   | 46:BZ:90:VAL:HG21  | 1.73                     | 0.69              |
| 55:B8:11:LYS:HE2    | 55:B8:64:TYR:HE1   | 1.56                     | 0.69              |
| 13:CM:4:ILE:HG22    | 13:CM:5:ALA:N      | 2.08                     | 0.69              |
| 22:CV:53:G:C2'      | 22:CV:54:G:C5'     | 2.70                     | 0.69              |
| 25:DA:2311:A:H1'    | 31:DG:82:LEU:HD11  | 1.73                     | 0.69              |
| 29:DE:11:MET:HB3    | 29:DE:24:THR:HA    | 1.73                     | 0.69              |
| 34:DN:125:GLY:HA3   | 34:DN:126:PRO:O    | 1.91                     | 0.69              |
| 34:DN:133:GLN:HG2   | 34:DN:135:PRO:HD3  | 1.72                     | 0.69              |
| 36:DP:15:ARG:O      | 36:DP:16:ARG:C     | 2.34                     | 0.69              |
| 5:AE:78:HIS:CE1     | 5:AE:143:ARG:H     | 2.10                     | 0.69              |
| 9:AI:21:PRO:HA      | 9:AI:59:PHE:HA     | 1.74                     | 0.69              |
| 13:AM:3:ARG:NH1     | 31:BG:113:ARG:NH2  | 2.40                     | 0.69              |
| 25:BA:388:G:H5'     | 48:B1:25:LYS:CB    | 2.22                     | 0.69              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:BA:819:A:OP2   | 25:BA:1187:G:N2    | 2.20                     | 0.69              |
| 25:BA:1340:U:O2   | 25:BA:1602:U:C5'   | 2.41                     | 0.69              |
| 25:BA:2458:G:C8   | 25:BA:2490:G:O6    | 2.45                     | 0.69              |
| 31:BG:44:GLY:CA   | 31:BG:88:ILE:HG21  | 2.20                     | 0.69              |
| 33:BI:101:LEU:HB3 | 33:BI:109:ILE:HD13 | 1.72                     | 0.69              |
| 53:B6:35:GLU:HB3  | 53:B6:51:GLU:CD    | 2.18                     | 0.69              |
| 1:CA:31:G:O6      | 1:CA:48:C:H1'      | 1.91                     | 0.69              |
| 2:CB:179:LYS:HA   | 8:CH:72:PRO:HD3    | 1.74                     | 0.69              |
| 9:CI:53:VAL:HB    | 9:CI:92:TYR:HE2    | 1.56                     | 0.69              |
| 13:CM:116:THR:O   | 13:CM:117:VAL:HG12 | 1.92                     | 0.69              |
| 17:CQ:44:ALA:HA   | 17:CQ:71:PHE:O     | 1.92                     | 0.69              |
| 20:CT:72:LEU:CD2  | 20:CT:73:HIS:H     | 2.04                     | 0.69              |
| 44:DX:12:VAL:CG2  | 44:DX:17:ALA:CB    | 2.71                     | 0.69              |
| 46:DZ:117:LEU:HA  | 46:DZ:174:VAL:HG22 | 1.75                     | 0.69              |
| 1:AA:878:G:H5'    | 8:AH:89:PRO:HG2    | 1.74                     | 0.69              |
| 13:AM:15:VAL:HG12 | 13:AM:45:VAL:HG22  | 1.74                     | 0.69              |
| 25:BA:448:U:O2'   | 30:BF:84:VAL:CG1   | 2.38                     | 0.69              |
| 25:BA:529:A:H62   | 25:BA:2041:U:H3    | 1.41                     | 0.69              |
| 25:BA:1326:U:O4   | 25:BA:1647:G:H1'   | 1.93                     | 0.69              |
| 25:BA:1385:G:C4'  | 25:BA:1386:C:OP1   | 2.35                     | 0.69              |
| 25:BA:2528:U:P    | 56:B9:30:PRO:HG2   | 2.32                     | 0.69              |
| 28:BD:130:ALA:HB2 | 28:BD:192:THR:HB   | 1.75                     | 0.69              |
| 36:BP:66:GLY:O    | 36:BP:67:MET:CB    | 2.41                     | 0.69              |
| 40:BT:31:SER:C    | 40:BT:32:TYR:CD2   | 2.70                     | 0.69              |
| 45:BY:27:VAL:C    | 45:BY:28:LYS:HE3   | 2.17                     | 0.69              |
| 45:BY:95:LYS:CG   | 45:BY:100:ALA:HA   | 2.22                     | 0.69              |
| 1:CA:1152:A:H5''  | 10:CJ:13:HIS:CD2   | 2.27                     | 0.69              |
| 1:CA:1399:C:H4'   | 1:CA:1400:C:O5'    | 1.91                     | 0.69              |
| 4:CD:198:VAL:HG12 | 4:CD:199:ASN:N     | 2.07                     | 0.69              |
| 22:CV:20:G:H3'    | 22:CV:21:U:O2      | 1.92                     | 0.69              |
| 22:CV:20:G:H4'    | 22:CV:21:U:OP2     | 1.91                     | 0.69              |
| 31:DG:7:LEU:O     | 31:DG:7:LEU:HD23   | 1.92                     | 0.69              |
| 39:DS:106:ARG:CA  | 39:DS:110:LEU:CD1  | 2.50                     | 0.69              |
| 43:DW:73:ALA:HB3  | 43:DW:106:ILE:HD11 | 1.74                     | 0.69              |
| 48:D1:56:GLN:HE21 | 48:D1:56:GLN:CA    | 2.04                     | 0.69              |
| 52:D5:58:LEU:O    | 52:D5:59:GLU:CD    | 2.35                     | 0.69              |
| 1:AA:1049:U:H4'   | 1:AA:1050:G:H5'    | 1.75                     | 0.69              |
| 2:AB:178:ARG:HH21 | 8:AH:74:PRO:HG3    | 1.58                     | 0.69              |
| 3:AC:41:GLY:O     | 3:AC:45:LYS:HG3    | 1.92                     | 0.69              |
| 12:AL:83:VAL:CG1  | 12:AL:100:ILE:HG12 | 2.23                     | 0.69              |
| 20:AT:81:LYS:O    | 20:AT:85:MET:CB    | 2.40                     | 0.69              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:BA:2168:G:N2    | 25:BA:2170:A:H3'   | 2.07                     | 0.69              |
| 30:BF:32:LEU:HD23  | 30:BF:32:LEU:C     | 2.18                     | 0.69              |
| 31:BG:43:LEU:CB    | 31:BG:88:ILE:CD1   | 2.42                     | 0.69              |
| 40:BT:31:SER:HB3   | 40:BT:43:GLN:C     | 2.18                     | 0.69              |
| 41:BU:34:LYS:CE    | 41:BU:34:LYS:CA    | 2.55                     | 0.69              |
| 1:CA:428:G:C4'     | 1:CA:429:U:O5'     | 2.34                     | 0.69              |
| 1:CA:1077:G:N2     | 1:CA:1080:A:OP2    | 2.26                     | 0.69              |
| 2:CB:18:GLY:N      | 2:CB:42:ILE:HG22   | 2.07                     | 0.69              |
| 12:CL:113:ARG:HB3  | 12:CL:122:THR:HG21 | 1.74                     | 0.69              |
| 25:DA:2331:G:O2'   | 47:D0:43:THR:HG22  | 1.93                     | 0.69              |
| 25:DA:2331:G:H4'   | 47:D0:43:THR:H     | 1.57                     | 0.69              |
| 25:DA:2336:A:H61   | 47:D0:43:THR:HG21  | 1.58                     | 0.69              |
| 26:DB:43:C:P       | 31:DG:67:LYS:HE3   | 2.33                     | 0.69              |
| 31:DG:118:ARG:HA   | 31:DG:118:ARG:HE   | 1.57                     | 0.69              |
| 32:DH:59:ARG:HG3   | 32:DH:59:ARG:HH11  | 1.58                     | 0.69              |
| 33:DI:14:ASP:OD1   | 33:DI:15:VAL:HG22  | 1.92                     | 0.69              |
| 41:DU:92:ARG:NH2   | 41:DU:94:ASN:ND2   | 2.36                     | 0.69              |
| 1:AA:79:G:C1'      | 1:AA:80:G:OP1      | 2.41                     | 0.69              |
| 1:AA:251:G:N1      | 1:AA:266:G:C6      | 2.61                     | 0.69              |
| 1:AA:1347:G:N7     | 9:AI:10:ARG:NH2    | 2.40                     | 0.69              |
| 1:AA:1399:C:H4'    | 1:AA:1400:C:O5'    | 1.93                     | 0.69              |
| 2:AB:19:HIS:CE1    | 2:AB:20:GLU:CD     | 2.71                     | 0.69              |
| 3:AC:113:ALA:HB3   | 3:AC:114:PRO:HD3   | 1.75                     | 0.69              |
| 4:AD:146:ILE:H     | 4:AD:146:ILE:HD12  | 1.57                     | 0.69              |
| 5:AE:76:ILE:CG1    | 5:AE:77:PRO:HD2    | 2.22                     | 0.69              |
| 8:AH:112:LEU:HD22  | 8:AH:133:LEU:HA    | 1.74                     | 0.69              |
| 13:AM:83:ASP:OD1   | 19:AS:74:PHE:HE1   | 1.75                     | 0.69              |
| 25:BA:243:U:C4     | 25:BA:254:G:C2     | 2.81                     | 0.69              |
| 25:BA:481:G:O5'    | 45:BY:47:LYS:HE3   | 1.93                     | 0.69              |
| 25:BA:1301:A:O2'   | 25:BA:1302:A:C5'   | 2.40                     | 0.69              |
| 29:BE:11:MET:HB3   | 29:BE:24:THR:HA    | 1.75                     | 0.69              |
| 29:BE:51:PHE:CE1   | 29:BE:52:LEU:HD13  | 2.28                     | 0.69              |
| 29:BE:104:VAL:HG11 | 29:BE:188:VAL:HG23 | 1.73                     | 0.69              |
| 30:BF:63:LYS:CE    | 30:BF:67:GLN:HB3   | 2.23                     | 0.69              |
| 40:BT:50:ILE:HD12  | 40:BT:99:LEU:HD13  | 1.74                     | 0.69              |
| 45:BY:14:LEU:HD12  | 45:BY:15:VAL:N     | 2.06                     | 0.69              |
| 45:BY:67:LEU:HD11  | 45:BY:71:LYS:HB2   | 1.73                     | 0.69              |
| 45:BY:95:LYS:HG3   | 45:BY:100:ALA:HA   | 1.74                     | 0.69              |
| 51:B4:52:SER:OG    | 51:B4:53:THR:N     | 2.22                     | 0.69              |
| 9:CI:53:VAL:O      | 9:CI:54:ASP:HB2    | 1.93                     | 0.69              |
| 10:CJ:58:ASP:O     | 10:CJ:60:ARG:HG3   | 1.92                     | 0.69              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:CK:41:THR:HG21 | 11:CK:71:LYS:HB3  | 1.73                     | 0.69              |
| 25:DA:604:G:H2'   | 25:DA:605:C:C6    | 2.28                     | 0.69              |
| 25:DA:660:G:N2    | 36:DP:12:ALA:HA   | 2.03                     | 0.69              |
| 25:DA:768:G:O2'   | 25:DA:1379:A:N6   | 2.26                     | 0.69              |
| 25:DA:1287:A:C6   | 25:DA:1288:U:N3   | 2.61                     | 0.69              |
| 28:DD:33:LEU:H    | 28:DD:33:LEU:HD12 | 1.58                     | 0.69              |
| 29:DE:36:ARG:HH22 | 29:DE:88:GLY:CA   | 2.06                     | 0.69              |
| 34:DN:25:ARG:HH11 | 34:DN:25:ARG:HG3  | 1.57                     | 0.69              |
| 36:DP:48:PRO:HG2  | 36:DP:49:ARG:H    | 1.58                     | 0.69              |
| 37:DQ:12:GLN:HG2  | 37:DQ:73:PRO:HD2  | 1.75                     | 0.69              |
| 37:DQ:29:PHE:HB2  | 37:DQ:105:GLU:OE2 | 1.92                     | 0.69              |
| 38:DR:26:LYS:HE2  | 38:DR:71:GLN:H    | 1.56                     | 0.69              |
| 41:DU:92:ARG:HH21 | 41:DU:95:LEU:HG   | 1.58                     | 0.69              |
| 53:D6:32:ASN:CG   | 53:D6:33:LYS:H    | 2.01                     | 0.69              |
| 53:D6:41:PRO:HG3  | 53:D6:46:HIS:O    | 1.93                     | 0.69              |
| 4:AD:108:LEU:HB3  | 4:AD:110:PHE:HE1  | 1.56                     | 0.69              |
| 23:AW:57:G:H2'    | 23:AW:58:A:H5'    | 1.75                     | 0.69              |
| 25:BA:2307:G:N1   | 31:BG:43:LEU:O    | 2.25                     | 0.69              |
| 33:BI:133:HIS:HB2 | 33:BI:134:PRO:CD  | 2.22                     | 0.69              |
| 36:BP:31:ALA:O    | 36:BP:32:THR:HG23 | 1.93                     | 0.69              |
| 36:BP:48:PRO:HG2  | 36:BP:49:ARG:H    | 1.58                     | 0.69              |
| 40:BT:27:THR:CG2  | 40:BT:49:VAL:HG23 | 2.23                     | 0.69              |
| 8:CH:30:ARG:HH11  | 8:CH:30:ARG:HB3   | 1.56                     | 0.69              |
| 20:CT:14:LYS:HA   | 20:CT:17:ARG:HE   | 1.58                     | 0.69              |
| 25:DA:530:G:N3    | 25:DA:2021:C:O2'  | 2.26                     | 0.69              |
| 25:DA:1739:U:O2   | 25:DA:1739:U:C5'  | 2.39                     | 0.69              |
| 31:DG:8:LYS:O     | 31:DG:11:TYR:HB3  | 1.93                     | 0.69              |
| 33:DI:1:MET:HG3   | 33:DI:23:PRO:HB3  | 1.74                     | 0.69              |
| 33:DI:23:PRO:HB2  | 33:DI:27:ARG:NH1  | 2.08                     | 0.69              |
| 48:D1:66:HIS:C    | 48:D1:68:PRO:HD2  | 2.18                     | 0.69              |
| 48:D1:67:ILE:N    | 48:D1:68:PRO:HD2  | 2.08                     | 0.69              |
| 5:AE:12:LEU:HD22  | 5:AE:13:ILE:N     | 2.06                     | 0.69              |
| 13:AM:83:ASP:C    | 13:AM:85:GLY:N    | 2.46                     | 0.69              |
| 25:BA:243:U:C4    | 25:BA:254:G:N2    | 2.62                     | 0.69              |
| 35:BO:68:GLU:HB3  | 35:BO:78:ARG:HB2  | 1.74                     | 0.69              |
| 38:BR:9:LYS:O     | 38:BR:10:LEU:CG   | 2.40                     | 0.69              |
| 48:B1:45:ASN:HD22 | 48:B1:45:ASN:C    | 2.01                     | 0.69              |
| 12:CL:24:VAL:HG13 | 12:CL:98:TYR:CE2  | 2.25                     | 0.69              |
| 13:CM:4:ILE:HG22  | 13:CM:5:ALA:H     | 1.56                     | 0.69              |
| 25:DA:2700:C:O2'  | 25:DA:2701:C:H5'  | 1.93                     | 0.69              |
| 29:DE:117:MET:O   | 29:DE:118:LYS:HB2 | 1.92                     | 0.69              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:DG:101:ILE:HD13 | 51:D4:9:LEU:HD11   | 1.75                     | 0.69              |
| 45:DY:39:VAL:HG12  | 45:DY:40:GLU:N     | 2.06                     | 0.69              |
| 46:DZ:175:VAL:HB   | 46:DZ:176:PRO:HD2  | 1.75                     | 0.69              |
| 1:AA:79:G:H1'      | 1:AA:80:G:OP1      | 1.94                     | 0.68              |
| 1:AA:1452:C:O2'    | 1:AA:1456:G:N2     | 2.26                     | 0.68              |
| 19:AS:9:VAL:C      | 19:AS:10:PHE:CG    | 2.72                     | 0.68              |
| 20:AT:26:ASN:CB    | 20:AT:71:THR:OG1   | 2.39                     | 0.68              |
| 25:BA:1902:C:O2'   | 28:BD:244:ARG:HB2  | 1.93                     | 0.68              |
| 25:BA:2406:U:O4    | 36:BP:70:GLN:HB2   | 1.94                     | 0.68              |
| 29:BE:104:VAL:HG11 | 29:BE:188:VAL:CG2  | 2.23                     | 0.68              |
| 29:BE:129:HIS:O    | 29:BE:130:GLY:O    | 2.10                     | 0.68              |
| 31:BG:43:LEU:CG    | 31:BG:88:ILE:HD11  | 2.22                     | 0.68              |
| 35:BO:112:MET:HE2  | 35:BO:112:MET:HA   | 1.73                     | 0.68              |
| 40:BT:30:VAL:HG12  | 40:BT:31:SER:N     | 2.08                     | 0.68              |
| 45:BY:28:LYS:HA    | 45:BY:39:VAL:H     | 1.58                     | 0.68              |
| 45:BY:52:SER:O     | 45:BY:54:LYS:N     | 2.26                     | 0.68              |
| 1:CA:1029:C:H4'    | 1:CA:1033:G:H22    | 1.57                     | 0.68              |
| 2:CB:77:ALA:HB2    | 2:CB:211:ILE:HD13  | 1.74                     | 0.68              |
| 3:CC:64:VAL:HG23   | 3:CC:98:ASN:O      | 1.93                     | 0.68              |
| 13:CM:15:VAL:HG23  | 13:CM:43:THR:O     | 1.93                     | 0.68              |
| 32:DH:35:VAL:HG13  | 32:DH:71:LEU:HG    | 1.75                     | 0.68              |
| 36:DP:63:PRO:HB3   | 55:D8:13:ARG:CB    | 2.15                     | 0.68              |
| 36:DP:63:PRO:C     | 36:DP:65:ARG:N     | 2.49                     | 0.68              |
| 44:DX:13:LEU:HA    | 44:DX:18:TYR:CE1   | 2.28                     | 0.68              |
| 1:AA:1157:A:H5'    | 1:AA:1158:C:C6     | 2.28                     | 0.68              |
| 7:AG:60:LYS:HA     | 7:AG:60:LYS:NZ     | 2.09                     | 0.68              |
| 25:BA:1270:C:C4    | 25:BA:1648:C:N4    | 2.60                     | 0.68              |
| 25:BA:1820:U:O2'   | 28:BD:201:HIS:HD2  | 1.75                     | 0.68              |
| 25:BA:2745:C:C5    | 25:BA:2746:U:C4    | 2.81                     | 0.68              |
| 31:BG:108:ASN:O    | 31:BG:112:PRO:HG2  | 1.93                     | 0.68              |
| 36:BP:57:THR:C     | 36:BP:59:LEU:H     | 2.01                     | 0.68              |
| 50:B3:46:ASN:O     | 50:B3:50:VAL:HG22  | 1.93                     | 0.68              |
| 1:CA:484:G:C4'     | 1:CA:485:G:O5'     | 2.36                     | 0.68              |
| 13:CM:116:THR:CG2  | 13:CM:117:VAL:N    | 2.56                     | 0.68              |
| 23:CW:67:C:O2'     | 23:CW:68:C:H5'     | 1.93                     | 0.68              |
| 25:DA:614:U:H5''   | 25:DA:614:U:O2     | 1.93                     | 0.68              |
| 29:DE:32:PRO:HB3   | 29:DE:69:LYS:HB3   | 1.76                     | 0.68              |
| 30:DF:65:TRP:HB2   | 30:DF:66:PRO:CD    | 2.24                     | 0.68              |
| 33:DI:130:TYR:C    | 33:DI:131:LYS:HD2  | 2.18                     | 0.68              |
| 40:DT:100:TYR:HD2  | 40:DT:103:ARG:HH21 | 1.40                     | 0.68              |
| 42:DV:25:LEU:HD12  | 42:DV:94:LEU:HD21  | 1.74                     | 0.68              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:AA:970:C:H4'     | 1:AA:972:C:C5     | 2.28                     | 0.68              |
| 1:AA:1363(A):A:H1' | 1:AA:1365:G:N7    | 2.07                     | 0.68              |
| 19:AS:6:LYS:HE3    | 19:AS:6:LYS:N     | 2.08                     | 0.68              |
| 25:BA:1698:A:O2'   | 25:BA:1699:G:H5'' | 1.93                     | 0.68              |
| 25:BA:1754:C:OP1   | 40:BT:96:ARG:NH1  | 2.25                     | 0.68              |
| 25:BA:1799:G:H4'   | 25:BA:1800:C:O5'  | 1.93                     | 0.68              |
| 25:BA:1902:C:C1'   | 28:BD:244:ARG:HG3 | 2.22                     | 0.68              |
| 28:BD:224:ALA:O    | 28:BD:225:ALA:HB3 | 1.92                     | 0.68              |
| 32:BH:40:GLU:HB2   | 32:BH:41:MET:SD   | 2.33                     | 0.68              |
| 40:BT:133:GLU:OE2  | 40:BT:137:LYS:HB2 | 1.93                     | 0.68              |
| 1:CA:1298:C:C4     | 7:CG:114:ARG:HD2  | 2.28                     | 0.68              |
| 5:CE:72:GLN:O      | 5:CE:73:ASN:CB    | 2.38                     | 0.68              |
| 6:CF:44:GLY:HA2    | 6:CF:59:TYR:CZ    | 2.28                     | 0.68              |
| 8:CH:20:TYR:CE2    | 8:CH:75:ARG:HB3   | 2.28                     | 0.68              |
| 25:DA:1187:G:H5''  | 42:DV:81:TYR:CE2  | 2.28                     | 0.68              |
| 25:DA:2377:A:H4'   | 39:DS:111:GLU:O   | 1.93                     | 0.68              |
| 32:DH:152:ARG:HG3  | 32:DH:153:LYS:HE2 | 1.74                     | 0.68              |
| 33:DI:52:ARG:HH11  | 33:DI:52:ARG:HB2  | 1.58                     | 0.68              |
| 36:DP:66:GLY:O     | 36:DP:67:MET:CB   | 2.41                     | 0.68              |
| 45:DY:50:ARG:HB3   | 45:DY:53:PRO:HD2  | 1.75                     | 0.68              |
| 47:D0:72:ARG:HB3   | 47:D0:75:LEU:HB3  | 1.76                     | 0.68              |
| 1:AA:251:G:C6      | 1:AA:266:G:N1     | 2.62                     | 0.68              |
| 4:AD:101:LEU:HD23  | 4:AD:121:VAL:CG1  | 2.23                     | 0.68              |
| 5:AE:70:PRO:HB2    | 5:AE:144:THR:HG21 | 1.76                     | 0.68              |
| 12:AL:55:VAL:HG13  | 12:AL:68:ALA:O    | 1.93                     | 0.68              |
| 19:AS:32:LYS:HG2   | 19:AS:57:HIS:CD2  | 2.29                     | 0.68              |
| 23:AW:34:G:C4      | 24:AX:14:A:H2     | 2.07                     | 0.68              |
| 25:BA:1283:G:N2    | 25:BA:1286:A:OP2  | 2.24                     | 0.68              |
| 28:BD:127:VAL:HA   | 28:BD:193:VAL:CG2 | 2.24                     | 0.68              |
| 29:BE:116:VAL:HG22 | 29:BE:117:MET:H   | 1.58                     | 0.68              |
| 38:BR:11:ASN:O     | 38:BR:12:ARG:HD2  | 1.94                     | 0.68              |
| 46:BZ:10:ARG:HH21  | 46:BZ:26:GLY:H    | 1.40                     | 0.68              |
| 46:BZ:140:ASP:O    | 46:BZ:140:ASP:CG  | 2.36                     | 0.68              |
| 50:B3:4:LEU:HB2    | 50:B3:39:ASP:HB2  | 1.75                     | 0.68              |
| 9:CI:4:TYR:N       | 9:CI:4:TYR:CD1    | 2.62                     | 0.68              |
| 12:CL:53:ARG:CB    | 12:CL:93:LEU:HD11 | 2.24                     | 0.68              |
| 19:CS:53:ASN:OD1   | 19:CS:54:GLY:N    | 2.27                     | 0.68              |
| 23:CW:24:G:H2'     | 23:CW:25:C:C6     | 2.28                     | 0.68              |
| 23:CY:34:G:H2'     | 23:CY:35:A:C8     | 2.29                     | 0.68              |
| 25:DA:630:G:N2     | 25:DA:633:A:OP2   | 2.26                     | 0.68              |
| 25:DA:866:A:C6     | 25:DA:914:C:C5    | 2.82                     | 0.68              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:DA:2285:C:C5   | 53:D6:27:LYS:HE3   | 2.27                     | 0.68              |
| 25:DA:2392:A:H2   | 25:DA:2424:C:H42   | 1.41                     | 0.68              |
| 28:DD:172:TYR:HD1 | 28:DD:186:HIS:HA   | 1.58                     | 0.68              |
| 31:DG:88:ILE:HG23 | 31:DG:88:ILE:O     | 1.92                     | 0.68              |
| 32:DH:20:ALA:CB   | 32:DH:21:PRO:CD    | 2.71                     | 0.68              |
| 36:DP:11:GLY:O    | 36:DP:12:ALA:CB    | 2.40                     | 0.68              |
| 36:DP:57:THR:HG21 | 36:DP:59:LEU:HB3   | 1.75                     | 0.68              |
| 37:DQ:51:ARG:HH11 | 37:DQ:51:ARG:CG    | 2.06                     | 0.68              |
| 40:DT:53:ARG:HH11 | 40:DT:53:ARG:HG2   | 1.59                     | 0.68              |
| 41:DU:40:PHE:CD1  | 42:DV:75:PHE:CE2   | 2.82                     | 0.68              |
| 43:DW:111:HIS:CG  | 43:DW:112:GLY:H    | 2.11                     | 0.68              |
| 2:AB:200:ILE:HG22 | 2:AB:202:PRO:HD3   | 1.75                     | 0.68              |
| 4:AD:9:CYS:HB2    | 4:AD:22:LYS:NZ     | 2.07                     | 0.68              |
| 25:BA:527:C:H1'   | 25:BA:528:A:C5     | 2.29                     | 0.68              |
| 25:BA:2259:G:H1'  | 25:BA:2427:C:H2'   | 1.74                     | 0.68              |
| 25:BA:2304:G:H1   | 25:BA:2312:U:H3    | 1.41                     | 0.68              |
| 25:BA:2320:A:N6   | 25:BA:2333:A:C5    | 2.59                     | 0.68              |
| 25:BA:2457:U:H2'  | 25:BA:2458:G:C5'   | 2.20                     | 0.68              |
| 25:BA:2780:G:C5'  | 25:BA:2781:A:OP2   | 2.41                     | 0.68              |
| 32:BH:126:PRO:HB2 | 32:BH:130:ARG:HH11 | 1.59                     | 0.68              |
| 32:BH:156:ALA:H   | 32:BH:158:HIS:H    | 1.42                     | 0.68              |
| 39:BS:78:LEU:HD11 | 39:BS:103:GLU:HB3  | 1.75                     | 0.68              |
| 51:B4:42:CYS:HB2  | 51:B4:46:ASN:O     | 1.93                     | 0.68              |
| 54:B7:24:THR:HG23 | 54:B7:27:GLY:HA3   | 1.75                     | 0.68              |
| 2:CB:223:ILE:HA   | 2:CB:226:ARG:HD2   | 1.74                     | 0.68              |
| 3:CC:23:TYR:CD2   | 3:CC:24:ALA:N      | 2.62                     | 0.68              |
| 5:CE:9:LYS:HB3    | 5:CE:112:LEU:HD11  | 1.75                     | 0.68              |
| 9:CI:4:TYR:CE2    | 9:CI:59:PHE:HE2    | 2.10                     | 0.68              |
| 22:CV:41:C:C2'    | 22:CV:42:C:H5'     | 2.22                     | 0.68              |
| 23:CW:1:G:C6      | 23:CW:73:A:C2      | 2.82                     | 0.68              |
| 25:DA:390:A:C6    | 36:DP:71:VAL:HG11  | 2.28                     | 0.68              |
| 25:DA:613:G:C2    | 25:DA:615:G:C5     | 2.80                     | 0.68              |
| 25:DA:620:G:H4'   | 25:DA:621:A:H5''   | 1.75                     | 0.68              |
| 25:DA:729:G:OP2   | 28:DD:13:ARG:NH1   | 2.26                     | 0.68              |
| 28:DD:26:LYS:NZ   | 28:DD:82:ILE:H     | 1.92                     | 0.68              |
| 30:DF:59:TYR:CD1  | 30:DF:78:ILE:HB    | 2.28                     | 0.68              |
| 36:DP:85:LEU:HA   | 36:DP:88:LEU:CB    | 2.22                     | 0.68              |
| 37:DQ:43:THR:HA   | 37:DQ:94:VAL:HG12  | 1.75                     | 0.68              |
| 40:DT:30:VAL:HG23 | 40:DT:31:SER:N     | 2.08                     | 0.68              |
| 41:DU:92:ARG:HH11 | 41:DU:92:ARG:CG    | 2.06                     | 0.68              |
| 47:D0:60:PHE:CD1  | 47:D0:60:PHE:O     | 2.47                     | 0.68              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 12:AL:41:ARG:HH22 | 12:AL:57:LYS:HZ3  | 1.41                     | 0.68              |
| 25:BA:662:G:OP1   | 36:BP:15:ARG:NE   | 2.27                     | 0.68              |
| 34:BN:67:LEU:HB3  | 34:BN:88:GLU:HG2  | 1.75                     | 0.68              |
| 40:BT:28:VAL:CB   | 40:BT:46:GLU:HA   | 2.23                     | 0.68              |
| 49:B2:46:GLN:OE1  | 49:B2:46:GLN:HA   | 1.93                     | 0.68              |
| 5:CE:91:LEU:HD21  | 5:CE:138:ALA:HB1  | 1.76                     | 0.68              |
| 23:CW:38:A:C3'    | 23:CW:39:U:H5''   | 2.24                     | 0.68              |
| 25:DA:660:G:H21   | 36:DP:12:ALA:CA   | 2.01                     | 0.68              |
| 25:DA:662:G:H5'   | 36:DP:15:ARG:HA   | 1.75                     | 0.68              |
| 25:DA:2068:U:H3   | 25:DA:2430:A:H2   | 1.40                     | 0.68              |
| 29:DE:179:GLU:O   | 29:DE:180:ASN:HB2 | 1.92                     | 0.68              |
| 32:DH:37:VAL:HG12 | 32:DH:38:SER:N    | 2.07                     | 0.68              |
| 40:DT:132:LYS:C   | 40:DT:134:GLU:H   | 2.01                     | 0.68              |
| 2:AB:111:ARG:HG2  | 2:AB:111:ARG:NH1  | 2.08                     | 0.68              |
| 12:AL:113:ARG:HG3 | 12:AL:117:ARG:HG2 | 1.75                     | 0.68              |
| 15:AO:65:ARG:HG2  | 15:AO:65:ARG:NH1  | 2.07                     | 0.68              |
| 19:AS:32:LYS:HA   | 19:AS:50:ALA:HB3  | 1.74                     | 0.68              |
| 25:BA:125:G:C5'   | 25:BA:126:A:OP2   | 2.41                     | 0.68              |
| 25:BA:1451:C:H6   | 25:BA:1451:C:O5'  | 1.76                     | 0.68              |
| 25:BA:1918:A:O2'  | 25:BA:1920:C:N4   | 2.27                     | 0.68              |
| 30:BF:45:ARG:HG3  | 30:BF:46:ARG:H    | 1.59                     | 0.68              |
| 33:BI:8:PRO:C     | 33:BI:9:LEU:HG    | 2.18                     | 0.68              |
| 37:BQ:68:ILE:CG2  | 37:BQ:101:ARG:HD3 | 2.23                     | 0.68              |
| 40:BT:80:SER:HB3  | 40:BT:81:PRO:CD   | 2.23                     | 0.68              |
| 42:BV:64:HIS:CG   | 42:BV:92:THR:HG22 | 2.29                     | 0.68              |
| 1:CA:429:U:O2'    | 1:CA:430:A:P      | 2.52                     | 0.68              |
| 1:CA:575:G:H4'    | 1:CA:576:G:O5'    | 1.93                     | 0.68              |
| 2:CB:17:PHE:HB3   | 2:CB:44:LEU:HD21  | 1.76                     | 0.68              |
| 4:CD:79:PHE:CD2   | 4:CD:207:TYR:HD1  | 2.11                     | 0.68              |
| 6:CF:19:LEU:O     | 6:CF:23:LYS:HG3   | 1.93                     | 0.68              |
| 8:CH:13:ILE:O     | 8:CH:17:THR:HG23  | 1.93                     | 0.68              |
| 9:CI:17:VAL:HG11  | 9:CI:81:ILE:HD13  | 1.76                     | 0.68              |
| 16:CP:8:ARG:HG2   | 16:CP:8:ARG:NH1   | 2.07                     | 0.68              |
| 22:CV:51:U:H3     | 22:CV:65:G:H1     | 1.42                     | 0.68              |
| 24:CX:16:A:C2     | 24:CX:17:U:C2     | 2.81                     | 0.68              |
| 28:DD:35:LYS:HZ2  | 28:DD:103:ARG:HA  | 1.57                     | 0.68              |
| 38:DR:78:LYS:O    | 38:DR:83:ILE:HG12 | 1.93                     | 0.68              |
| 45:DY:14:LEU:HD23 | 45:DY:14:LEU:C    | 2.18                     | 0.68              |
| 1:AA:90:U:H5''    | 1:AA:91:C:H5'     | 1.76                     | 0.68              |
| 2:AB:87:ARG:NH2   | 2:AB:233:SER:CB   | 2.57                     | 0.68              |
| 23:AW:34:G:C8     | 24:AX:14:A:N1     | 2.61                     | 0.68              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:BA:1299:G:H5''  | 25:BA:1300:U:OP1   | 1.94                     | 0.68              |
| 25:BA:1340:U:O2    | 25:BA:1602:U:H5'   | 1.93                     | 0.68              |
| 28:BD:80:ALA:HB2   | 28:BD:96:HIS:HD2   | 1.52                     | 0.68              |
| 34:BN:67:LEU:O     | 34:BN:68:GLU:HB2   | 1.92                     | 0.68              |
| 45:BY:48:ALA:O     | 45:BY:58:GLY:HA3   | 1.94                     | 0.68              |
| 50:B3:7:LYS:HB2    | 50:B3:34:GLU:HG2   | 1.74                     | 0.68              |
| 2:CB:91:PRO:HG2    | 2:CB:155:LEU:HD23  | 1.74                     | 0.68              |
| 4:CD:4:TYR:O       | 4:CD:5:ILE:HB      | 1.92                     | 0.68              |
| 6:CF:22:GLU:O      | 6:CF:26:ILE:HG13   | 1.94                     | 0.68              |
| 20:CT:43:LEU:HD12  | 20:CT:51:GLU:HB3   | 1.75                     | 0.68              |
| 25:DA:614(B):G:H1' | 30:DF:44:ARG:HD2   | 1.74                     | 0.68              |
| 25:DA:1287:A:C5    | 25:DA:1288:U:C4    | 2.81                     | 0.68              |
| 25:DA:1963:U:C4'   | 25:DA:1964:G:OP1   | 2.36                     | 0.68              |
| 28:DD:31:LYS:NZ    | 28:DD:102:LYS:HZ2  | 1.92                     | 0.68              |
| 31:DG:101:ILE:HG13 | 31:DG:102:PHE:N    | 2.08                     | 0.68              |
| 34:DN:58:ASP:O     | 34:DN:60:ILE:N     | 2.27                     | 0.68              |
| 40:DT:129:ARG:O    | 40:DT:129:ARG:HG3  | 1.93                     | 0.68              |
| 3:AC:150:LYS:HB3   | 3:AC:201:TYR:HB2   | 1.75                     | 0.68              |
| 3:AC:206:GLU:O     | 3:AC:208:ILE:N     | 2.26                     | 0.68              |
| 5:AE:76:ILE:HG12   | 5:AE:142:LEU:HD13  | 1.76                     | 0.68              |
| 7:AG:15:ASP:N      | 7:AG:24:THR:CG2    | 2.57                     | 0.68              |
| 14:AN:12:ARG:O     | 14:AN:14:PRO:HD2   | 1.93                     | 0.68              |
| 25:BA:1428:C:N4    | 25:BA:1570:A:OP2   | 2.21                     | 0.68              |
| 30:BF:149:ASP:OD2  | 30:BF:151:SER:N    | 2.27                     | 0.68              |
| 39:BS:31:SER:HB3   | 39:BS:34:HIS:O     | 1.94                     | 0.68              |
| 43:BW:50:VAL:HG22  | 43:BW:105:VAL:HG23 | 1.76                     | 0.68              |
| 1:CA:31:G:O6       | 1:CA:48:C:C1'      | 2.42                     | 0.68              |
| 25:DA:1434:A:H61   | 25:DA:1558:A:H62   | 1.42                     | 0.68              |
| 28:DD:181:GLU:HA   | 28:DD:272:ALA:CB   | 2.22                     | 0.68              |
| 29:DE:34:VAL:O     | 29:DE:35:GLN:HB2   | 1.91                     | 0.68              |
| 30:DF:66:PRO:O     | 30:DF:67:GLN:HB3   | 1.93                     | 0.68              |
| 36:DP:9:ASN:O      | 36:DP:10:PRO:C     | 2.36                     | 0.68              |
| 36:DP:31:ALA:O     | 36:DP:32:THR:HG23  | 1.93                     | 0.68              |
| 39:DS:59:LYS:HG2   | 39:DS:60:GLY:N     | 1.99                     | 0.68              |
| 42:DV:89:GLN:HA    | 42:DV:89:GLN:NE2   | 2.09                     | 0.68              |
| 5:AE:75:THR:HA     | 5:AE:115:VAL:HG13  | 1.75                     | 0.68              |
| 5:AE:78:HIS:CE1    | 5:AE:142:LEU:HD23  | 2.29                     | 0.68              |
| 10:AJ:49:VAL:O     | 10:AJ:60:ARG:HB3   | 1.93                     | 0.68              |
| 12:AL:46:LYS:HG2   | 12:AL:47:LYS:H     | 1.58                     | 0.68              |
| 13:AM:3:ARG:HE     | 13:AM:9:ILE:HD11   | 1.59                     | 0.68              |
| 23:AW:18:G:H1      | 23:AW:55:U:H1'     | 1.59                     | 0.68              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:BA:1300:U:C5'  | 25:BA:1301:A:C2    | 2.77                     | 0.68              |
| 28:BD:231:HIS:ND1 | 28:BD:232:PRO:CD   | 2.57                     | 0.68              |
| 31:BG:110:ALA:HA  | 31:BG:140:ILE:HG22 | 1.76                     | 0.68              |
| 41:BU:95:LEU:HD13 | 42:BV:4:ILE:CG1    | 2.24                     | 0.68              |
| 43:BW:59:VAL:CG1  | 43:BW:60:ASN:OD1   | 2.41                     | 0.68              |
| 2:CB:132:LYS:HA   | 2:CB:135:GLN:HG3   | 1.76                     | 0.68              |
| 29:DE:52:LEU:HD12 | 29:DE:53:PRO:HD2   | 1.76                     | 0.68              |
| 30:DF:178:PRO:HB2 | 30:DF:201:VAL:HG11 | 1.76                     | 0.68              |
| 32:DH:109:PHE:HZ  | 32:DH:152:ARG:HG2  | 1.58                     | 0.68              |
| 33:DI:76:THR:HG23 | 33:DI:139:GLN:HE22 | 1.57                     | 0.68              |
| 38:DR:45:ARG:HG3  | 38:DR:46:GLY:H     | 1.59                     | 0.68              |
| 39:DS:61:ASN:O    | 39:DS:65:VAL:HG23  | 1.92                     | 0.68              |
| 1:AA:1054:C:N4    | 23:AY:34:G:C1'     | 2.57                     | 0.67              |
| 22:AV:48:U:C5     | 22:AV:51:U:OP1     | 2.47                     | 0.67              |
| 25:BA:2178:C:H4'  | 27:BC:46:LYS:HE2   | 1.76                     | 0.67              |
| 28:BD:96:HIS:HD1  | 28:BD:102:LYS:HD3  | 1.59                     | 0.67              |
| 30:BF:24:LEU:HB3  | 30:BF:25:PRO:CD    | 2.24                     | 0.67              |
| 40:BT:28:VAL:HG11 | 40:BT:46:GLU:CB    | 2.23                     | 0.67              |
| 40:BT:28:VAL:CG2  | 40:BT:46:GLU:C     | 2.66                     | 0.67              |
| 1:CA:8:A:H62      | 4:CD:208:SER:HB2   | 1.59                     | 0.67              |
| 1:CA:48:C:H4'     | 1:CA:49:U:OP2      | 1.94                     | 0.67              |
| 1:CA:1399:C:C2    | 1:CA:1502:A:N6     | 2.62                     | 0.67              |
| 3:CC:139:GLN:O    | 3:CC:143:GLU:HB2   | 1.93                     | 0.67              |
| 3:CC:140:ARG:HH11 | 3:CC:140:ARG:CG    | 2.08                     | 0.67              |
| 13:CM:84:ILE:CD1  | 19:CS:65:ASN:HB3   | 2.24                     | 0.67              |
| 25:DA:2712:U:OP1  | 25:DA:2714:G:H4'   | 1.93                     | 0.67              |
| 45:DY:97:ARG:HD3  | 45:DY:97:ARG:N     | 2.09                     | 0.67              |
| 1:AA:1307:U:OP1   | 13:AM:101:GLN:NE2  | 2.27                     | 0.67              |
| 2:AB:25:ASN:CG    | 2:AB:26:PRO:HD2    | 2.20                     | 0.67              |
| 25:BA:1039:G:O6   | 25:BA:1116:C:N4    | 2.27                     | 0.67              |
| 25:BA:2002:G:C5'  | 38:BR:13:HIS:HA    | 2.24                     | 0.67              |
| 29:BE:176:ILE:CG2 | 29:BE:178:GLU:HB3  | 2.24                     | 0.67              |
| 36:BP:88:LEU:HD11 | 36:BP:95:VAL:HG21  | 1.77                     | 0.67              |
| 2:CB:61:LEU:HD21  | 2:CB:68:ILE:CD1    | 2.22                     | 0.67              |
| 10:CJ:30:SER:HA   | 10:CJ:80:LYS:HD3   | 1.75                     | 0.67              |
| 12:CL:36:VAL:CG1  | 12:CL:80:HIS:HA    | 2.23                     | 0.67              |
| 14:CN:44:LEU:HD12 | 14:CN:44:LEU:O     | 1.94                     | 0.67              |
| 20:CT:89:ARG:HB2  | 20:CT:104:LEU:HD11 | 1.76                     | 0.67              |
| 31:DG:26:GLN:NE2  | 31:DG:27:ASN:HB2   | 2.10                     | 0.67              |
| 31:DG:81:LYS:O    | 31:DG:82:LEU:HB2   | 1.92                     | 0.67              |
| 34:DN:30:ILE:HG23 | 34:DN:52:VAL:HG11  | 1.76                     | 0.67              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 42:DV:1:MET:HE2    | 42:DV:43:GLU:CG   | 2.23                     | 0.67              |
| 43:DW:9:TYR:N      | 43:DW:102:HIS:HD2 | 1.90                     | 0.67              |
| 17:AQ:66:SER:OG    | 17:AQ:69:LYS:HB3  | 1.94                     | 0.67              |
| 25:BA:987:G:O2'    | 25:BA:1000:A:N3   | 2.27                     | 0.67              |
| 36:BP:14:LYS:O     | 36:BP:16:ARG:N    | 2.27                     | 0.67              |
| 36:BP:85:LEU:HD23  | 36:BP:85:LEU:H    | 1.59                     | 0.67              |
| 40:BT:89:VAL:HG11  | 40:BT:91:ARG:HE   | 1.59                     | 0.67              |
| 5:CE:86:ALA:HB3    | 5:CE:130:ASN:ND2  | 2.09                     | 0.67              |
| 11:CK:34:ASP:HB3   | 11:CK:40:ILE:HD11 | 1.75                     | 0.67              |
| 20:CT:43:LEU:CD1   | 20:CT:51:GLU:HG2  | 2.15                     | 0.67              |
| 22:CV:53:G:C2'     | 22:CV:54:G:H5'    | 2.24                     | 0.67              |
| 25:DA:221:A:H5'    | 25:DA:222:A:C5'   | 2.24                     | 0.67              |
| 25:DA:1817:G:C2'   | 25:DA:1818:U:H5'  | 2.24                     | 0.67              |
| 31:DG:76:SER:O     | 31:DG:77:ILE:HD12 | 1.94                     | 0.67              |
| 34:DN:10:GLU:CD    | 34:DN:11:PRO:HD2  | 2.19                     | 0.67              |
| 34:DN:15:LEU:HD13  | 34:DN:16:ILE:H    | 1.59                     | 0.67              |
| 41:DU:102:GLU:OE2  | 42:DV:2:PHE:CD2   | 2.47                     | 0.67              |
| 41:DU:104:GLN:HE21 | 41:DU:105:VAL:N   | 1.92                     | 0.67              |
| 1:AA:79:G:C4'      | 1:AA:80:G:OP1     | 2.42                     | 0.67              |
| 3:AC:113:ALA:HA    | 3:AC:202:ILE:HD11 | 1.75                     | 0.67              |
| 4:AD:10:ARG:HH11   | 4:AD:10:ARG:CG    | 2.07                     | 0.67              |
| 8:AH:29:SER:HB3    | 8:AH:32:LYS:HG3   | 1.77                     | 0.67              |
| 17:AQ:18:THR:HG23  | 17:AQ:44:ALA:O    | 1.95                     | 0.67              |
| 33:BI:14:ASP:HB2   | 33:BI:17:GLN:NE2  | 2.08                     | 0.67              |
| 39:BS:74:ALA:HB1   | 39:BS:103:GLU:CG  | 2.25                     | 0.67              |
| 5:CE:142:LEU:C     | 5:CE:143:ARG:HG2  | 2.19                     | 0.67              |
| 9:CI:10:ARG:HD3    | 9:CI:75:ASP:CB    | 2.23                     | 0.67              |
| 10:CJ:6:ILE:HG22   | 10:CJ:98:ILE:HG12 | 1.76                     | 0.67              |
| 11:CK:59:TYR:CE1   | 11:CK:63:LEU:HD12 | 2.28                     | 0.67              |
| 25:DA:301:G:N2     | 25:DA:316:C:N3    | 2.41                     | 0.67              |
| 31:DG:77:ILE:HG22  | 31:DG:77:ILE:O    | 1.95                     | 0.67              |
| 33:DI:88:ILE:HG12  | 33:DI:122:GLU:N   | 2.10                     | 0.67              |
| 40:DT:65:LYS:HZ2   | 40:DT:66:VAL:N    | 1.90                     | 0.67              |
| 41:DU:91:ASP:OD2   | 41:DU:96:ALA:N    | 2.28                     | 0.67              |
| 43:DW:92:ARG:HH11  | 43:DW:92:ARG:HG2  | 1.58                     | 0.67              |
| 2:AB:44:LEU:H      | 2:AB:44:LEU:HD12  | 1.59                     | 0.67              |
| 3:AC:83:ARG:O      | 3:AC:87:LEU:HG    | 1.95                     | 0.67              |
| 7:AG:23:VAL:HG13   | 7:AG:43:PHE:CE2   | 2.24                     | 0.67              |
| 7:AG:60:LYS:HA     | 7:AG:60:LYS:HZ2   | 1.59                     | 0.67              |
| 10:AJ:95:GLU:OE2   | 10:AJ:95:GLU:HA   | 1.94                     | 0.67              |
| 12:AL:25:PRO:C     | 12:AL:27:LEU:N    | 2.49                     | 0.67              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:AV:15:G:H22     | 22:AV:49:C:N4      | 1.93                     | 0.67              |
| 24:AX:12:A:C5'     | 24:AX:12:A:N3      | 2.57                     | 0.67              |
| 25:BA:705:A:C8     | 25:BA:727:A:C2     | 2.83                     | 0.67              |
| 25:BA:1452:A:H5'   | 25:BA:1453:U:OP2   | 1.93                     | 0.67              |
| 25:BA:2259:G:N7    | 25:BA:2427:C:C4    | 2.63                     | 0.67              |
| 25:BA:2519:U:C5'   | 25:BA:2520:C:OP1   | 2.43                     | 0.67              |
| 27:BC:38:ASP:HB2   | 27:BC:181:PRO:CB   | 2.24                     | 0.67              |
| 28:BD:105:ILE:HD12 | 28:BD:106:ILE:HG22 | 1.75                     | 0.67              |
| 31:BG:43:LEU:HB2   | 31:BG:88:ILE:CG1   | 2.25                     | 0.67              |
| 32:BH:20:ALA:HB1   | 32:BH:21:PRO:HD2   | 1.76                     | 0.67              |
| 33:BI:133:HIS:N    | 33:BI:133:HIS:ND1  | 2.42                     | 0.67              |
| 36:BP:97:PRO:O     | 36:BP:98:GLU:HB3   | 1.94                     | 0.67              |
| 40:BT:13:ARG:HA    | 40:BT:13:ARG:NH1   | 2.09                     | 0.67              |
| 52:B5:46:CYS:HB3   | 52:B5:50:GLY:H     | 1.59                     | 0.67              |
| 1:CA:1226:C:HO2'   | 1:CA:1227:A:C5'    | 2.08                     | 0.67              |
| 1:CA:1226:C:C4'    | 1:CA:1227:A:OP1    | 2.30                     | 0.67              |
| 1:CA:1239:A:H62    | 1:CA:1299:A:H62    | 1.42                     | 0.67              |
| 5:CE:8:GLU:HA      | 5:CE:34:VAL:HG22   | 1.75                     | 0.67              |
| 19:CS:62:ILE:HD12  | 19:CS:63:THR:H     | 1.59                     | 0.67              |
| 36:DP:97:PRO:O     | 36:DP:98:GLU:HB3   | 1.94                     | 0.67              |
| 38:DR:47:PHE:O     | 38:DR:51:LEU:HD12  | 1.94                     | 0.67              |
| 46:DZ:58:VAL:CG1   | 46:DZ:66:SER:HB3   | 2.25                     | 0.67              |
| 1:AA:707:C:OP1     | 11:AK:85:ARG:NH1   | 2.28                     | 0.67              |
| 1:AA:1054:C:H42    | 23:AY:34:G:C1'     | 2.07                     | 0.67              |
| 19:AS:39:THR:HG22  | 19:AS:40:ILE:N     | 2.10                     | 0.67              |
| 25:BA:458:G:N2     | 25:BA:470:A:OP2    | 2.27                     | 0.67              |
| 25:BA:1779:U:OP2   | 25:BA:1784:A:N6    | 2.27                     | 0.67              |
| 25:BA:2680:C:OP2   | 29:BE:111:ARG:NH2  | 2.27                     | 0.67              |
| 29:BE:203:LYS:HE2  | 29:BE:204:ALA:HB2  | 1.75                     | 0.67              |
| 30:BF:64:ILE:C     | 30:BF:65:TRP:CD1   | 2.72                     | 0.67              |
| 31:BG:15:VAL:HG13  | 31:BG:175:LEU:HB3  | 1.76                     | 0.67              |
| 33:BI:29:TYR:CD2   | 33:BI:30:LEU:HD23  | 2.30                     | 0.67              |
| 34:BN:49:GLY:O     | 34:BN:119:ARG:NH1  | 2.28                     | 0.67              |
| 34:BN:62:VAL:CG2   | 34:BN:66:LYS:CG    | 2.72                     | 0.67              |
| 35:BO:17:ARG:HD3   | 35:BO:47:ILE:HD13  | 1.77                     | 0.67              |
| 46:BZ:150:LEU:HD23 | 46:BZ:171:ILE:HG12 | 1.77                     | 0.67              |
| 1:CA:1457:G:H8     | 1:CA:1457:G:O5'    | 1.78                     | 0.67              |
| 25:DA:77:C:OP1     | 49:D2:59:ARG:NH1   | 2.27                     | 0.67              |
| 25:DA:1799:G:O6    | 28:DD:179:SER:CB   | 2.42                     | 0.67              |
| 30:DF:157:VAL:HB   | 30:DF:194:MET:HB3  | 1.75                     | 0.67              |
| 41:DU:52:ARG:HD3   | 41:DU:55:ARG:HE    | 1.59                     | 0.67              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 52:D5:49:CYS:O    | 52:D5:56:LYS:HB3  | 1.95                     | 0.67              |
| 1:AA:1067:A:O2'   | 1:AA:1068:G:P     | 2.53                     | 0.67              |
| 4:AD:138:TYR:CD2  | 4:AD:138:TYR:C    | 2.71                     | 0.67              |
| 10:AJ:29:ARG:HH11 | 1:CA:1163:C:H5''  | 1.59                     | 0.67              |
| 10:AJ:40:LEU:HG   | 10:AJ:69:ASN:HB3  | 1.77                     | 0.67              |
| 31:BG:125:PHE:CD2 | 31:BG:131:TYR:HB2 | 2.30                     | 0.67              |
| 36:BP:79:ARG:HH21 | 36:BP:81:GLN:HG2  | 1.60                     | 0.67              |
| 41:BU:95:LEU:HD13 | 42:BV:4:ILE:CG2   | 2.24                     | 0.67              |
| 49:B2:10:LEU:HD22 | 49:B2:14:ARG:NH1  | 2.10                     | 0.67              |
| 1:CA:1445:C:C2'   | 1:CA:1446:U:H5'   | 2.24                     | 0.67              |
| 3:CC:40:ARG:O     | 3:CC:44:GLU:HG3   | 1.94                     | 0.67              |
| 3:CC:84:ILE:O     | 3:CC:88:ARG:HG3   | 1.95                     | 0.67              |
| 9:CI:21:PRO:HA    | 9:CI:58:HIS:O     | 1.94                     | 0.67              |
| 9:CI:59:PHE:N     | 9:CI:59:PHE:HD1   | 1.92                     | 0.67              |
| 11:CK:32:ILE:HD11 | 11:CK:68:ALA:O    | 1.95                     | 0.67              |
| 13:CM:119:GLY:C   | 13:CM:120:LYS:HD3 | 2.19                     | 0.67              |
| 18:CR:70:ILE:HG22 | 18:CR:74:ARG:HD2  | 1.77                     | 0.67              |
| 20:CT:72:LEU:HD22 | 20:CT:77:ALA:HB2  | 1.75                     | 0.67              |
| 32:DH:150:ALA:O   | 32:DH:152:ARG:N   | 2.26                     | 0.67              |
| 55:D8:6:THR:CG2   | 55:D8:63:PRO:HD3  | 2.25                     | 0.67              |
| 2:AB:144:ARG:HA   | 2:AB:147:LYS:HB3  | 1.75                     | 0.67              |
| 4:AD:138:TYR:C    | 4:AD:138:TYR:HD2  | 2.03                     | 0.67              |
| 27:BC:65:PRO:HG2  | 27:BC:189:ILE:HA  | 1.76                     | 0.67              |
| 29:BE:117:MET:HA  | 29:BE:122:PHE:H   | 1.58                     | 0.67              |
| 38:BR:2:ARG:CZ    | 38:BR:5:LYS:CE    | 2.73                     | 0.67              |
| 43:BW:12:ILE:HD13 | 43:BW:46:PHE:HD2  | 1.59                     | 0.67              |
| 1:CA:992:U:H1'    | 1:CA:993:G:C2     | 2.30                     | 0.67              |
| 5:CE:6:PHE:HD2    | 5:CE:36:ASP:HB3   | 1.59                     | 0.67              |
| 5:CE:102:ALA:O    | 5:CE:106:PRO:CG   | 2.30                     | 0.67              |
| 25:DA:560:C:H4'   | 41:DU:52:ARG:NH2  | 2.09                     | 0.67              |
| 25:DA:1496:A:H8   | 25:DA:1577:C:HO2' | 1.41                     | 0.67              |
| 30:DF:184:TYR:O   | 30:DF:188:ARG:HG3 | 1.95                     | 0.67              |
| 39:DS:103:GLU:O   | 39:DS:106:ARG:HG3 | 1.93                     | 0.67              |
| 43:DW:60:ASN:N    | 43:DW:60:ASN:HD22 | 1.91                     | 0.67              |
| 46:DZ:63:ASP:O    | 46:DZ:65:GLN:HG2  | 1.94                     | 0.67              |
| 1:AA:1343:G:H4'   | 9:AI:122:ALA:HB3  | 1.76                     | 0.67              |
| 2:AB:236:TYR:HA   | 2:AB:239:VAL:CG2  | 2.25                     | 0.67              |
| 3:AC:175:LEU:HD23 | 3:AC:201:TYR:CE2  | 2.28                     | 0.67              |
| 4:AD:18:LYS:HB2   | 4:AD:33:MET:HG2   | 1.77                     | 0.67              |
| 6:AF:37:VAL:O     | 6:AF:38:GLU:HG3   | 1.95                     | 0.67              |
| 25:BA:2302:G:H21  | 31:BG:128:ARG:HG3 | 1.58                     | 0.67              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:BG:46:ALA:O     | 31:BG:82:LEU:HD21  | 1.94                     | 0.67              |
| 41:BU:78:THR:O     | 41:BU:81:HIS:HB3   | 1.95                     | 0.67              |
| 44:BX:16:LYS:O     | 44:BX:19:ALA:HB3   | 1.95                     | 0.67              |
| 1:CA:484:G:C1'     | 1:CA:486:U:C5      | 2.77                     | 0.67              |
| 12:CL:23:LYS:O     | 12:CL:24:VAL:HG23  | 1.93                     | 0.67              |
| 16:CP:26:ARG:HD3   | 16:CP:31:LYS:O     | 1.95                     | 0.67              |
| 25:DA:1340:U:O2'   | 25:DA:1602:U:H2'   | 1.95                     | 0.67              |
| 37:DQ:39:PRO:HB3   | 37:DQ:99:PRO:HD3   | 1.76                     | 0.67              |
| 40:DT:91:ARG:HA    | 40:DT:117:ASP:H    | 1.59                     | 0.67              |
| 46:DZ:13:GLU:O     | 46:DZ:15:PRO:HD3   | 1.94                     | 0.67              |
| 7:AG:14:PRO:CG     | 7:AG:21:VAL:HG12   | 2.22                     | 0.67              |
| 19:AS:29:ARG:HD2   | 19:AS:29:ARG:C     | 2.21                     | 0.67              |
| 20:AT:16:HIS:O     | 20:AT:19:SER:HB3   | 1.95                     | 0.67              |
| 23:AW:68:C:H2'     | 23:AW:69:G:C8      | 2.25                     | 0.67              |
| 25:BA:322:A:H5''   | 25:BA:323:G:OP2    | 1.95                     | 0.67              |
| 28:BD:172:TYR:CD1  | 28:BD:186:HIS:HA   | 2.30                     | 0.67              |
| 33:BI:101:LEU:HB3  | 33:BI:109:ILE:HD11 | 1.77                     | 0.67              |
| 45:BY:81:LYS:CD    | 45:BY:97:ARG:HB3   | 2.23                     | 0.67              |
| 5:CE:100:VAL:HA    | 5:CE:118:ILE:O     | 1.94                     | 0.67              |
| 20:CT:42:GLN:O     | 20:CT:42:GLN:HG3   | 1.95                     | 0.67              |
| 25:DA:1170:G:H1    | 25:DA:1179:C:H42   | 1.42                     | 0.67              |
| 25:DA:2788:C:O2'   | 25:DA:2809:A:N3    | 2.26                     | 0.67              |
| 28:DD:65:ILE:HD11  | 28:DD:67:PHE:CE1   | 2.29                     | 0.67              |
| 31:DG:131:TYR:HB3  | 31:DG:159:VAL:HG13 | 1.76                     | 0.67              |
| 33:DI:114:LEU:CD1  | 33:DI:128:LEU:HD12 | 2.25                     | 0.67              |
| 42:DV:35:LEU:O     | 42:DV:35:LEU:HD23  | 1.95                     | 0.67              |
| 46:DZ:48:PHE:CE2   | 46:DZ:52:SER:HA    | 2.30                     | 0.67              |
| 50:D3:59:VAL:HG12  | 50:D3:60:GLU:N     | 2.09                     | 0.67              |
| 9:AI:5:TYR:O       | 9:AI:84:ALA:HA     | 1.95                     | 0.66              |
| 11:AK:21:ILE:HA    | 11:AK:30:VAL:CG1   | 2.25                     | 0.66              |
| 12:AL:101:VAL:HG12 | 12:AL:101:VAL:O    | 1.93                     | 0.66              |
| 19:AS:43:GLU:C     | 19:AS:45:VAL:HG13  | 2.19                     | 0.66              |
| 25:BA:1784:A:H4'   | 25:BA:1785:A:O5'   | 1.95                     | 0.66              |
| 25:BA:2197:U:O2'   | 25:BA:2198:A:H3'   | 1.95                     | 0.66              |
| 28:BD:69:ARG:NH2   | 28:BD:192:THR:HB   | 2.11                     | 0.66              |
| 31:BG:37:VAL:HG12  | 31:BG:94:LEU:HD12  | 1.77                     | 0.66              |
| 42:BV:64:HIS:ND1   | 42:BV:92:THR:HG22  | 2.10                     | 0.66              |
| 23:CW:31:A:C2      | 23:CW:40:C:N3      | 2.62                     | 0.66              |
| 25:DA:82:G:C6      | 25:DA:83:G:C6      | 2.83                     | 0.66              |
| 25:DA:2414:G:H21   | 36:DP:67:MET:HE1   | 1.60                     | 0.66              |
| 30:DF:107:LYS:CD   | 30:DF:206:ILE:HD13 | 2.21                     | 0.66              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 32:DH:148:ILE:O    | 32:DH:151:ILE:HG12 | 1.95                     | 0.66              |
| 38:DR:10:LEU:O     | 38:DR:12:ARG:HG3   | 1.94                     | 0.66              |
| 40:DT:29:ARG:HG3   | 40:DT:30:VAL:CG1   | 2.26                     | 0.66              |
| 41:DU:91:ASP:OD2   | 41:DU:96:ALA:CA    | 2.43                     | 0.66              |
| 53:D6:20:ASN:ND2   | 53:D6:21:TYR:H     | 1.94                     | 0.66              |
| 3:AC:18:TRP:HE1    | 14:AN:55:GLY:H     | 1.41                     | 0.66              |
| 5:AE:101:ILE:CG1   | 5:AE:119:LEU:HD23  | 2.24                     | 0.66              |
| 25:BA:892:G:H2'    | 25:BA:893:C:C6     | 2.30                     | 0.66              |
| 25:BA:1902:C:O2'   | 28:BD:244:ARG:HG3  | 1.95                     | 0.66              |
| 25:BA:1930:G:HO2'  | 25:BA:1968:G:H1    | 1.43                     | 0.66              |
| 25:BA:2504:U:H1'   | 25:BA:2572:A:N1    | 2.10                     | 0.66              |
| 26:BB:57:A:H5'     | 31:BG:27:ASN:HD22  | 1.60                     | 0.66              |
| 27:BC:59:ARG:HB2   | 27:BC:62:VAL:HG22  | 1.75                     | 0.66              |
| 28:BD:25:THR:HG22  | 28:BD:26:LYS:H     | 1.60                     | 0.66              |
| 34:BN:123:TYR:CE1  | 34:BN:130:HIS:NE2  | 2.63                     | 0.66              |
| 38:BR:10:LEU:HB3   | 38:BR:17:ARG:HD3   | 0.77                     | 0.66              |
| 1:CA:792:A:H4'     | 1:CA:793:U:O5'     | 1.93                     | 0.66              |
| 8:CH:118:VAL:C     | 8:CH:119:LEU:HD23  | 2.19                     | 0.66              |
| 12:CL:24:VAL:O     | 12:CL:24:VAL:HG12  | 1.95                     | 0.66              |
| 25:DA:83:G:H22     | 25:DA:102:G:H2'    | 1.58                     | 0.66              |
| 25:DA:90:U:HO2'    | 25:DA:92:A:H8      | 1.42                     | 0.66              |
| 25:DA:2615:U:H2'   | 25:DA:2616:C:H6    | 1.61                     | 0.66              |
| 31:DG:77:ILE:HG22  | 31:DG:80:PHE:H     | 1.60                     | 0.66              |
| 32:DH:124:GLU:HB3  | 32:DH:126:PRO:HD3  | 1.77                     | 0.66              |
| 35:DO:77:ILE:CD1   | 40:DT:74:ARG:HG2   | 2.25                     | 0.66              |
| 35:DO:87:ILE:CG2   | 35:DO:91:LEU:HA    | 2.24                     | 0.66              |
| 45:DY:57:GLN:HE21  | 45:DY:57:GLN:C     | 2.02                     | 0.66              |
| 1:AA:8:A:N6        | 4:AD:205:GLU:O     | 2.28                     | 0.66              |
| 1:AA:993:G:H2'     | 1:AA:993:G:N3      | 2.11                     | 0.66              |
| 9:AI:55:ALA:O      | 9:AI:56:LEU:C      | 2.36                     | 0.66              |
| 11:AK:29:ILE:HB    | 11:AK:44:SER:HB3   | 1.76                     | 0.66              |
| 19:AS:6:LYS:H      | 19:AS:6:LYS:CE     | 2.07                     | 0.66              |
| 25:BA:1598:C:H5'   | 44:BX:36:LYS:HB2   | 1.78                     | 0.66              |
| 25:BA:1963:U:H4'   | 25:BA:1964:G:OP1   | 1.94                     | 0.66              |
| 29:BE:92:THR:O     | 29:BE:95:ILE:HD13  | 1.95                     | 0.66              |
| 29:BE:102:VAL:HG12 | 29:BE:199:ARG:O    | 1.95                     | 0.66              |
| 32:BH:44:VAL:HG12  | 32:BH:45:VAL:H     | 1.61                     | 0.66              |
| 36:BP:18:ARG:O     | 36:BP:19:VAL:HB    | 1.95                     | 0.66              |
| 37:BQ:30:GLY:CA    | 37:BQ:107:ALA:HB2  | 2.24                     | 0.66              |
| 41:BU:74:LEU:HD12  | 41:BU:75:ASN:N     | 2.11                     | 0.66              |
| 42:BV:45:THR:O     | 42:BV:46:VAL:HG12  | 1.95                     | 0.66              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 55:B8:23:VAL:HG12  | 55:B8:46:ARG:HH11 | 1.61                     | 0.66              |
| 1:CA:872:A:H4'     | 1:CA:873:A:OP1    | 1.94                     | 0.66              |
| 2:CB:131:PRO:HG2   | 2:CB:134:GLU:HB2  | 1.76                     | 0.66              |
| 4:CD:125:HIS:O     | 4:CD:126:ILE:HD13 | 1.96                     | 0.66              |
| 8:CH:104:ARG:O     | 8:CH:106:GLY:N    | 2.27                     | 0.66              |
| 15:CO:56:LEU:O     | 15:CO:60:VAL:HG23 | 1.96                     | 0.66              |
| 16:CP:9:PHE:HE1    | 16:CP:18:ARG:NH2  | 1.94                     | 0.66              |
| 25:DA:1799:G:O2'   | 25:DA:1800:C:C5'  | 2.44                     | 0.66              |
| 31:DG:113:ARG:NH1  | 31:DG:142:PRO:HA  | 2.10                     | 0.66              |
| 40:DT:13:ARG:HA    | 40:DT:13:ARG:NE   | 2.09                     | 0.66              |
| 48:D1:12:PRO:HB3   | 48:D1:43:TYR:HD2  | 1.59                     | 0.66              |
| 56:D9:9:ARG:NH1    | 56:D9:9:ARG:HB3   | 2.10                     | 0.66              |
| 2:AB:170:GLU:O     | 2:AB:173:ALA:HB3  | 1.95                     | 0.66              |
| 11:AK:43:SER:HB3   | 11:AK:68:ALA:HB2  | 1.78                     | 0.66              |
| 12:AL:53:ARG:HH12  | 12:AL:92:ASP:CB   | 2.09                     | 0.66              |
| 29:BE:30:PRO:C     | 29:BE:32:PRO:HD3  | 2.20                     | 0.66              |
| 29:BE:176:ILE:HD12 | 29:BE:176:ILE:N   | 2.11                     | 0.66              |
| 30:BF:34:TRP:N     | 36:BP:6:LEU:HD12  | 2.11                     | 0.66              |
| 31:BG:76:SER:CB    | 31:BG:83:ARG:HB2  | 2.25                     | 0.66              |
| 32:BH:23:ARG:HD2   | 32:BH:34:GLU:OE2  | 1.94                     | 0.66              |
| 33:BI:113:ARG:O    | 33:BI:130:TYR:HA  | 1.94                     | 0.66              |
| 47:B0:38:VAL:HG12  | 47:B0:40:GLN:HG2  | 1.76                     | 0.66              |
| 56:B9:24:TYR:O     | 56:B9:25:VAL:HG23 | 1.95                     | 0.66              |
| 1:CA:1456:G:C2     | 1:CA:1457:G:C8    | 2.83                     | 0.66              |
| 7:CG:38:LEU:O      | 7:CG:42:ILE:HG13  | 1.95                     | 0.66              |
| 21:CU:18:TYR:CD2   | 21:CU:22:ARG:HD3  | 2.31                     | 0.66              |
| 22:CV:29:C:O2      | 22:CV:30:G:C8     | 2.49                     | 0.66              |
| 25:DA:1648:C:C4    | 25:DA:2010:G:N1   | 2.63                     | 0.66              |
| 29:DE:76:ARG:O     | 29:DE:77:ILE:O    | 2.13                     | 0.66              |
| 31:DG:173:LEU:HD22 | 31:DG:178:PHE:CZ  | 2.30                     | 0.66              |
| 32:DH:80:SER:O     | 32:DH:81:GLU:HB2  | 1.95                     | 0.66              |
| 33:DI:92:VAL:HG22  | 33:DI:92:VAL:O    | 1.96                     | 0.66              |
| 33:DI:133:HIS:O    | 33:DI:134:PRO:C   | 2.38                     | 0.66              |
| 34:DN:46:VAL:O     | 34:DN:47:ALA:HB3  | 1.95                     | 0.66              |
| 53:D6:33:LYS:HE2   | 53:D6:33:LYS:HA   | 1.77                     | 0.66              |
| 1:AA:686:U:C1'     | 11:AK:42:TRP:HE1  | 2.04                     | 0.66              |
| 5:AE:101:ILE:N     | 5:AE:101:ILE:HD13 | 2.10                     | 0.66              |
| 11:AK:12:ARG:O     | 11:AK:13:GLN:HG3  | 1.95                     | 0.66              |
| 13:AM:4:ILE:HG22   | 13:AM:5:ALA:N     | 2.09                     | 0.66              |
| 25:BA:2092:U:H4'   | 25:BA:2093:G:O5'  | 1.96                     | 0.66              |
| 30:BF:132:VAL:HG22 | 30:BF:133:ASN:N   | 2.09                     | 0.66              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 36:BP:59:LEU:HG    | 55:B8:13:ARG:CZ    | 2.26                     | 0.66              |
| 41:BU:14:HIS:C     | 41:BU:16:LYS:H     | 2.02                     | 0.66              |
| 45:BY:66:PRO:O     | 45:BY:67:LEU:CG    | 2.43                     | 0.66              |
| 1:CA:819:A:C4'     | 1:CA:820:U:OP2     | 2.43                     | 0.66              |
| 1:CA:968:A:C5'     | 1:CA:969:A:OP2     | 2.43                     | 0.66              |
| 8:CH:20:TYR:HE2    | 8:CH:75:ARG:HB3    | 1.59                     | 0.66              |
| 12:CL:54:LYS:O     | 12:CL:70:ILE:HG13  | 1.95                     | 0.66              |
| 14:CN:59:ALA:O     | 14:CN:60:SER:HB2   | 1.94                     | 0.66              |
| 25:DA:307:G:H21    | 25:DA:330:A:H62    | 1.42                     | 0.66              |
| 25:DA:1827:C:OP2   | 28:DD:222:ARG:NH1  | 2.27                     | 0.66              |
| 25:DA:2393:A:H4'   | 36:DP:60:MET:O     | 1.95                     | 0.66              |
| 36:DP:88:LEU:HD11  | 36:DP:95:VAL:HG21  | 1.76                     | 0.66              |
| 40:DT:24:PRO:CD    | 40:DT:52:ILE:CD1   | 2.71                     | 0.66              |
| 45:DY:52:SER:OG    | 45:DY:53:PRO:HD3   | 1.95                     | 0.66              |
| 4:AD:30:LYS:C      | 4:AD:32:ALA:N      | 2.48                     | 0.66              |
| 8:AH:109:ILE:HG22  | 8:AH:137:VAL:HB    | 1.76                     | 0.66              |
| 12:AL:26:ALA:C     | 12:AL:27:LEU:HD22  | 2.21                     | 0.66              |
| 12:AL:38:THR:O     | 12:AL:79:GLU:HG3   | 1.96                     | 0.66              |
| 14:AN:15:LYS:HE3   | 14:AN:16:PHE:HE2   | 1.61                     | 0.66              |
| 20:AT:44:ALA:O     | 20:AT:91:LEU:HB3   | 1.96                     | 0.66              |
| 20:AT:89:ARG:HB2   | 20:AT:104:LEU:HD11 | 1.77                     | 0.66              |
| 23:AW:18:G:N1      | 23:AW:55:U:H1'     | 2.10                     | 0.66              |
| 25:BA:265:A:H1'    | 25:BA:266:G:O4'    | 1.95                     | 0.66              |
| 25:BA:1740:G:H4'   | 25:BA:1741:A:OP1   | 1.95                     | 0.66              |
| 34:BN:14:VAL:HG12  | 34:BN:15:LEU:N     | 2.11                     | 0.66              |
| 1:CA:992:U:O2'     | 1:CA:993:G:C5'     | 2.43                     | 0.66              |
| 1:CA:1349:A:OP2    | 9:CI:118:LYS:NZ    | 2.28                     | 0.66              |
| 12:CL:126:LYS:HG3  | 12:CL:127:GLU:N    | 2.10                     | 0.66              |
| 16:CP:2:VAL:HG22   | 16:CP:64:ALA:HB2   | 1.78                     | 0.66              |
| 22:CV:53:G:H2'     | 22:CV:54:G:H5'     | 1.78                     | 0.66              |
| 29:DE:199:ARG:HH11 | 29:DE:199:ARG:HB2  | 1.60                     | 0.66              |
| 30:DF:46:ARG:HH11  | 30:DF:46:ARG:CG    | 2.08                     | 0.66              |
| 46:DZ:16:SER:O     | 46:DZ:20:ARG:HG3   | 1.96                     | 0.66              |
| 51:D4:8:LYS:O      | 51:D4:27:THR:CG2   | 2.43                     | 0.66              |
| 53:D6:17:LYS:C     | 53:D6:18:ARG:HD3   | 2.21                     | 0.66              |
| 1:AA:9:G:H2'       | 1:AA:10:A:H8       | 1.60                     | 0.66              |
| 3:AC:157:ILE:HD11  | 3:AC:166:GLU:HB2   | 1.77                     | 0.66              |
| 4:AD:116:GLN:NE2   | 4:AD:157:LEU:HD11  | 2.11                     | 0.66              |
| 24:AX:13:A:C2      | 24:AX:14:A:H8      | 2.13                     | 0.66              |
| 25:BA:242:G:O3'    | 25:BA:243:U:C5     | 2.48                     | 0.66              |
| 25:BA:1252:G:C6    | 25:BA:1253:A:N1    | 2.63                     | 0.66              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:BA:2500:U:O2    | 25:BA:2504:U:C4    | 2.48                     | 0.66              |
| 30:BF:46:ARG:HH11  | 30:BF:46:ARG:CG    | 2.08                     | 0.66              |
| 40:BT:19:LEU:HD22  | 40:BT:85:LYS:HD3   | 1.78                     | 0.66              |
| 45:BY:67:LEU:CD1   | 45:BY:68:HIS:H     | 2.08                     | 0.66              |
| 1:CA:1442(B):A:C2  | 40:DT:118:ARG:NH1  | 2.64                     | 0.66              |
| 3:CC:15:THR:HG22   | 3:CC:16:ARG:N      | 2.10                     | 0.66              |
| 5:CE:76:ILE:CG1    | 5:CE:77:PRO:HD2    | 2.24                     | 0.66              |
| 25:DA:1129:A:N6    | 25:DA:2491:U:OP1   | 2.29                     | 0.66              |
| 27:DC:38:ASP:HB2   | 27:DC:181:PRO:CB   | 2.25                     | 0.66              |
| 29:DE:23:VAL:HA    | 29:DE:184:VAL:O    | 1.95                     | 0.66              |
| 34:DN:19:GLU:HG3   | 34:DN:20:GLY:N     | 2.10                     | 0.66              |
| 39:DS:107:GLU:N    | 39:DS:110:LEU:CD1  | 2.46                     | 0.66              |
| 44:DX:70:LEU:HD23  | 44:DX:71:GLY:N     | 2.11                     | 0.66              |
| 46:DZ:108:PRO:HB3  | 46:DZ:117:LEU:HD22 | 1.78                     | 0.66              |
| 4:AD:60:GLU:HG3    | 4:AD:198:VAL:HG13  | 1.77                     | 0.66              |
| 10:AJ:44:VAL:HG22  | 10:AJ:66:ARG:HG2   | 1.78                     | 0.66              |
| 16:AP:58:TYR:HA    | 16:AP:61:SER:HB3   | 1.77                     | 0.66              |
| 28:BD:28:GLU:H     | 28:BD:29:PRO:HD2   | 1.59                     | 0.66              |
| 29:BE:114:ALA:HB1  | 29:BE:118:LYS:HD2  | 1.77                     | 0.66              |
| 33:BI:78:THR:HA    | 33:BI:141:LYS:O    | 1.96                     | 0.66              |
| 53:B6:43:CYS:O     | 53:B6:44:ARG:C     | 2.38                     | 0.66              |
| 1:CA:60:A:C4'      | 1:CA:61:G:O5'      | 2.42                     | 0.66              |
| 1:CA:1149:C:O2'    | 1:CA:1280:A:N1     | 2.27                     | 0.66              |
| 3:CC:24:ALA:HB1    | 3:CC:28:GLN:O      | 1.96                     | 0.66              |
| 4:CD:152:SER:O     | 4:CD:158:ILE:HD12  | 1.95                     | 0.66              |
| 4:CD:172:PRO:HB2   | 4:CD:187:ARG:HH22  | 1.59                     | 0.66              |
| 25:DA:943:U:P      | 36:DP:36:LYS:HG3   | 2.35                     | 0.66              |
| 33:DI:41:GLU:CD    | 33:DI:41:GLU:H     | 2.04                     | 0.66              |
| 33:DI:69:LYS:HE2   | 33:DI:73:GLU:OE2   | 1.96                     | 0.66              |
| 43:DW:9:TYR:HD2    | 43:DW:102:HIS:NE2  | 1.89                     | 0.66              |
| 1:AA:652:U:O2'     | 1:AA:653:A:N3      | 2.29                     | 0.66              |
| 11:AK:127:LYS:HE2  | 11:AK:127:LYS:HA   | 1.77                     | 0.66              |
| 24:AX:13:A:C2      | 24:AX:14:A:C8      | 2.84                     | 0.66              |
| 25:BA:322:A:H4'    | 25:BA:323:G:OP2    | 1.96                     | 0.66              |
| 32:BH:121:ILE:HD11 | 32:BH:140:LYS:HG2  | 1.77                     | 0.66              |
| 38:BR:37:THR:CG2   | 38:BR:40:LYS:HE3   | 2.26                     | 0.66              |
| 42:BV:19:LYS:CG    | 42:BV:94:LEU:HB2   | 2.25                     | 0.66              |
| 46:BZ:97:GLU:HB3   | 46:BZ:125:LEU:HD11 | 1.77                     | 0.66              |
| 55:B8:51:ALA:C     | 55:B8:53:PRO:HD2   | 2.21                     | 0.66              |
| 1:CA:61:G:OP2      | 20:CT:10:LEU:HD21  | 1.96                     | 0.66              |
| 1:CA:1305:G:N2     | 1:CA:1331:G:O2'    | 2.29                     | 0.66              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 5:CE:11:ILE:HG13   | 5:CE:31:LEU:HB3    | 1.78                     | 0.66              |
| 12:CL:25:PRO:C     | 12:CL:27:LEU:H     | 2.04                     | 0.66              |
| 28:DD:218:ARG:HH11 | 28:DD:218:ARG:HG3  | 1.59                     | 0.66              |
| 29:DE:120:TRP:O    | 29:DE:121:ASN:HB2  | 1.94                     | 0.66              |
| 30:DF:29:ASN:H     | 30:DF:112:MET:HE3  | 1.61                     | 0.66              |
| 32:DH:19:VAL:HG12  | 32:DH:20:ALA:N     | 2.10                     | 0.66              |
| 32:DH:89:ILE:HD13  | 32:DH:89:ILE:C     | 2.19                     | 0.66              |
| 38:DR:3:HIS:O      | 38:DR:5:LYS:N      | 2.22                     | 0.66              |
| 40:DT:65:LYS:HZ1   | 40:DT:66:VAL:HB    | 1.61                     | 0.66              |
| 41:DU:83:LEU:HG    | 41:DU:88:ILE:CD1   | 2.25                     | 0.66              |
| 45:DY:35:TYR:CE1   | 45:DY:69:ALA:HB3   | 2.31                     | 0.66              |
| 1:AA:625:G:C4'     | 16:AP:16:HIS:HD2   | 2.09                     | 0.66              |
| 1:AA:914:A:O2'     | 1:AA:915:A:H5'     | 1.96                     | 0.66              |
| 4:AD:88:VAL:O      | 4:AD:92:VAL:HG23   | 1.96                     | 0.66              |
| 27:BC:55:ASP:CG    | 27:BC:56:GLN:H     | 2.01                     | 0.66              |
| 39:BS:89:ARG:HD3   | 39:BS:92:TYR:HA    | 1.76                     | 0.66              |
| 41:BU:33:ARG:O     | 41:BU:37:GLU:HG2   | 1.95                     | 0.66              |
| 1:CA:255:G:H1'     | 17:CQ:16:GLN:OE1   | 1.95                     | 0.66              |
| 1:CA:993:G:N3      | 1:CA:993:G:H2'     | 2.10                     | 0.66              |
| 11:CK:20:TYR:O     | 11:CK:30:VAL:CA    | 2.44                     | 0.66              |
| 25:DA:1819:A:H5''  | 25:DA:1820:U:C5'   | 2.26                     | 0.66              |
| 25:DA:2700:C:H2'   | 25:DA:2701:C:H5'   | 1.78                     | 0.66              |
| 30:DF:178:PRO:HG2  | 30:DF:179:GLU:OE2  | 1.94                     | 0.66              |
| 31:DG:133:LEU:HD21 | 31:DG:157:ILE:HB   | 1.78                     | 0.66              |
| 34:DN:54:VAL:HB    | 34:DN:122:VAL:HG22 | 1.78                     | 0.66              |
| 34:DN:128:HIS:NE2  | 34:DN:134:ARG:HG2  | 2.11                     | 0.66              |
| 53:D6:10:LEU:HD12  | 55:D8:34:TRP:NE1   | 2.11                     | 0.66              |
| 1:AA:1346:A:C8     | 1:AA:1348:U:C2     | 2.84                     | 0.65              |
| 2:AB:32:ILE:HD11   | 2:AB:190:THR:HG22  | 1.77                     | 0.65              |
| 8:AH:51:VAL:HG23   | 8:AH:52:ASP:N      | 2.11                     | 0.65              |
| 20:AT:49:ALA:C     | 20:AT:100:ILE:CD1  | 2.68                     | 0.65              |
| 22:AV:3:C:H2'      | 22:AV:4:G:H5'      | 1.78                     | 0.65              |
| 25:BA:1365:A:OP1   | 48:B1:41:ARG:NH1   | 2.29                     | 0.65              |
| 25:BA:1620:G:O2'   | 54:B7:2:LYS:HG3    | 1.96                     | 0.65              |
| 25:BA:2443:C:OP1   | 30:BF:68:LYS:HG2   | 1.96                     | 0.65              |
| 28:BD:44:ASN:OD1   | 28:BD:44:ASN:N     | 2.29                     | 0.65              |
| 28:BD:131:LEU:HD12 | 28:BD:131:LEU:N    | 2.11                     | 0.65              |
| 29:BE:9:VAL:HG13   | 29:BE:25:VAL:O     | 1.97                     | 0.65              |
| 34:BN:125:GLY:HA3  | 34:BN:126:PRO:C    | 2.21                     | 0.65              |
| 4:CD:108:LEU:CG    | 4:CD:110:PHE:CD1   | 2.77                     | 0.65              |
| 6:CF:37:VAL:HA     | 6:CF:65:VAL:HG12   | 1.78                     | 0.65              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:CH:68:ARG:HH11   | 8:CH:68:ARG:HG3    | 1.59                     | 0.65              |
| 10:CJ:45:ARG:HG3   | 10:CJ:45:ARG:NH1   | 2.11                     | 0.65              |
| 11:CK:125:PHE:CD1  | 11:CK:125:PHE:N    | 2.59                     | 0.65              |
| 18:CR:76:LEU:N     | 18:CR:76:LEU:CD2   | 2.59                     | 0.65              |
| 23:CW:36:A:H2'     | 23:CW:37:A:O4'     | 1.96                     | 0.65              |
| 25:DA:614(C):A:C4' | 25:DA:615:G:OP1    | 2.44                     | 0.65              |
| 25:DA:747:U:C5     | 52:D5:3:LYS:HB2    | 2.30                     | 0.65              |
| 25:DA:1141:U:OP2   | 34:DN:22:THR:HG21  | 1.96                     | 0.65              |
| 30:DF:34:TRP:HA    | 36:DP:6:LEU:HD12   | 1.78                     | 0.65              |
| 30:DF:127:GLU:O    | 30:DF:129:PHE:N    | 2.29                     | 0.65              |
| 33:DI:110:ASP:HB2  | 33:DI:112:LYS:N    | 2.11                     | 0.65              |
| 36:DP:124:LYS:HZ2  | 36:DP:143:GLY:HA3  | 1.60                     | 0.65              |
| 39:DS:49:VAL:HG22  | 39:DS:80:LEU:HD12  | 1.78                     | 0.65              |
| 39:DS:58:LEU:HD23  | 39:DS:58:LEU:H     | 1.60                     | 0.65              |
| 39:DS:66:ALA:O     | 39:DS:69:VAL:HG13  | 1.96                     | 0.65              |
| 40:DT:11:GLU:CD    | 40:DT:11:GLU:H     | 2.04                     | 0.65              |
| 46:DZ:150:LEU:HB2  | 46:DZ:154:ASP:OD1  | 1.96                     | 0.65              |
| 1:AA:242:C:H3'     | 1:AA:242:C:H6      | 1.61                     | 0.65              |
| 1:AA:955:U:OP1     | 13:AM:120:LYS:NZ   | 2.29                     | 0.65              |
| 10:AJ:47:PHE:CE2   | 14:AN:37:PHE:HE2   | 2.14                     | 0.65              |
| 20:AT:26:ASN:O     | 20:AT:30:LYS:HB2   | 1.95                     | 0.65              |
| 20:AT:45:GLN:CA    | 20:AT:91:LEU:HD13  | 2.26                     | 0.65              |
| 24:AX:11:U:OP2     | 24:AX:11:U:H5      | 1.78                     | 0.65              |
| 25:BA:995:C:C4     | 34:BN:1:MET:CG     | 2.75                     | 0.65              |
| 28:BD:32:SER:O     | 28:BD:36:PRO:HD2   | 1.97                     | 0.65              |
| 28:BD:36:PRO:HA    | 28:BD:62:TYR:O     | 1.95                     | 0.65              |
| 28:BD:226:MET:O    | 28:BD:234:GLY:HA3  | 1.96                     | 0.65              |
| 29:BE:16:ARG:O     | 29:BE:17:ASP:HB2   | 1.96                     | 0.65              |
| 29:BE:186:GLY:O    | 29:BE:188:VAL:N    | 2.29                     | 0.65              |
| 34:BN:3:THR:HG22   | 34:BN:5:VAL:HG12   | 1.78                     | 0.65              |
| 36:BP:83:VAL:HG23  | 36:BP:105:LEU:HD22 | 1.79                     | 0.65              |
| 41:BU:112:ARG:HG2  | 41:BU:112:ARG:NH1  | 2.12                     | 0.65              |
| 46:BZ:53:ILE:HG21  | 46:BZ:71:VAL:O     | 1.96                     | 0.65              |
| 49:B2:63:VAL:HA    | 49:B2:66:GLU:HG2   | 1.78                     | 0.65              |
| 1:CA:251:G:N9      | 1:CA:252:U:H5      | 1.92                     | 0.65              |
| 4:CD:30:LYS:C      | 4:CD:32:ALA:N      | 2.51                     | 0.65              |
| 25:DA:483:A:H5'    | 45:DY:49:VAL:HG13  | 1.77                     | 0.65              |
| 25:DA:1615:C:C5    | 25:DA:1617:C:C4    | 2.84                     | 0.65              |
| 36:DP:79:ARG:HH21  | 36:DP:81:GLN:HG2   | 1.60                     | 0.65              |
| 46:DZ:11:GLU:CD    | 46:DZ:11:GLU:N     | 2.41                     | 0.65              |
| 46:DZ:23:LYS:HE2   | 46:DZ:38:TYR:HE1   | 1.60                     | 0.65              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:AA:1226:C:C4'    | 1:AA:1227:A:OP1   | 2.30                     | 0.65              |
| 4:AD:173:TRP:HA    | 4:AD:187:ARG:HH12 | 1.59                     | 0.65              |
| 13:AM:20:THR:C     | 13:AM:22:ILE:H    | 2.04                     | 0.65              |
| 13:AM:29:ARG:HB3   | 13:AM:64:TRP:CZ2  | 2.31                     | 0.65              |
| 25:BA:242:G:C2     | 25:BA:254:G:N7    | 2.64                     | 0.65              |
| 25:BA:322:A:C4'    | 25:BA:323:G:OP2   | 2.44                     | 0.65              |
| 25:BA:2128:C:OP1   | 27:BC:35:ALA:HB1  | 1.96                     | 0.65              |
| 30:BF:11:VAL:C     | 30:BF:13:SER:H    | 2.04                     | 0.65              |
| 31:BG:16:ARG:HG3   | 31:BG:16:ARG:NH1  | 2.10                     | 0.65              |
| 31:BG:117:PHE:HD1  | 31:BG:118:ARG:N   | 1.94                     | 0.65              |
| 34:BN:134:ARG:N    | 34:BN:135:PRO:HD3 | 2.09                     | 0.65              |
| 36:BP:55:ARG:O     | 36:BP:56:SER:C    | 2.39                     | 0.65              |
| 36:BP:78:PRO:HB3   | 36:BP:111:ARG:CZ  | 2.27                     | 0.65              |
| 40:BT:102:ILE:HD12 | 40:BT:103:ARG:N   | 2.12                     | 0.65              |
| 41:BU:12:ARG:C     | 41:BU:14:HIS:H    | 2.03                     | 0.65              |
| 46:BZ:39:VAL:HG21  | 46:BZ:44:PHE:HB2  | 1.78                     | 0.65              |
| 51:B4:62:CYS:SG    | 51:B4:63:SER:N    | 2.69                     | 0.65              |
| 1:CA:119:A:H4'     | 1:CA:120:A:O5'    | 1.97                     | 0.65              |
| 1:CA:1446:U:C2     | 1:CA:1457:G:N1    | 2.64                     | 0.65              |
| 2:CB:168:THR:OG1   | 2:CB:169:LYS:N    | 2.24                     | 0.65              |
| 5:CE:81:GLU:HG2    | 5:CE:90:VAL:HG12  | 1.77                     | 0.65              |
| 20:CT:50:GLU:O     | 20:CT:52:ALA:N    | 2.29                     | 0.65              |
| 25:DA:1205:U:H5'   | 25:DA:1206:G:OP2  | 1.96                     | 0.65              |
| 25:DA:1899:G:N2    | 25:DA:1902:C:H41  | 1.94                     | 0.65              |
| 33:DI:74:ASN:HD22  | 33:DI:74:ASN:N    | 1.93                     | 0.65              |
| 36:DP:3:LEU:HA     | 36:DP:6:LEU:HD23  | 1.78                     | 0.65              |
| 36:DP:20:GLY:O     | 36:DP:21:ARG:CD   | 2.44                     | 0.65              |
| 36:DP:85:LEU:HD23  | 36:DP:85:LEU:H    | 1.59                     | 0.65              |
| 41:DU:92:ARG:C     | 41:DU:94:ASN:H    | 2.04                     | 0.65              |
| 42:DV:1:MET:HG3    | 42:DV:43:GLU:HG2  | 1.77                     | 0.65              |
| 45:DY:95:LYS:HB3   | 45:DY:100:ALA:CA  | 2.19                     | 0.65              |
| 46:DZ:53:ILE:H     | 46:DZ:71:VAL:CG2  | 2.09                     | 0.65              |
| 53:D6:45:LYS:O     | 53:D6:46:HIS:HB3  | 1.95                     | 0.65              |
| 2:AB:7:VAL:N       | 2:AB:8:LYS:HE2    | 2.11                     | 0.65              |
| 6:AF:1:MET:CE      | 6:AF:68:PRO:HB3   | 2.27                     | 0.65              |
| 13:AM:47:ASP:O     | 13:AM:48:LEU:HB3  | 1.95                     | 0.65              |
| 25:BA:1301:A:C5'   | 25:BA:1301:A:N3   | 2.58                     | 0.65              |
| 25:BA:1899:G:H21   | 25:BA:1902:C:H41  | 1.44                     | 0.65              |
| 25:BA:2447:G:C1'   | 25:BA:2501:C:C5   | 2.79                     | 0.65              |
| 26:BB:44:G:H1'     | 26:BB:47:C:H42    | 1.62                     | 0.65              |
| 38:BR:76:VAL:O     | 38:BR:80:PHE:N    | 2.29                     | 0.65              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 39:BS:66:ALA:O     | 39:BS:67:ARG:C     | 2.39                     | 0.65              |
| 41:BU:108:GLU:OE2  | 42:BV:44:LYS:CD    | 2.40                     | 0.65              |
| 45:BY:17:SER:OG    | 45:BY:18:GLY:N     | 2.23                     | 0.65              |
| 45:BY:28:LYS:CG    | 45:BY:37:VAL:HB    | 2.26                     | 0.65              |
| 1:CA:913:A:C4'     | 1:CA:914:A:O5'     | 2.33                     | 0.65              |
| 31:DG:67:LYS:CG    | 51:D4:5:ILE:HG22   | 2.18                     | 0.65              |
| 33:DI:69:LYS:HG3   | 33:DI:136:VAL:HB   | 1.79                     | 0.65              |
| 36:DP:79:ARG:HD3   | 36:DP:109:GLY:C    | 2.21                     | 0.65              |
| 55:D8:60:LEU:C     | 55:D8:63:PRO:HD2   | 2.22                     | 0.65              |
| 1:AA:962:C:H2'     | 1:AA:963:G:H8      | 1.62                     | 0.65              |
| 4:AD:8:VAL:CA      | 4:AD:11:LEU:HD21   | 2.23                     | 0.65              |
| 7:AG:10:ARG:HH11   | 7:AG:10:ARG:CG     | 2.05                     | 0.65              |
| 19:AS:39:THR:HG22  | 19:AS:40:ILE:O     | 1.97                     | 0.65              |
| 23:AW:7:A:H61      | 23:AW:66:U:H3      | 1.42                     | 0.65              |
| 25:BA:2168:G:N2    | 25:BA:2171:A:OP2   | 2.30                     | 0.65              |
| 25:BA:2466:C:H5''  | 56:B9:6:SER:HB3    | 1.79                     | 0.65              |
| 28:BD:49:ILE:HD11  | 28:BD:52:ARG:HA    | 1.79                     | 0.65              |
| 28:BD:210:GLY:O    | 28:BD:213:ARG:N    | 2.30                     | 0.65              |
| 36:BP:83:VAL:CG1   | 36:BP:112:LEU:HD21 | 2.26                     | 0.65              |
| 40:BT:64:ARG:NH1   | 40:BT:103:ARG:HA   | 2.11                     | 0.65              |
| 42:BV:20:LEU:C     | 42:BV:21:ARG:HD3   | 2.21                     | 0.65              |
| 43:BW:5:ALA:O      | 43:BW:6:ILE:HG13   | 1.96                     | 0.65              |
| 1:CA:624:C:H4'     | 16:CP:10:GLY:C     | 2.21                     | 0.65              |
| 11:CK:21:ILE:HD12  | 11:CK:21:ILE:N     | 2.11                     | 0.65              |
| 20:CT:29:LYS:HD2   | 20:CT:66:ALA:HA    | 1.79                     | 0.65              |
| 33:DI:77:LEU:HD11  | 33:DI:140:LEU:CA   | 2.27                     | 0.65              |
| 41:DU:92:ARG:HD3   | 41:DU:92:ARG:N     | 2.10                     | 0.65              |
| 43:DW:55:ALA:HA    | 43:DW:107:LEU:CD2  | 2.26                     | 0.65              |
| 45:DY:50:ARG:HB3   | 45:DY:53:PRO:CG    | 2.27                     | 0.65              |
| 1:AA:971:G:H3'     | 1:AA:971:G:P       | 2.37                     | 0.65              |
| 8:AH:97:VAL:O      | 8:AH:100:ILE:HG13  | 1.96                     | 0.65              |
| 11:AK:51:LYS:HA    | 11:AK:55:LYS:HG3   | 1.77                     | 0.65              |
| 13:AM:35:GLU:HG3   | 13:AM:36:LYS:N     | 2.11                     | 0.65              |
| 14:AN:13:THR:O     | 14:AN:15:LYS:N     | 2.30                     | 0.65              |
| 19:AS:6:LYS:CG     | 19:AS:7:LYS:CD     | 2.70                     | 0.65              |
| 25:BA:668:G:N7     | 25:BA:670:A:C8     | 2.65                     | 0.65              |
| 28:BD:79:VAL:HG21  | 28:BD:111:LEU:HD11 | 1.77                     | 0.65              |
| 30:BF:154:VAL:HG22 | 30:BF:191:ARG:CB   | 2.21                     | 0.65              |
| 31:BG:66:GLN:NE2   | 31:BG:94:LEU:HD23  | 2.12                     | 0.65              |
| 38:BR:2:ARG:HH12   | 38:BR:5:LYS:HE2    | 1.60                     | 0.65              |
| 45:BY:31:LEU:CB    | 45:BY:32:PRO:HA    | 2.27                     | 0.65              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:CB:236:TYR:HA    | 2:CB:239:VAL:CG2   | 2.27                     | 0.65              |
| 3:CC:70:VAL:HG12   | 3:CC:71:ALA:N      | 2.11                     | 0.65              |
| 8:CH:68:ARG:HG2    | 8:CH:68:ARG:NH1    | 2.12                     | 0.65              |
| 11:CK:78:GLN:O     | 11:CK:103:LEU:HD22 | 1.96                     | 0.65              |
| 13:CM:82:MET:HE2   | 13:CM:93:ARG:HA    | 1.79                     | 0.65              |
| 22:CV:24:C:C2      | 22:CV:25:U:C5      | 2.85                     | 0.65              |
| 25:DA:896:A:C2     | 46:DZ:113:ALA:HB3  | 2.32                     | 0.65              |
| 25:DA:1559:G:N2    | 25:DA:1559:G:OP1   | 2.30                     | 0.65              |
| 2:AB:106:LYS:O     | 2:AB:110:GLN:HG3   | 1.96                     | 0.65              |
| 25:BA:1396:U:O2    | 25:BA:1396:U:C2'   | 2.45                     | 0.65              |
| 26:BB:109:C:C6     | 26:BB:109:C:OP2    | 2.50                     | 0.65              |
| 30:BF:32:LEU:HD13  | 30:BF:112:MET:HE1  | 1.78                     | 0.65              |
| 35:BO:64:ARG:HG2   | 35:BO:79:PHE:CG    | 2.30                     | 0.65              |
| 35:BO:105:GLU:HA   | 35:BO:108:GLU:OE2  | 1.97                     | 0.65              |
| 45:BY:14:LEU:CG    | 45:BY:15:VAL:H     | 2.10                     | 0.65              |
| 1:CA:643:C:H5'     | 8:CH:31:PHE:CD1    | 2.31                     | 0.65              |
| 4:CD:146:ILE:H     | 4:CD:146:ILE:HD12  | 1.60                     | 0.65              |
| 17:CQ:11:VAL:HG12  | 17:CQ:85:VAL:HG22  | 1.77                     | 0.65              |
| 20:CT:40:ALA:CB    | 20:CT:55:ILE:HG21  | 2.27                     | 0.65              |
| 25:DA:2258:C:H4'   | 25:DA:2259:G:OP2   | 1.94                     | 0.65              |
| 28:DD:227:ASN:HB3  | 28:DD:228:PRO:CD   | 2.26                     | 0.65              |
| 30:DF:20:LEU:HD12  | 30:DF:21:ALA:N     | 2.12                     | 0.65              |
| 30:DF:57:VAL:HG12  | 30:DF:59:TYR:H     | 1.61                     | 0.65              |
| 31:DG:16:ARG:HB3   | 31:DG:17:PRO:CD    | 2.26                     | 0.65              |
| 33:DI:114:LEU:HD22 | 33:DI:130:TYR:CD1  | 2.31                     | 0.65              |
| 36:DP:78:PRO:HB3   | 36:DP:111:ARG:CZ   | 2.27                     | 0.65              |
| 40:DT:36:GLU:HB3   | 40:DT:38:ASN:CG    | 2.22                     | 0.65              |
| 42:DV:41:GLY:HA3   | 42:DV:46:VAL:HG11  | 1.79                     | 0.65              |
| 45:DY:95:LYS:HE3   | 45:DY:95:LYS:O     | 1.96                     | 0.65              |
| 3:AC:153:VAL:HG22  | 3:AC:198:VAL:HG13  | 1.79                     | 0.65              |
| 7:AG:46:ALA:HB1    | 7:AG:121:ALA:HB2   | 1.79                     | 0.65              |
| 12:AL:35:GLY:O     | 12:AL:82:VAL:HG13  | 1.97                     | 0.65              |
| 14:AN:15:LYS:HD2   | 14:AN:16:PHE:CE2   | 2.31                     | 0.65              |
| 23:AW:38:A:C3'     | 23:AW:39:U:C5'     | 2.75                     | 0.65              |
| 25:BA:2318:G:C2'   | 25:BA:2319:G:OP1   | 2.44                     | 0.65              |
| 39:BS:89:ARG:CD    | 39:BS:92:TYR:HA    | 2.27                     | 0.65              |
| 40:BT:30:VAL:CG2   | 40:BT:84:GLN:O     | 2.42                     | 0.65              |
| 1:CA:429:U:O2'     | 1:CA:430:A:C5'     | 2.45                     | 0.65              |
| 7:CG:26:PHE:HB2    | 7:CG:101:LEU:HD22  | 1.79                     | 0.65              |
| 8:CH:82:HIS:CD2    | 8:CH:138:TRP:CZ2   | 2.85                     | 0.65              |
| 28:DD:74:GLY:O     | 28:DD:76:PRO:HD3   | 1.96                     | 0.65              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 30:DF:34:TRP:CA    | 36:DP:6:LEU:HD12   | 2.25                     | 0.65              |
| 30:DF:185:ASP:HA   | 30:DF:188:ARG:HD3  | 1.78                     | 0.65              |
| 31:DG:135:LEU:HD23 | 31:DG:140:ILE:HD11 | 1.79                     | 0.65              |
| 33:DI:29:TYR:C     | 33:DI:32:PRO:HD2   | 2.22                     | 0.65              |
| 33:DI:77:LEU:HD13  | 33:DI:78:THR:H     | 1.61                     | 0.65              |
| 36:DP:42:SER:O     | 36:DP:43:GLY:C     | 2.40                     | 0.65              |
| 38:DR:32:GLY:C     | 38:DR:33:ARG:HD2   | 2.22                     | 0.65              |
| 40:DT:50:ILE:HD11  | 40:DT:102:ILE:CD1  | 2.25                     | 0.65              |
| 44:DX:60:ARG:NH1   | 54:D7:47:ARG:NH2   | 2.41                     | 0.65              |
| 46:DZ:42:VAL:HG13  | 46:DZ:43:GLU:OE1   | 1.96                     | 0.65              |
| 46:DZ:99:TYR:HD2   | 46:DZ:99:TYR:H     | 1.45                     | 0.65              |
| 2:AB:74:LYS:O      | 2:AB:78:GLN:HG3    | 1.96                     | 0.65              |
| 6:AF:12:PRO:HB3    | 6:AF:57:GLN:O      | 1.96                     | 0.65              |
| 13:AM:57:ARG:CZ    | 51:B4:60:GLU:HG3   | 2.26                     | 0.65              |
| 25:BA:196:A:C4     | 25:BA:805:G:C6     | 2.84                     | 0.65              |
| 25:BA:1396:U:O2    | 25:BA:1396:U:C3'   | 2.44                     | 0.65              |
| 25:BA:1858:G:O2'   | 25:BA:1884:A:N6    | 2.30                     | 0.65              |
| 30:BF:24:LEU:HB3   | 30:BF:25:PRO:HD2   | 1.77                     | 0.65              |
| 36:BP:3:LEU:HA     | 36:BP:6:LEU:HD23   | 1.78                     | 0.65              |
| 39:BS:12:PHE:CG    | 39:BS:12:PHE:O     | 2.49                     | 0.65              |
| 42:BV:82:ARG:HG2   | 42:BV:82:ARG:NH1   | 2.04                     | 0.65              |
| 43:BW:111:HIS:CD2  | 43:BW:112:GLY:H    | 2.14                     | 0.65              |
| 51:B4:60:GLU:O     | 51:B4:61:VAL:HB    | 1.95                     | 0.65              |
| 1:CA:566:G:H4'     | 1:CA:567:G:OP1     | 1.97                     | 0.65              |
| 11:CK:41:THR:HG21  | 11:CK:71:LYS:CB    | 2.27                     | 0.65              |
| 16:CP:3:LYS:O      | 16:CP:21:VAL:HA    | 1.95                     | 0.65              |
| 20:CT:29:LYS:CD    | 20:CT:66:ALA:CB    | 2.75                     | 0.65              |
| 20:CT:43:LEU:CD1   | 20:CT:51:GLU:HB3   | 2.27                     | 0.65              |
| 23:CW:55:U:C4      | 23:CW:57:G:H5'     | 2.32                     | 0.65              |
| 25:DA:819:A:OP2    | 25:DA:1187:G:N2    | 2.20                     | 0.65              |
| 25:DA:1310:G:OP2   | 54:D7:9:ARG:NH1    | 2.29                     | 0.65              |
| 25:DA:2377:A:O2'   | 39:DS:112:PHE:HB3  | 1.97                     | 0.65              |
| 25:DA:2520:C:C6    | 25:DA:2567:G:H1'   | 2.32                     | 0.65              |
| 29:DE:111:ARG:CB   | 38:DR:1:MET:SD     | 2.85                     | 0.65              |
| 30:DF:63:LYS:HE3   | 30:DF:65:TRP:O     | 1.95                     | 0.65              |
| 30:DF:123:LEU:HD12 | 30:DF:192:LEU:O    | 1.97                     | 0.65              |
| 31:DG:55:LYS:NZ    | 31:DG:148:MET:HG3  | 2.12                     | 0.65              |
| 33:DI:4:ILE:HG12   | 33:DI:18:VAL:CG2   | 2.25                     | 0.65              |
| 36:DP:52:GLU:CD    | 36:DP:55:ARG:HH21  | 2.04                     | 0.65              |
| 42:DV:58:VAL:CB    | 42:DV:98:GLU:HB2   | 2.18                     | 0.65              |
| 48:D1:56:GLN:HA    | 48:D1:56:GLN:NE2   | 2.11                     | 0.65              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 49:D2:48:HIS:O    | 49:D2:52:ASP:HB2   | 1.96                     | 0.65              |
| 4:AD:146:ILE:HD12 | 4:AD:146:ILE:N     | 2.12                     | 0.65              |
| 16:AP:82:GLN:O    | 16:AP:83:GLU:HB2   | 1.96                     | 0.65              |
| 22:AV:53:G:O2'    | 22:AV:54:G:P       | 2.55                     | 0.65              |
| 25:BA:1287:A:N6   | 25:BA:1288:U:O4    | 2.30                     | 0.65              |
| 25:BA:2002:G:H5'  | 38:BR:13:HIS:HA    | 1.79                     | 0.65              |
| 25:BA:2779:U:H5'' | 25:BA:2780:G:H3'   | 1.79                     | 0.65              |
| 28:BD:17:THR:O    | 28:BD:211:ARG:NH2  | 2.28                     | 0.65              |
| 30:BF:40:GLN:HE22 | 30:BF:182:ASN:HB2  | 1.60                     | 0.65              |
| 30:BF:123:LEU:CD1 | 30:BF:124:LEU:H    | 2.03                     | 0.65              |
| 32:BH:126:PRO:HB2 | 32:BH:130:ARG:NH1  | 2.11                     | 0.65              |
| 33:BI:53:ALA:O    | 33:BI:57:ARG:CB    | 2.44                     | 0.65              |
| 33:BI:79:ILE:HB   | 33:BI:142:VAL:HG13 | 1.78                     | 0.65              |
| 39:BS:12:PHE:CD1  | 39:BS:12:PHE:O     | 2.50                     | 0.65              |
| 41:BU:80:ILE:HG22 | 41:BU:81:HIS:N     | 2.12                     | 0.65              |
| 41:BU:90:VAL:HG22 | 42:BV:39:LEU:HG    | 1.79                     | 0.65              |
| 47:B0:53:MET:HB2  | 47:B0:59:LEU:CD2   | 2.26                     | 0.65              |
| 48:B1:70:VAL:O    | 48:B1:74:VAL:HG23  | 1.97                     | 0.65              |
| 1:CA:1203:C:OP1   | 14:CN:3:ARG:HD3    | 1.97                     | 0.65              |
| 1:CA:1452:C:O2'   | 1:CA:1456:G:N2     | 2.30                     | 0.65              |
| 17:CQ:29:HIS:O    | 17:CQ:31:LEU:N     | 2.30                     | 0.65              |
| 19:CS:43:GLU:C    | 19:CS:45:VAL:H     | 2.04                     | 0.65              |
| 19:CS:63:THR:HG23 | 19:CS:66:MET:HG3   | 1.78                     | 0.65              |
| 20:CT:82:SER:O    | 20:CT:85:MET:N     | 2.30                     | 0.65              |
| 25:DA:340:A:O2'   | 25:DA:341:G:H5'    | 1.97                     | 0.65              |
| 25:DA:447:A:N1    | 25:DA:454:A:H2'    | 2.12                     | 0.65              |
| 25:DA:483:A:C5'   | 45:DY:49:VAL:HG13  | 2.26                     | 0.65              |
| 25:DA:1455:G:N2   | 25:DA:1456:G:C1'   | 2.61                     | 0.65              |
| 36:DP:57:THR:O    | 36:DP:60:MET:CG    | 2.42                     | 0.65              |
| 39:DS:85:VAL:HG23 | 39:DS:112:PHE:CZ   | 2.32                     | 0.65              |
| 46:DZ:6:LYS:N     | 46:DZ:6:LYS:HD2    | 2.12                     | 0.65              |
| 46:DZ:14:LYS:H    | 46:DZ:14:LYS:NZ    | 1.95                     | 0.65              |
| 13:AM:93:ARG:HA   | 13:AM:93:ARG:HE    | 1.62                     | 0.64              |
| 21:AU:25:LYS:HB2  | 21:AU:25:LYS:NZ    | 2.12                     | 0.64              |
| 23:AW:49:C:H42    | 23:AW:65:G:H1      | 1.45                     | 0.64              |
| 25:BA:1481:U:H5'  | 25:BA:1482:G:OP2   | 1.96                     | 0.64              |
| 28:BD:10:THR:HG23 | 28:BD:13:ARG:HB3   | 1.78                     | 0.64              |
| 33:BI:125:GLU:OE1 | 33:BI:141:LYS:HG2  | 1.96                     | 0.64              |
| 34:BN:99:LEU:HD22 | 34:BN:103:VAL:HG23 | 1.79                     | 0.64              |
| 36:BP:63:PRO:HB3  | 55:B8:13:ARG:CB    | 2.14                     | 0.64              |
| 37:BQ:42:ILE:HD13 | 37:BQ:97:VAL:HB    | 1.79                     | 0.64              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 45:BY:67:LEU:CG    | 45:BY:68:HIS:H     | 2.10                     | 0.64              |
| 52:B5:32:PRO:O     | 52:B5:33:CYS:HB3   | 1.96                     | 0.64              |
| 2:CB:18:GLY:H      | 2:CB:42:ILE:HG23   | 1.60                     | 0.64              |
| 2:CB:178:ARG:HH22  | 2:CB:196:LEU:HA    | 1.62                     | 0.64              |
| 10:CJ:38:ILE:HD11  | 10:CJ:71:LEU:CD2   | 2.24                     | 0.64              |
| 14:CN:26:ARG:HD2   | 14:CN:43:CYS:HB3   | 1.78                     | 0.64              |
| 25:DA:1819:A:H1'   | 25:DA:1821:A:N6    | 2.12                     | 0.64              |
| 25:DA:2712:U:O2    | 25:DA:2712:U:H5''  | 1.97                     | 0.64              |
| 28:DD:36:PRO:HA    | 28:DD:62:TYR:O     | 1.97                     | 0.64              |
| 34:DN:23:LEU:CD1   | 34:DN:98:VAL:HG12  | 2.27                     | 0.64              |
| 41:DU:104:GLN:HE22 | 41:DU:105:VAL:CG2  | 2.05                     | 0.64              |
| 51:D4:4:GLY:O      | 51:D4:5:ILE:HB     | 1.96                     | 0.64              |
| 1:AA:748:C:H4'     | 1:AA:749:C:O5'     | 1.96                     | 0.64              |
| 2:AB:181:PHE:HD1   | 8:AH:70:GLN:HB3    | 1.62                     | 0.64              |
| 3:AC:54:ARG:HD3    | 3:AC:56:ASP:HB2    | 1.80                     | 0.64              |
| 4:AD:128:VAL:HG12  | 4:AD:129:ASN:HD22  | 1.61                     | 0.64              |
| 22:AV:35:C:HO2'    | 22:AV:36:A:P       | 2.20                     | 0.64              |
| 25:BA:614:U:O2'    | 25:BA:614(C):A:N7  | 2.30                     | 0.64              |
| 25:BA:630:G:N2     | 25:BA:633:A:OP2    | 2.26                     | 0.64              |
| 36:BP:42:SER:O     | 36:BP:43:GLY:C     | 2.40                     | 0.64              |
| 36:BP:57:THR:O     | 36:BP:59:LEU:N     | 2.30                     | 0.64              |
| 36:BP:146:VAL:HG13 | 36:BP:147:LEU:HD13 | 1.80                     | 0.64              |
| 41:BU:91:ASP:O     | 41:BU:92:ARG:HD3   | 1.96                     | 0.64              |
| 1:CA:60:A:O2'      | 1:CA:61:G:P        | 2.55                     | 0.64              |
| 1:CA:751:U:C2'     | 1:CA:752:G:H5'     | 2.26                     | 0.64              |
| 1:CA:881:G:P       | 12:CL:12:ARG:HH22  | 2.20                     | 0.64              |
| 1:CA:1128:C:H1'    | 1:CA:1146:A:H61    | 1.62                     | 0.64              |
| 2:CB:7:VAL:N       | 2:CB:217:ARG:HH22  | 1.95                     | 0.64              |
| 5:CE:105:VAL:O     | 5:CE:108:ALA:HB3   | 1.97                     | 0.64              |
| 13:CM:116:THR:C    | 13:CM:117:VAL:CG1  | 2.70                     | 0.64              |
| 19:CS:29:ARG:O     | 19:CS:31:ILE:N     | 2.30                     | 0.64              |
| 25:DA:1963:U:O2    | 25:DA:1963:U:C3'   | 2.44                     | 0.64              |
| 25:DA:2396:G:O2'   | 48:D1:29:GLY:HA3   | 1.97                     | 0.64              |
| 25:DA:2577:A:H5''  | 25:DA:2578:G:H5'   | 1.80                     | 0.64              |
| 28:DD:182:LEU:O    | 28:DD:271:ILE:HG13 | 1.97                     | 0.64              |
| 29:DE:3:GLY:O      | 29:DE:4:ILE:HB     | 1.97                     | 0.64              |
| 31:DG:44:GLY:HA2   | 31:DG:88:ILE:HG12  | 1.79                     | 0.64              |
| 31:DG:116:ASP:O    | 31:DG:117:PHE:HB3  | 1.96                     | 0.64              |
| 32:DH:30:LYS:HE3   | 32:DH:81:GLU:HG3   | 1.79                     | 0.64              |
| 36:DP:71:VAL:HG23  | 36:DP:72:PRO:HD3   | 1.79                     | 0.64              |
| 36:DP:78:PRO:CB    | 36:DP:111:ARG:HD3  | 2.26                     | 0.64              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 36:DP:146:VAL:HG13 | 36:DP:147:LEU:HD13 | 1.80                     | 0.64              |
| 37:DQ:51:ARG:HG2   | 37:DQ:51:ARG:NH1   | 2.12                     | 0.64              |
| 42:DV:35:LEU:O     | 42:DV:37:VAL:N     | 2.30                     | 0.64              |
| 1:AA:189(F):U:H2'  | 17:AQ:63:ARG:HH21  | 1.63                     | 0.64              |
| 1:AA:832:C:O2      | 1:AA:854:G:N2      | 2.29                     | 0.64              |
| 1:AA:925:G:H1'     | 1:AA:1502:A:C4     | 2.32                     | 0.64              |
| 12:AL:71:PRO:HD2   | 12:AL:102:ARG:HD3  | 1.79                     | 0.64              |
| 15:AO:17:ARG:CD    | 15:AO:26:GLU:HG3   | 2.28                     | 0.64              |
| 25:BA:2238:G:H4'   | 25:BA:2239:G:OP1   | 1.98                     | 0.64              |
| 28:BD:260:ARG:NH1  | 28:BD:267:SER:OG   | 2.30                     | 0.64              |
| 28:BD:264:LYS:HG2  | 28:BD:266:SER:H    | 1.63                     | 0.64              |
| 32:BH:146:ALA:HA   | 32:BH:149:ARG:HG2  | 1.79                     | 0.64              |
| 34:BN:42:TRP:HZ3   | 34:BN:48:MET:HE1   | 1.56                     | 0.64              |
| 36:BP:57:THR:CG2   | 36:BP:59:LEU:HB3   | 2.28                     | 0.64              |
| 36:BP:79:ARG:HD3   | 36:BP:109:GLY:C    | 2.21                     | 0.64              |
| 37:BQ:29:PHE:HB2   | 37:BQ:105:GLU:OE2  | 1.97                     | 0.64              |
| 55:B8:16:ILE:HG22  | 55:B8:64:TYR:CD2   | 2.32                     | 0.64              |
| 1:CA:8:A:O4'       | 5:CE:101:ILE:HG22  | 1.97                     | 0.64              |
| 2:CB:213:LEU:CD2   | 2:CB:214:ILE:HG12  | 2.24                     | 0.64              |
| 3:CC:14:ILE:CG1    | 3:CC:15:THR:H      | 2.11                     | 0.64              |
| 8:CH:25:ASP:HA     | 8:CH:59:LEU:O      | 1.96                     | 0.64              |
| 25:DA:1740:G:H4'   | 25:DA:1741:A:OP1   | 1.97                     | 0.64              |
| 28:DD:218:ARG:HB3  | 28:DD:219:PRO:HD2  | 1.79                     | 0.64              |
| 38:DR:8:ARG:N      | 38:DR:43:GLU:OE1   | 2.27                     | 0.64              |
| 41:DU:95:LEU:CD1   | 42:DV:4:ILE:HG21   | 2.27                     | 0.64              |
| 41:DU:107:ALA:O    | 41:DU:110:VAL:HB   | 1.97                     | 0.64              |
| 45:DY:76:CYS:HB3   | 45:DY:96:ILE:CD1   | 2.26                     | 0.64              |
| 12:AL:23:LYS:O     | 12:AL:24:VAL:HG23  | 1.98                     | 0.64              |
| 19:AS:12:ASP:OD1   | 19:AS:37:ARG:HD2   | 1.98                     | 0.64              |
| 25:BA:1299:G:H5'   | 25:BA:1301:A:O4'   | 1.98                     | 0.64              |
| 28:BD:65:ILE:HD11  | 28:BD:67:PHE:CZ    | 2.32                     | 0.64              |
| 31:BG:143:GLU:OE1  | 31:BG:143:GLU:N    | 2.30                     | 0.64              |
| 34:BN:32:THR:CG2   | 34:BN:37:LYS:HB3   | 2.28                     | 0.64              |
| 36:BP:23:PRO:HB3   | 42:BV:80:GLN:HG3   | 1.79                     | 0.64              |
| 36:BP:78:PRO:CB    | 36:BP:111:ARG:HD3  | 2.26                     | 0.64              |
| 38:BR:10:LEU:HB2   | 38:BR:17:ARG:CD    | 2.21                     | 0.64              |
| 39:BS:49:VAL:HG12  | 39:BS:50:SER:N     | 2.12                     | 0.64              |
| 40:BT:57:PHE:O     | 40:BT:59:THR:N     | 2.30                     | 0.64              |
| 45:BY:75:ILE:HG13  | 45:BY:79:CYS:CA    | 2.18                     | 0.64              |
| 4:CD:198:VAL:HG12  | 4:CD:199:ASN:H     | 1.62                     | 0.64              |
| 25:DA:975(A):G:H2' | 25:DA:976:C:H5'    | 1.78                     | 0.64              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:DA:2590:A:OP2  | 28:DD:238:GLY:HA2 | 1.98                     | 0.64              |
| 26:DB:14:U:C5'    | 26:DB:15:A:OP2    | 2.45                     | 0.64              |
| 33:DI:77:LEU:CD1  | 33:DI:140:LEU:HB2 | 2.23                     | 0.64              |
| 35:DO:49:ARG:HG2  | 35:DO:49:ARG:NH1  | 2.12                     | 0.64              |
| 36:DP:9:ASN:HB2   | 36:DP:10:PRO:HD2  | 1.78                     | 0.64              |
| 36:DP:61:ARG:NH1  | 55:D8:13:ARG:HD2  | 2.12                     | 0.64              |
| 40:DT:81:PRO:O    | 40:DT:82:LEU:HG   | 1.97                     | 0.64              |
| 45:DY:47:LYS:C    | 45:DY:49:VAL:H    | 2.05                     | 0.64              |
| 25:BA:373:U:H2'   | 25:BA:374:A:H8    | 1.61                     | 0.64              |
| 28:BD:4:LYS:HB2   | 28:BD:18:VAL:HG23 | 1.79                     | 0.64              |
| 29:BE:68:ALA:O    | 29:BE:70:ALA:N    | 2.31                     | 0.64              |
| 36:BP:58:THR:O    | 36:BP:61:ARG:NE   | 2.30                     | 0.64              |
| 55:B8:29:LYS:HG2  | 55:B8:29:LYS:O    | 1.95                     | 0.64              |
| 1:CA:49:U:C6      | 1:CA:364:A:N6     | 2.66                     | 0.64              |
| 1:CA:61:G:O2'     | 1:CA:62:U:H5'     | 1.98                     | 0.64              |
| 1:CA:1452:C:C2'   | 1:CA:1456:G:OP2   | 2.46                     | 0.64              |
| 2:CB:18:GLY:N     | 2:CB:42:ILE:CG2   | 2.57                     | 0.64              |
| 2:CB:71:VAL:HG13  | 2:CB:93:VAL:HG21  | 1.79                     | 0.64              |
| 13:CM:88:ARG:HH11 | 13:CM:88:ARG:CB   | 2.01                     | 0.64              |
| 13:CM:93:ARG:HH12 | 25:DA:888:C:C4'   | 2.10                     | 0.64              |
| 16:CP:8:ARG:O     | 16:CP:9:PHE:HD2   | 1.80                     | 0.64              |
| 34:DN:42:TRP:CD1  | 41:DU:63:VAL:HG11 | 2.32                     | 0.64              |
| 42:DV:11:GLN:NE2  | 42:DV:39:LEU:CD2  | 2.55                     | 0.64              |
| 42:DV:44:LYS:O    | 42:DV:46:VAL:N    | 2.30                     | 0.64              |
| 45:DY:53:PRO:O    | 45:DY:54:LYS:C    | 2.39                     | 0.64              |
| 1:AA:867:G:O2'    | 1:AA:873:A:N1     | 2.27                     | 0.64              |
| 2:AB:36:ARG:N     | 2:AB:36:ARG:NE    | 2.45                     | 0.64              |
| 3:AC:39:ILE:HG22  | 3:AC:40:ARG:N     | 2.12                     | 0.64              |
| 3:AC:125:GLU:OE2  | 3:AC:189:ALA:HA   | 1.98                     | 0.64              |
| 24:AX:11:U:OP2    | 24:AX:11:U:C5     | 2.51                     | 0.64              |
| 25:BA:805:G:H5'   | 25:BA:806:C:C5    | 2.33                     | 0.64              |
| 25:BA:2110:G:H2'  | 25:BA:2120:G:H5'  | 1.78                     | 0.64              |
| 29:BE:71:GLY:O    | 29:BE:72:VAL:C    | 2.40                     | 0.64              |
| 33:BI:72:LEU:HD13 | 33:BI:72:LEU:C    | 2.22                     | 0.64              |
| 35:BO:87:ILE:CG2  | 35:BO:91:LEU:HA   | 2.26                     | 0.64              |
| 38:BR:106:GLY:O   | 38:BR:107:ASP:HB3 | 1.98                     | 0.64              |
| 1:CA:31:G:N2      | 1:CA:48:C:OP1     | 2.31                     | 0.64              |
| 1:CA:76:C:H42     | 1:CA:93:G:H1      | 1.46                     | 0.64              |
| 1:CA:748:C:O2'    | 1:CA:749:C:P      | 2.56                     | 0.64              |
| 2:CB:7:VAL:N      | 2:CB:217:ARG:NH2  | 2.46                     | 0.64              |
| 34:DN:57:ALA:H    | 34:DN:124:ALA:HA  | 1.62                     | 0.64              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 36:DP:83:VAL:CG1  | 36:DP:112:LEU:HD21 | 2.26                     | 0.64              |
| 37:DQ:69:PHE:HD1  | 37:DQ:70:PRO:HD2   | 1.61                     | 0.64              |
| 41:DU:49:HIS:HA   | 41:DU:52:ARG:HB2   | 1.80                     | 0.64              |
| 51:D4:9:LEU:HG    | 51:D4:26:SER:HA    | 1.80                     | 0.64              |
| 55:D8:50:LEU:HD12 | 55:D8:51:ALA:N     | 2.09                     | 0.64              |
| 1:AA:1279:A:N3    | 1:AA:1279:A:O5'    | 2.30                     | 0.64              |
| 1:AA:1305:G:H22   | 1:AA:1331:G:H2'    | 1.62                     | 0.64              |
| 7:AG:15:ASP:H     | 7:AG:24:THR:HG23   | 1.62                     | 0.64              |
| 9:AI:63:ILE:HD13  | 9:AI:77:ILE:HG23   | 1.79                     | 0.64              |
| 12:AL:82:VAL:O    | 12:AL:106:ASP:HB2  | 1.98                     | 0.64              |
| 17:AQ:51:TYR:CE1  | 17:AQ:73:VAL:HG11  | 2.33                     | 0.64              |
| 22:AV:57:C:H2'    | 22:AV:58:A:H5'     | 1.78                     | 0.64              |
| 25:BA:669:G:H2'   | 25:BA:669:G:N3     | 2.12                     | 0.64              |
| 29:BE:11:MET:CB   | 29:BE:24:THR:HA    | 2.28                     | 0.64              |
| 29:BE:37:ARG:HB2  | 29:BE:46:ALA:HB3   | 1.80                     | 0.64              |
| 31:BG:109:VAL:C   | 31:BG:112:PRO:HD2  | 2.22                     | 0.64              |
| 32:BH:122:THR:O   | 32:BH:133:VAL:HG13 | 1.98                     | 0.64              |
| 39:BS:92:TYR:C    | 39:BS:94:TYR:N     | 2.54                     | 0.64              |
| 49:B2:42:GLY:O    | 49:B2:44:LEU:N     | 2.31                     | 0.64              |
| 2:CB:21:ARG:HB2   | 2:CB:38:GLY:O      | 1.96                     | 0.64              |
| 3:CC:6:HIS:CD2    | 3:CC:7:PRO:HD2     | 2.31                     | 0.64              |
| 5:CE:115:VAL:HG12 | 5:CE:116:THR:N     | 2.11                     | 0.64              |
| 6:CF:24:GLU:HG3   | 6:CF:25:ILE:HD13   | 1.80                     | 0.64              |
| 10:CJ:33:GLN:HB2  | 10:CJ:75:ILE:HD13  | 1.79                     | 0.64              |
| 20:CT:72:LEU:CD2  | 20:CT:73:HIS:N     | 2.61                     | 0.64              |
| 25:DA:943:U:OP1   | 36:DP:36:LYS:HG3   | 1.98                     | 0.64              |
| 28:DD:96:HIS:CE1  | 28:DD:102:LYS:HE2  | 2.33                     | 0.64              |
| 34:DN:17:ASP:OD1  | 34:DN:56:ASN:HB3   | 1.97                     | 0.64              |
| 36:DP:59:LEU:O    | 36:DP:61:ARG:NH1   | 2.30                     | 0.64              |
| 40:DT:78:LEU:C    | 40:DT:79:HIS:ND1   | 2.56                     | 0.64              |
| 44:DX:60:ARG:HH12 | 54:D7:47:ARG:HH22  | 1.44                     | 0.64              |
| 1:AA:241:C:H2'    | 1:AA:242:C:H5'     | 1.79                     | 0.64              |
| 8:AH:31:PHE:O     | 8:AH:34:GLU:HB2    | 1.98                     | 0.64              |
| 19:AS:20:LEU:O    | 19:AS:23:ASN:HB3   | 1.98                     | 0.64              |
| 23:AW:12:U:H3     | 23:AW:23:A:H61     | 1.46                     | 0.64              |
| 25:BA:601:C:H4'   | 30:BF:104:LYS:HZ1  | 1.63                     | 0.64              |
| 25:BA:703:U:H3    | 25:BA:727:A:N6     | 1.95                     | 0.64              |
| 25:BA:1799:G:N2   | 25:BA:1818:U:O2'   | 2.31                     | 0.64              |
| 28:BD:77:ALA:HB2  | 28:BD:97:TYR:CD2   | 2.32                     | 0.64              |
| 32:BH:53:GLU:O    | 32:BH:54:ARG:HB3   | 1.98                     | 0.64              |
| 34:BN:46:VAL:O    | 34:BN:47:ALA:HB3   | 1.96                     | 0.64              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 50:B3:29:ARG:HH11  | 50:B3:29:ARG:HG3   | 1.62                     | 0.64              |
| 50:B3:39:ASP:OD1   | 50:B3:44:ARG:HG2   | 1.97                     | 0.64              |
| 53:B6:32:ASN:C     | 53:B6:33:LYS:HG2   | 2.22                     | 0.64              |
| 1:CA:820:U:C4'     | 1:CA:821:G:OP2     | 2.40                     | 0.64              |
| 1:CA:926:G:H22     | 24:CX:15:A:H3'     | 1.62                     | 0.64              |
| 4:CD:22:LYS:CG     | 4:CD:26:CYS:SG     | 2.84                     | 0.64              |
| 14:CN:36:PHE:HD1   | 14:CN:37:PHE:CD2   | 2.16                     | 0.64              |
| 17:CQ:70:ARG:C     | 17:CQ:71:PHE:HD2   | 2.06                     | 0.64              |
| 20:CT:72:LEU:HD23  | 20:CT:73:HIS:N     | 2.13                     | 0.64              |
| 23:CW:18:G:N1      | 23:CW:55:U:H1'     | 2.12                     | 0.64              |
| 25:DA:265:A:H8     | 25:DA:266:G:H1'    | 1.63                     | 0.64              |
| 25:DA:1645:G:H5''  | 25:DA:1646:C:C5'   | 2.19                     | 0.64              |
| 28:DD:165:ILE:HD13 | 28:DD:175:LEU:HD21 | 1.80                     | 0.64              |
| 33:DI:57:ARG:NH1   | 33:DI:57:ARG:HB2   | 2.11                     | 0.64              |
| 37:DQ:141:GLN:HB2  | 46:DZ:98:MET:HA    | 1.79                     | 0.64              |
| 44:DX:71:GLY:C     | 44:DX:72:LYS:HD2   | 2.22                     | 0.64              |
| 46:DZ:97:GLU:HB3   | 46:DZ:125:LEU:HD11 | 1.77                     | 0.64              |
| 53:D6:46:HIS:O     | 53:D6:47:THR:OG1   | 2.16                     | 0.64              |
| 1:AA:984:C:H6      | 1:AA:984:C:O5'     | 1.81                     | 0.64              |
| 1:AA:1049:U:C4'    | 1:AA:1050:G:O5'    | 2.46                     | 0.64              |
| 2:AB:158:LEU:H     | 2:AB:158:LEU:HD12  | 1.63                     | 0.64              |
| 8:AH:2:LEU:C       | 8:AH:2:LEU:HD13    | 2.22                     | 0.64              |
| 8:AH:91:ARG:NH1    | 17:AQ:33:GLY:HA3   | 2.12                     | 0.64              |
| 23:AW:38:A:C3'     | 23:AW:39:U:H5''    | 2.28                     | 0.64              |
| 25:BA:34:C:N4      | 25:BA:454:A:O2'    | 2.30                     | 0.64              |
| 25:BA:614(A):U:C2' | 25:BA:614(B):G:OP1 | 2.45                     | 0.64              |
| 25:BA:957:A:OP1    | 37:BQ:76:LYS:HE3   | 1.98                     | 0.64              |
| 25:BA:2528:U:OP1   | 56:B9:30:PRO:HG2   | 1.97                     | 0.64              |
| 30:BF:85:GLY:O     | 30:BF:86:GLY:O     | 2.16                     | 0.64              |
| 33:BI:77:LEU:HD21  | 33:BI:101:LEU:HA   | 1.80                     | 0.64              |
| 34:BN:55:VAL:HG22  | 34:BN:126:PRO:HA   | 1.80                     | 0.64              |
| 36:BP:79:ARG:CD    | 36:BP:109:GLY:CA   | 2.76                     | 0.64              |
| 37:BQ:141:GLN:CD   | 46:BZ:72:ARG:HD3   | 2.23                     | 0.64              |
| 40:BT:91:ARG:HB3   | 40:BT:115:ARG:O    | 1.98                     | 0.64              |
| 40:BT:113:LYS:C    | 40:BT:114:LEU:HD23 | 2.23                     | 0.64              |
| 45:BY:35:TYR:CD2   | 45:BY:69:ALA:HB3   | 2.32                     | 0.64              |
| 46:BZ:3:TYR:N      | 46:BZ:3:TYR:CD1    | 2.64                     | 0.64              |
| 1:CA:1067:A:O2'    | 1:CA:1068:G:P      | 2.55                     | 0.64              |
| 5:CE:147:ASP:HA    | 5:CE:150:ARG:HB2   | 1.80                     | 0.64              |
| 20:CT:22:ARG:O     | 20:CT:26:ASN:CG    | 2.40                     | 0.64              |
| 20:CT:53:LEU:HD21  | 20:CT:100:ILE:CB   | 2.27                     | 0.64              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 20:CT:53:LEU:HD21  | 20:CT:100:ILE:HB  | 1.79                     | 0.64              |
| 25:DA:1455:G:H21   | 25:DA:1456:G:H1'  | 1.62                     | 0.64              |
| 30:DF:32:LEU:HD21  | 30:DF:108:LYS:HB3 | 1.80                     | 0.64              |
| 41:DU:92:ARG:HH21  | 41:DU:94:ASN:HD22 | 1.43                     | 0.64              |
| 42:DV:76:LYS:O     | 42:DV:79:VAL:HG12 | 1.97                     | 0.64              |
| 45:DY:78:ALA:HB3   | 45:DY:81:LYS:HE3  | 1.79                     | 0.64              |
| 1:AA:1301:U:O2'    | 13:AM:13:LYS:NZ   | 2.30                     | 0.64              |
| 6:AF:62:TRP:CD1    | 18:AR:35:ARG:NH1  | 2.66                     | 0.64              |
| 9:AI:4:TYR:HB2     | 9:AI:19:LEU:HD12  | 1.79                     | 0.64              |
| 11:AK:101:SER:OG   | 11:AK:103:LEU:HB2 | 1.98                     | 0.64              |
| 13:AM:57:ARG:HH12  | 51:B4:60:GLU:HA   | 1.63                     | 0.64              |
| 19:AS:41:VAL:HB    | 19:AS:44:MET:HG2  | 1.80                     | 0.64              |
| 22:AV:53:G:HO2'    | 22:AV:54:G:P      | 2.21                     | 0.64              |
| 25:BA:27:G:H22     | 25:BA:512:G:H2'   | 1.62                     | 0.64              |
| 29:BE:106:GLY:HA3  | 29:BE:189:PRO:HG2 | 1.80                     | 0.64              |
| 36:BP:14:LYS:O     | 36:BP:15:ARG:C    | 2.39                     | 0.64              |
| 41:BU:61:TRP:CE2   | 41:BU:94:ASN:HA   | 2.33                     | 0.64              |
| 14:CN:13:THR:H     | 14:CN:14:PRO:HD2  | 1.61                     | 0.64              |
| 15:CO:10:LYS:HG3   | 15:CO:11:VAL:N    | 2.13                     | 0.64              |
| 23:CW:38:A:H8      | 23:CW:38:A:O5'    | 1.81                     | 0.64              |
| 25:DA:2519:U:C5'   | 25:DA:2520:C:OP1  | 2.46                     | 0.64              |
| 25:DA:2580:U:H4'   | 29:DE:130:GLY:HA3 | 1.79                     | 0.64              |
| 27:DC:86:ALA:HB1   | 27:DC:94:VAL:HG11 | 1.78                     | 0.64              |
| 32:DH:86:GLU:HG3   | 32:DH:165:ALA:CB  | 2.27                     | 0.64              |
| 33:DI:139:GLN:HE21 | 33:DI:139:GLN:C   | 2.05                     | 0.64              |
| 41:DU:69:CYS:SG    | 41:DU:79:PHE:CD1  | 2.88                     | 0.64              |
| 42:DV:46:VAL:O     | 42:DV:46:VAL:HG13 | 1.97                     | 0.64              |
| 44:DX:60:ARG:HH22  | 54:D7:47:ARG:CZ   | 2.10                     | 0.64              |
| 1:AA:792:A:C4      | 1:AA:794:A:C6     | 2.86                     | 0.63              |
| 5:AE:82:VAL:HG21   | 5:AE:138:ALA:HA   | 1.80                     | 0.63              |
| 8:AH:1:MET:HE2     | 8:AH:2:LEU:N      | 2.12                     | 0.63              |
| 19:AS:12:ASP:CB    | 19:AS:14:HIS:CE1  | 2.75                     | 0.63              |
| 25:BA:1174:A:H5''  | 25:BA:1175:U:H5'  | 1.80                     | 0.63              |
| 25:BA:1403:C:H5''  | 25:BA:1471:A:H1'  | 1.79                     | 0.63              |
| 25:BA:1666:G:H1'   | 35:BO:3:GLN:OE1   | 1.97                     | 0.63              |
| 25:BA:1917:U:C2'   | 25:BA:1918:A:H5'  | 2.27                     | 0.63              |
| 25:BA:2458:G:N9    | 25:BA:2490:G:N1   | 2.47                     | 0.63              |
| 34:BN:26:LEU:HD21  | 34:BN:30:ILE:HD11 | 1.80                     | 0.63              |
| 36:BP:9:ASN:HB2    | 36:BP:10:PRO:HD2  | 1.78                     | 0.63              |
| 37:BQ:116:GLU:HA   | 37:BQ:116:GLU:OE1 | 1.96                     | 0.63              |
| 44:BX:63:LYS:HB3   | 44:BX:72:LYS:HG3  | 1.80                     | 0.63              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 46:BZ:11:GLU:CD    | 46:BZ:11:GLU:H     | 2.04                     | 0.63              |
| 1:CA:528:C:H41     | 12:CL:49:ASN:CG    | 2.06                     | 0.63              |
| 2:CB:69:LEU:HD12   | 2:CB:70:PHE:H      | 1.60                     | 0.63              |
| 23:CW:36:A:C6      | 23:CW:37:A:C5      | 2.86                     | 0.63              |
| 28:DD:62:TYR:HA    | 28:DD:87:ASN:ND2   | 2.13                     | 0.63              |
| 32:DH:4:ILE:HD13   | 32:DH:4:ILE:N      | 2.12                     | 0.63              |
| 35:DO:1:MET:HE2    | 35:DO:67:LYS:HG2   | 1.79                     | 0.63              |
| 36:DP:59:LEU:HA    | 36:DP:61:ARG:NH2   | 2.11                     | 0.63              |
| 36:DP:79:ARG:CD    | 36:DP:109:GLY:CA   | 2.76                     | 0.63              |
| 37:DQ:45:GLN:CD    | 37:DQ:45:GLN:H     | 2.05                     | 0.63              |
| 40:DT:29:ARG:HG3   | 40:DT:30:VAL:HG13  | 1.80                     | 0.63              |
| 40:DT:88:ILE:HG22  | 40:DT:89:VAL:N     | 2.12                     | 0.63              |
| 40:DT:128:GLU:OE1  | 40:DT:129:ARG:N    | 2.30                     | 0.63              |
| 40:DT:129:ARG:NH1  | 40:DT:130:ALA:O    | 2.31                     | 0.63              |
| 41:DU:47:TYR:HA    | 41:DU:50:ARG:NH2   | 2.13                     | 0.63              |
| 46:DZ:126:VAL:HG12 | 46:DZ:163:LEU:HA   | 1.79                     | 0.63              |
| 54:D7:41:ARG:HD3   | 54:D7:45:ALA:HB2   | 1.80                     | 0.63              |
| 55:D8:30:ARG:HA    | 55:D8:30:ARG:NE    | 2.12                     | 0.63              |
| 1:AA:533:A:O2'     | 1:AA:534:U:P       | 2.55                     | 0.63              |
| 1:AA:1003:G:N2     | 1:AA:1038:C:N3     | 2.46                     | 0.63              |
| 13:AM:3:ARG:HD3    | 31:BG:113:ARG:NH2  | 2.13                     | 0.63              |
| 16:AP:12:LYS:O     | 16:AP:13:HIS:HB2   | 1.98                     | 0.63              |
| 17:AQ:9:VAL:HG22   | 17:AQ:56:VAL:HG22  | 1.79                     | 0.63              |
| 20:AT:45:GLN:N     | 20:AT:91:LEU:HD13  | 2.13                     | 0.63              |
| 25:BA:956:G:H4'    | 37:BQ:83:MET:HE1   | 1.80                     | 0.63              |
| 25:BA:2259:G:C5    | 25:BA:2427:C:C4    | 2.86                     | 0.63              |
| 28:BD:270:ILE:C    | 28:BD:271:ILE:HG13 | 2.24                     | 0.63              |
| 30:BF:46:ARG:HG3   | 30:BF:46:ARG:NH1   | 2.10                     | 0.63              |
| 38:BR:2:ARG:NH1    | 38:BR:5:LYS:CE     | 2.61                     | 0.63              |
| 39:BS:13:ARG:HG3   | 39:BS:13:ARG:HH11  | 1.62                     | 0.63              |
| 40:BT:50:ILE:CD1   | 40:BT:99:LEU:HD13  | 2.28                     | 0.63              |
| 41:BU:66:ASN:O     | 41:BU:70:ARG:HG3   | 1.98                     | 0.63              |
| 44:BX:29:TRP:CZ3   | 44:BX:78:LYS:HB3   | 2.34                     | 0.63              |
| 1:CA:61:G:C6       | 1:CA:107:G:N1      | 2.66                     | 0.63              |
| 1:CA:413:G:N2      | 1:CA:428:G:O2'     | 2.31                     | 0.63              |
| 2:CB:87:ARG:NH1    | 2:CB:219:VAL:HB    | 2.13                     | 0.63              |
| 2:CB:97:TRP:HH2    | 2:CB:176:GLU:CD    | 2.06                     | 0.63              |
| 23:CW:24:G:C5      | 23:CW:25:C:C4      | 2.87                     | 0.63              |
| 25:DA:1342:A:N6    | 25:DA:1397:U:C5    | 2.66                     | 0.63              |
| 25:DA:2820:A:OP1   | 38:DR:4:LEU:HD22   | 1.98                     | 0.63              |
| 25:DA:2848:G:H3'   | 40:DT:95:ARG:O     | 1.98                     | 0.63              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 28:DD:33:LEU:HD22 | 28:DD:102:LYS:HD2  | 1.79                     | 0.63              |
| 28:DD:44:ASN:OD1  | 28:DD:44:ASN:N     | 2.30                     | 0.63              |
| 28:DD:94:LEU:HD22 | 28:DD:94:LEU:C     | 2.22                     | 0.63              |
| 36:DP:20:GLY:O    | 36:DP:21:ARG:NE    | 2.31                     | 0.63              |
| 45:DY:49:VAL:O    | 45:DY:51:VAL:N     | 2.31                     | 0.63              |
| 48:D1:5:CYS:SG    | 48:D1:62:VAL:HG23  | 2.37                     | 0.63              |
| 1:AA:227:G:N2     | 16:AP:62:VAL:O     | 2.30                     | 0.63              |
| 1:AA:411:A:C5     | 1:AA:413:G:H1'     | 2.33                     | 0.63              |
| 1:AA:595:G:C5'    | 1:AA:596:C:OP1     | 2.46                     | 0.63              |
| 3:AC:70:VAL:C     | 3:AC:106:VAL:HG23  | 2.23                     | 0.63              |
| 5:AE:78:HIS:HE1   | 5:AE:142:LEU:HA    | 1.62                     | 0.63              |
| 7:AG:76:ARG:HD3   | 7:AG:89:MET:SD     | 2.39                     | 0.63              |
| 9:AI:3:GLN:O      | 9:AI:88:TYR:CE1    | 2.51                     | 0.63              |
| 13:AM:3:ARG:HB2   | 31:BG:113:ARG:HH22 | 1.62                     | 0.63              |
| 25:BA:34:C:H2'    | 25:BA:35:G:O5'     | 1.98                     | 0.63              |
| 25:BA:83:G:N2     | 25:BA:103:A:OP2    | 2.27                     | 0.63              |
| 25:BA:2177:C:H1'  | 27:BC:44:HIS:CD2   | 2.33                     | 0.63              |
| 25:BA:2306:C:H3'  | 25:BA:2307:G:H5''  | 1.80                     | 0.63              |
| 31:BG:5:VAL:HG12  | 51:B4:51:TYR:HE1   | 1.63                     | 0.63              |
| 31:BG:32:PRO:HB3  | 31:BG:172:LEU:HD22 | 1.80                     | 0.63              |
| 32:BH:107:VAL:CG2 | 32:BH:109:PHE:CE2  | 2.81                     | 0.63              |
| 34:BN:125:GLY:HA3 | 34:BN:126:PRO:O    | 1.98                     | 0.63              |
| 35:BO:68:GLU:HB3  | 35:BO:78:ARG:NH1   | 2.13                     | 0.63              |
| 36:BP:124:LYS:HG2 | 36:BP:145:PRO:HD3  | 1.80                     | 0.63              |
| 37:BQ:42:ILE:HG23 | 37:BQ:46:GLN:OE1   | 1.98                     | 0.63              |
| 45:BY:28:LYS:CB   | 45:BY:37:VAL:CB    | 2.40                     | 0.63              |
| 6:CF:100:ASN:HB3  | 18:CR:27:GLY:O     | 1.97                     | 0.63              |
| 25:DA:560:C:H4'   | 41:DU:52:ARG:HH22  | 1.62                     | 0.63              |
| 25:DA:2259:G:C5   | 25:DA:2427:C:N4    | 2.67                     | 0.63              |
| 25:DA:2847:U:H3'  | 25:DA:2848:G:H5'   | 1.79                     | 0.63              |
| 29:DE:4:ILE:HG12  | 29:DE:28:ALA:HB1   | 1.79                     | 0.63              |
| 43:DW:9:TYR:CD2   | 43:DW:102:HIS:NE2  | 2.55                     | 0.63              |
| 43:DW:50:VAL:HG13 | 43:DW:51:LEU:N     | 2.13                     | 0.63              |
| 44:DX:30:VAL:HG11 | 44:DX:39:ILE:HD12  | 1.80                     | 0.63              |
| 46:DZ:23:LYS:HD2  | 46:DZ:39:VAL:O     | 1.97                     | 0.63              |
| 1:AA:1124:G:O2'   | 10:AJ:38:ILE:HG21  | 1.99                     | 0.63              |
| 2:AB:201:ILE:HG21 | 2:AB:214:ILE:HG21  | 1.81                     | 0.63              |
| 3:AC:18:TRP:CD1   | 14:AN:54:PRO:HA    | 2.34                     | 0.63              |
| 3:AC:21:ARG:C     | 3:AC:22:TRP:CD1    | 2.77                     | 0.63              |
| 8:AH:97:VAL:HG13  | 8:AH:98:LYS:N      | 2.12                     | 0.63              |
| 25:BA:331:A:H5''  | 25:BA:332:A:OP2    | 1.98                     | 0.63              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:BA:1943:U:H4'   | 25:BA:1944:U:O5'   | 1.97                     | 0.63              |
| 25:BA:1963:U:H3'   | 25:BA:1963:U:O2    | 1.99                     | 0.63              |
| 28:BD:72:LYS:NZ    | 28:BD:99:ASP:OD1   | 2.28                     | 0.63              |
| 30:BF:45:ARG:CG    | 30:BF:46:ARG:H     | 2.12                     | 0.63              |
| 31:BG:111:LEU:HB2  | 31:BG:112:PRO:HD3  | 1.81                     | 0.63              |
| 31:BG:124:SER:HB2  | 31:BG:131:TYR:CE1  | 2.32                     | 0.63              |
| 45:BY:66:PRO:O     | 45:BY:67:LEU:HD23  | 1.98                     | 0.63              |
| 55:B8:43:GLN:C     | 55:B8:44:LYS:HD2   | 2.23                     | 0.63              |
| 2:CB:31:TYR:CD1    | 2:CB:202:PRO:HB3   | 2.33                     | 0.63              |
| 3:CC:32:LEU:HD22   | 3:CC:59:ARG:NH1    | 2.13                     | 0.63              |
| 6:CF:39:LYS:HG2    | 6:CF:40:VAL:H      | 1.64                     | 0.63              |
| 25:DA:458:G:N2     | 25:DA:470:A:OP2    | 2.31                     | 0.63              |
| 25:DA:1403:C:H5''  | 25:DA:1471:A:H1'   | 1.79                     | 0.63              |
| 36:DP:78:PRO:HB2   | 36:DP:111:ARG:HD3  | 1.81                     | 0.63              |
| 43:DW:9:TYR:N      | 43:DW:102:HIS:CD2  | 2.62                     | 0.63              |
| 1:AA:1224:G:N1     | 1:AA:1322:C:H1'    | 2.14                     | 0.63              |
| 5:AE:139:LEU:O     | 5:AE:141:GLN:N     | 2.31                     | 0.63              |
| 5:AE:139:LEU:O     | 5:AE:142:LEU:N     | 2.31                     | 0.63              |
| 18:AR:32:ARG:HA    | 18:AR:69:THR:HG21  | 1.81                     | 0.63              |
| 25:BA:1453:U:O2'   | 25:BA:1455:G:C8    | 2.49                     | 0.63              |
| 25:BA:2691:C:C4    | 25:BA:2719:G:N2    | 2.67                     | 0.63              |
| 28:BD:24:ILE:HG13  | 28:BD:83:GLU:HA    | 1.80                     | 0.63              |
| 30:BF:101:LEU:HD12 | 30:BF:102:PRO:HD2  | 1.81                     | 0.63              |
| 31:BG:42:GLY:C     | 31:BG:43:LEU:HD13  | 2.23                     | 0.63              |
| 41:BU:91:ASP:OD2   | 41:BU:96:ALA:HB2   | 1.99                     | 0.63              |
| 1:CA:66:G:C4'      | 1:CA:173:U:C4      | 2.82                     | 0.63              |
| 1:CA:992:U:O2'     | 1:CA:993:G:H5''    | 1.97                     | 0.63              |
| 3:CC:132:ARG:O     | 3:CC:136:GLN:HB2   | 1.98                     | 0.63              |
| 9:CI:4:TYR:HB2     | 9:CI:19:LEU:CB     | 2.27                     | 0.63              |
| 22:CV:40:C:H2'     | 22:CV:41:C:H6      | 1.64                     | 0.63              |
| 25:DA:915:C:N4     | 25:DA:916:G:C6     | 2.66                     | 0.63              |
| 25:DA:945:A:H2'    | 25:DA:945:A:N3     | 2.12                     | 0.63              |
| 29:DE:188:VAL:CG2  | 29:DE:189:PRO:HD2  | 2.28                     | 0.63              |
| 33:DI:82:ARG:HH11  | 33:DI:82:ARG:HG3   | 1.62                     | 0.63              |
| 36:DP:83:VAL:HG23  | 36:DP:105:LEU:HD22 | 1.79                     | 0.63              |
| 42:DV:28:GLU:O     | 42:DV:61:VAL:HG11  | 1.99                     | 0.63              |
| 42:DV:44:LYS:C     | 42:DV:46:VAL:H     | 2.06                     | 0.63              |
| 1:AA:197:A:H4'     | 1:AA:198:G:O5'     | 1.98                     | 0.63              |
| 1:AA:1279:A:O2'    | 1:AA:1282:C:N4     | 2.28                     | 0.63              |
| 4:AD:194:LEU:N     | 4:AD:194:LEU:HD22  | 2.14                     | 0.63              |
| 23:AW:38:A:H3'     | 23:AW:39:U:C5'     | 2.29                     | 0.63              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 24:AX:12:A:N3     | 24:AX:12:A:H5''    | 2.14                     | 0.63              |
| 25:BA:866:A:N3    | 25:BA:866:A:H2'    | 2.14                     | 0.63              |
| 40:BT:34:VAL:HG22 | 40:BT:39:ARG:CB    | 2.20                     | 0.63              |
| 41:BU:115:ALA:C   | 41:BU:117:GLN:H    | 2.06                     | 0.63              |
| 46:BZ:158:PRO:HG2 | 46:BZ:161:VAL:HG21 | 1.79                     | 0.63              |
| 55:B8:50:LEU:C    | 55:B8:53:PRO:CD    | 2.70                     | 0.63              |
| 2:CB:61:LEU:HD12  | 2:CB:61:LEU:O      | 1.99                     | 0.63              |
| 3:CC:6:HIS:ND1    | 14:CN:49:HIS:HB3   | 2.13                     | 0.63              |
| 5:CE:112:LEU:O    | 5:CE:113:ALA:C     | 2.41                     | 0.63              |
| 5:CE:127:ASN:O    | 5:CE:131:ILE:HB    | 1.98                     | 0.63              |
| 6:CF:7:ASN:HB2    | 6:CF:89:MET:HB3    | 1.81                     | 0.63              |
| 6:CF:29:ALA:O     | 6:CF:32:ASN:N      | 2.31                     | 0.63              |
| 12:CL:18:VAL:HG23 | 12:CL:19:ARG:H     | 1.62                     | 0.63              |
| 12:CL:92:ASP:O    | 12:CL:94:PRO:HD3   | 1.98                     | 0.63              |
| 24:CX:19:U:O2'    | 24:CX:20:U:H5'     | 1.98                     | 0.63              |
| 25:DA:482:A:H4'   | 45:DY:47:LYS:HD2   | 1.81                     | 0.63              |
| 29:DE:26:ILE:HG22 | 29:DE:27:LEU:H     | 1.63                     | 0.63              |
| 30:DF:47:GLY:HA3  | 30:DF:95:ARG:O     | 1.98                     | 0.63              |
| 37:DQ:30:GLY:CA   | 37:DQ:107:ALA:HB2  | 2.27                     | 0.63              |
| 39:DS:83:LYS:HE3  | 39:DS:109:GLY:HA2  | 1.81                     | 0.63              |
| 48:D1:23:LYS:HD3  | 48:D1:28:GLY:HA3   | 1.80                     | 0.63              |
| 1:AA:562:C:O2'    | 12:AL:15:ARG:HB3   | 1.98                     | 0.63              |
| 4:AD:3:ARG:HG2    | 4:AD:118:ARG:CD    | 2.29                     | 0.63              |
| 4:AD:33:MET:CE    | 4:AD:37:PRO:HA     | 2.29                     | 0.63              |
| 19:AS:9:VAL:C     | 19:AS:10:PHE:CD1   | 2.76                     | 0.63              |
| 25:BA:242:G:N1    | 55:B8:5:LYS:HE2    | 2.14                     | 0.63              |
| 25:BA:1299:G:H4'  | 25:BA:1301:A:C4    | 2.34                     | 0.63              |
| 28:BD:43:ARG:HH11 | 28:BD:44:ASN:HD21  | 1.41                     | 0.63              |
| 28:BD:65:ILE:HD11 | 28:BD:67:PHE:CE1   | 2.33                     | 0.63              |
| 30:BF:22:ALA:HB1  | 30:BF:26:ALA:HB1   | 1.81                     | 0.63              |
| 39:BS:19:LYS:O    | 39:BS:20:ARG:HD3   | 1.99                     | 0.63              |
| 40:BT:29:ARG:CD   | 40:BT:86:ILE:O     | 2.47                     | 0.63              |
| 42:BV:21:ARG:HB3  | 42:BV:91:TYR:HB2   | 1.81                     | 0.63              |
| 46:BZ:144:LEU:HG  | 46:BZ:150:LEU:HD12 | 1.80                     | 0.63              |
| 55:B8:30:ARG:HD3  | 55:B8:30:ARG:C     | 2.20                     | 0.63              |
| 1:CA:1325:C:H4'   | 21:CU:17:THR:HG21  | 1.81                     | 0.63              |
| 1:CA:1442(A):G:N1 | 25:DA:2864:G:OP1   | 2.31                     | 0.63              |
| 4:CD:64:LEU:HB2   | 4:CD:198:VAL:HG21  | 1.80                     | 0.63              |
| 5:CE:41:VAL:HG22  | 5:CE:113:ALA:HA    | 1.81                     | 0.63              |
| 5:CE:150:ARG:HG3  | 5:CE:150:ARG:NH1   | 2.09                     | 0.63              |
| 9:CI:106:ALA:O    | 9:CI:108:VAL:HG22  | 1.99                     | 0.63              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 16:CP:43:LYS:HG2    | 16:CP:48:TRP:CE2   | 2.32                     | 0.63              |
| 25:DA:99:U:H1'      | 25:DA:102:G:N3     | 2.14                     | 0.63              |
| 25:DA:389:G:N1      | 36:DP:71:VAL:HG22  | 2.14                     | 0.63              |
| 25:DA:750:A:C2'     | 25:DA:752:A:OP1    | 2.47                     | 0.63              |
| 32:DH:153:LYS:HG3   | 32:DH:161:GLY:HA2  | 1.79                     | 0.63              |
| 36:DP:124:LYS:HG2   | 36:DP:145:PRO:HD3  | 1.80                     | 0.63              |
| 37:DQ:12:GLN:HE21   | 37:DQ:73:PRO:HD2   | 1.62                     | 0.63              |
| 39:DS:19:LYS:O      | 39:DS:21:THR:N     | 2.31                     | 0.63              |
| 39:DS:52:SER:HB2    | 39:DS:55:ALA:H     | 1.61                     | 0.63              |
| 39:DS:58:LEU:HD23   | 39:DS:58:LEU:N     | 2.14                     | 0.63              |
| 40:DT:91:ARG:HB3    | 40:DT:116:ALA:HA   | 1.80                     | 0.63              |
| 45:DY:79:CYS:O      | 45:DY:80:GLY:O     | 2.17                     | 0.63              |
| 1:AA:451:A:H5''     | 1:AA:452:A:OP1     | 1.99                     | 0.63              |
| 1:AA:1238:A:N7      | 1:AA:1301:U:O4     | 2.31                     | 0.63              |
| 2:AB:55:PHE:HA      | 2:AB:58:ILE:CG1    | 2.27                     | 0.63              |
| 2:AB:178:ARG:NH2    | 8:AH:74:PRO:HG3    | 2.14                     | 0.63              |
| 7:AG:105:VAL:O      | 7:AG:108:ALA:HB3   | 1.99                     | 0.63              |
| 8:AH:89:PRO:HA      | 8:AH:92:ARG:HH11   | 1.62                     | 0.63              |
| 9:AI:97:LYS:HB3     | 9:AI:98:PRO:HD3    | 1.79                     | 0.63              |
| 12:AL:36:VAL:O      | 12:AL:58:VAL:HA    | 1.98                     | 0.63              |
| 15:AO:24:SER:O      | 15:AO:28:GLN:CG    | 2.36                     | 0.63              |
| 24:AX:20:U:C4       | 24:AX:21:C:N4      | 2.66                     | 0.63              |
| 25:BA:2171:A:N3     | 25:BA:2172:U:C4    | 2.67                     | 0.63              |
| 25:BA:2320:A:C6     | 25:BA:2333:A:N7    | 2.66                     | 0.63              |
| 25:BA:2683:C:OP1    | 40:BT:53:ARG:NH2   | 2.31                     | 0.63              |
| 25:BA:2712(A):A:H5' | 38:BR:13:HIS:HD2   | 1.64                     | 0.63              |
| 25:BA:2779:U:H1'    | 25:BA:2781:A:C6    | 2.33                     | 0.63              |
| 46:BZ:23:LYS:HG2    | 46:BZ:38:TYR:CE1   | 2.31                     | 0.63              |
| 46:BZ:75:ASN:O      | 46:BZ:84:GLU:HB2   | 1.98                     | 0.63              |
| 53:B6:19:ARG:HG2    | 53:B6:20:ASN:N     | 2.13                     | 0.63              |
| 1:CA:1054:C:N4      | 23:CY:34:G:C1'     | 2.55                     | 0.63              |
| 2:CB:74:LYS:HB3     | 2:CB:169:LYS:HE3   | 1.81                     | 0.63              |
| 4:CD:10:ARG:HG3     | 4:CD:10:ARG:HH11   | 1.64                     | 0.63              |
| 5:CE:31:LEU:HD13    | 5:CE:43:LEU:HD11   | 1.80                     | 0.63              |
| 11:CK:13:GLN:HB3    | 11:CK:75:TYR:O     | 1.99                     | 0.63              |
| 25:DA:1105:U:H2'    | 25:DA:1106:G:H8    | 1.64                     | 0.63              |
| 25:DA:1287:A:N6     | 38:DR:106:GLY:O    | 2.32                     | 0.63              |
| 25:DA:2542:A:O2'    | 25:DA:2544:G:N7    | 2.31                     | 0.63              |
| 29:DE:100:GLU:O     | 29:DE:172:VAL:HG23 | 1.99                     | 0.63              |
| 30:DF:129:PHE:HA    | 30:DF:142:TRP:NE1  | 2.14                     | 0.63              |
| 31:DG:76:SER:OG     | 31:DG:83:ARG:HA    | 1.99                     | 0.63              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:DG:81:LYS:N     | 31:DG:81:LYS:HD3   | 2.14                     | 0.63              |
| 32:DH:136:ILE:HG22 | 32:DH:136:ILE:O    | 1.98                     | 0.63              |
| 41:DU:101:ARG:C    | 41:DU:102:GLU:HG2  | 2.22                     | 0.63              |
| 42:DV:38:LEU:HB3   | 42:DV:52:VAL:HG22  | 1.81                     | 0.63              |
| 2:AB:96:ARG:NH1    | 2:AB:148:TYR:HE1   | 1.97                     | 0.63              |
| 8:AH:109:ILE:CG2   | 8:AH:137:VAL:HB    | 2.28                     | 0.63              |
| 11:AK:21:ILE:HD13  | 11:AK:84:VAL:HG12  | 1.81                     | 0.63              |
| 13:AM:49:THR:HB    | 13:AM:51:ALA:HB3   | 1.80                     | 0.63              |
| 19:AS:63:THR:HG22  | 19:AS:66:MET:CE    | 2.28                     | 0.63              |
| 25:BA:32:C:O5'     | 25:BA:32:C:H6      | 1.82                     | 0.63              |
| 25:BA:311:A:N9     | 25:BA:332:A:N7     | 2.47                     | 0.63              |
| 25:BA:865:C:H5'    | 25:BA:866:A:OP1    | 1.99                     | 0.63              |
| 25:BA:2712:U:H5''  | 25:BA:2714:G:C5'   | 2.29                     | 0.63              |
| 31:BG:102:PHE:HE2  | 31:BG:141:PHE:CE1  | 2.17                     | 0.63              |
| 39:BS:30:ARG:HH22  | 39:BS:62:LYS:HD2   | 1.62                     | 0.63              |
| 44:BX:11:PRO:HG2   | 44:BX:13:LEU:HG    | 1.81                     | 0.63              |
| 45:BY:55:TYR:CD1   | 45:BY:56:PRO:HG2   | 2.34                     | 0.63              |
| 46:BZ:103:ARG:HD3  | 46:BZ:136:PHE:CD1  | 2.34                     | 0.63              |
| 1:CA:339:C:OP2     | 35:DO:97:ARG:NH1   | 2.32                     | 0.63              |
| 11:CK:20:TYR:HB2   | 11:CK:31:THR:HG22  | 1.80                     | 0.63              |
| 11:CK:82:VAL:HG11  | 11:CK:108:ILE:HG12 | 1.80                     | 0.63              |
| 16:CP:8:ARG:C      | 16:CP:9:PHE:CD2    | 2.73                     | 0.63              |
| 19:CS:46:GLY:H     | 19:CS:62:ILE:HG23  | 1.61                     | 0.63              |
| 23:CW:31:A:N1      | 23:CW:39:U:O4      | 2.32                     | 0.63              |
| 25:DA:389:G:H1     | 36:DP:71:VAL:HG22  | 1.63                     | 0.63              |
| 31:DG:16:ARG:HG2   | 31:DG:16:ARG:NH1   | 2.12                     | 0.63              |
| 32:DH:89:ILE:HD11  | 32:DH:129:THR:CB   | 2.18                     | 0.63              |
| 39:DS:20:ARG:HD3   | 39:DS:21:THR:N     | 2.13                     | 0.63              |
| 40:DT:86:ILE:HG12  | 40:DT:87:ASP:N     | 2.12                     | 0.63              |
| 43:DW:64:MET:O     | 43:DW:65:LEU:HB3   | 1.98                     | 0.63              |
| 3:AC:6:HIS:HD2     | 3:AC:7:PRO:HD2     | 1.64                     | 0.62              |
| 4:AD:20:TYR:HE2    | 4:AD:27:TYR:CE2    | 2.16                     | 0.62              |
| 7:AG:27:ILE:HD11   | 7:AG:43:PHE:HD2    | 1.63                     | 0.62              |
| 15:AO:8:LYS:O      | 15:AO:12:ILE:HG13  | 2.00                     | 0.62              |
| 22:AV:36:A:C2      | 24:AX:18:G:C2      | 2.87                     | 0.62              |
| 25:BA:536:A:OP1    | 41:BU:53:ARG:NH1   | 2.32                     | 0.62              |
| 25:BA:866:A:N6     | 25:BA:914:C:C5     | 2.67                     | 0.62              |
| 25:BA:2258:C:H6    | 25:BA:2258:C:O5'   | 1.82                     | 0.62              |
| 25:BA:2458:G:C4    | 25:BA:2490:G:C2    | 2.87                     | 0.62              |
| 28:BD:69:ARG:HH22  | 28:BD:192:THR:HB   | 1.64                     | 0.62              |
| 28:BD:129:ASN:O    | 28:BD:193:VAL:HG13 | 1.98                     | 0.62              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 28:BD:243:GLY:O    | 28:BD:244:ARG:HB3  | 1.99                     | 0.62              |
| 30:BF:124:LEU:C    | 30:BF:124:LEU:HD12 | 2.24                     | 0.62              |
| 37:BQ:54:MET:HG3   | 37:BQ:117:ALA:HB1  | 1.80                     | 0.62              |
| 41:BU:8:VAL:HG12   | 41:BU:9:VAL:N      | 2.14                     | 0.62              |
| 47:B0:26:TYR:N     | 47:B0:29:GLN:HE21  | 1.96                     | 0.62              |
| 54:B7:46:VAL:HG12  | 54:B7:48:LYS:NZ    | 2.14                     | 0.62              |
| 2:CB:19:HIS:CE1    | 2:CB:20:GLU:HG2    | 2.34                     | 0.62              |
| 2:CB:85:ALA:CB     | 2:CB:92:TYR:HB3    | 2.29                     | 0.62              |
| 10:CJ:30:SER:CB    | 10:CJ:80:LYS:HB3   | 2.29                     | 0.62              |
| 22:CV:53:G:O2'     | 22:CV:54:G:P       | 2.57                     | 0.62              |
| 25:DA:242:G:C8     | 55:D8:3:LYS:CD     | 2.82                     | 0.62              |
| 25:DA:9271:G:N2    | 25:DA:9272:G:H1'   | 2.14                     | 0.62              |
| 25:DA:627:A:H4'    | 25:DA:628:G:H5'    | 1.81                     | 0.62              |
| 28:DD:227:ASN:HB3  | 28:DD:228:PRO:HD2  | 1.80                     | 0.62              |
| 10:AJ:42:THR:HG23  | 10:AJ:68:HIS:HA    | 1.79                     | 0.62              |
| 10:AJ:49:VAL:HG12  | 10:AJ:61:GLU:O     | 1.99                     | 0.62              |
| 19:AS:43:GLU:HA    | 19:AS:45:VAL:HG13  | 1.80                     | 0.62              |
| 25:BA:311:A:OP1    | 25:BA:311:A:H8     | 1.80                     | 0.62              |
| 25:BA:832:G:H21    | 36:BP:53:GLY:HA3   | 1.63                     | 0.62              |
| 25:BA:1523:U:H2'   | 25:BA:1524:G:H8    | 1.64                     | 0.62              |
| 25:BA:2051:A:H61   | 25:BA:2614:A:H2'   | 1.63                     | 0.62              |
| 25:BA:2345:G:O2'   | 25:BA:2382:G:C4'   | 2.47                     | 0.62              |
| 36:BP:59:LEU:HD21  | 55:B8:13:ARG:HH22  | 1.63                     | 0.62              |
| 39:BS:89:ARG:HD3   | 39:BS:92:TYR:N     | 2.14                     | 0.62              |
| 41:BU:12:ARG:C     | 41:BU:14:HIS:N     | 2.56                     | 0.62              |
| 43:BW:2:GLU:HA     | 43:BW:107:LEU:O    | 1.99                     | 0.62              |
| 44:BX:66:LEU:O     | 44:BX:69:TYR:HB2   | 1.99                     | 0.62              |
| 1:CA:119:A:N6      | 1:CA:288:A:C4      | 2.68                     | 0.62              |
| 2:CB:235:SER:O     | 2:CB:237:ALA:N     | 2.31                     | 0.62              |
| 11:CK:20:TYR:O     | 11:CK:31:THR:N     | 2.31                     | 0.62              |
| 17:CQ:22:LEU:HD12  | 17:CQ:40:LYS:O     | 1.99                     | 0.62              |
| 17:CQ:77:VAL:O     | 17:CQ:78:GLU:HB3   | 1.99                     | 0.62              |
| 18:CR:56:THR:OG1   | 18:CR:58:LEU:HD13  | 1.99                     | 0.62              |
| 25:DA:13:A:C4      | 25:DA:15:G:O6      | 2.53                     | 0.62              |
| 29:DE:61:ARG:HB3   | 29:DE:62:PRO:CD    | 2.29                     | 0.62              |
| 29:DE:116:VAL:HG22 | 29:DE:117:MET:N    | 2.14                     | 0.62              |
| 30:DF:9:ILE:HD11   | 30:DF:125:LEU:CG   | 2.28                     | 0.62              |
| 35:DO:47:ILE:HG23  | 35:DO:48:PRO:HD2   | 1.81                     | 0.62              |
| 42:DV:6:LYS:HG3    | 42:DV:10:LYS:O     | 1.98                     | 0.62              |
| 50:D3:56:VAL:HG12  | 50:D3:57:GLU:N     | 2.11                     | 0.62              |
| 1:AA:1128:C:H5'    | 9:AI:16:ARG:HH22   | 1.65                     | 0.62              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:AA:1330:U:H4'    | 13:AM:23:TYR:CE2  | 2.34                     | 0.62              |
| 10:AJ:90:LEU:N     | 10:AJ:91:PRO:HD3  | 2.14                     | 0.62              |
| 11:AK:58:PRO:HB3   | 11:AK:93:GLN:HG3  | 1.80                     | 0.62              |
| 13:AM:28:ALA:C     | 13:AM:30:ALA:N    | 2.55                     | 0.62              |
| 13:AM:90:LEU:HA    | 13:AM:93:ARG:HB2  | 1.82                     | 0.62              |
| 20:AT:12:ALA:O     | 20:AT:15:ARG:N    | 2.30                     | 0.62              |
| 25:BA:620:G:H4'    | 25:BA:621:A:O5'   | 1.99                     | 0.62              |
| 37:BQ:110:THR:HG23 | 37:BQ:113:GLN:HB2 | 1.80                     | 0.62              |
| 41:BU:25:TRP:CD1   | 41:BU:26:GLY:N    | 2.67                     | 0.62              |
| 41:BU:62:ILE:HG13  | 41:BU:76:TYR:CE1  | 2.34                     | 0.62              |
| 46:BZ:108:PRO:HB2  | 46:BZ:144:LEU:O   | 1.99                     | 0.62              |
| 54:B7:11:LYS:O     | 54:B7:11:LYS:HD2  | 1.99                     | 0.62              |
| 2:CB:68:ILE:HD13   | 2:CB:161:ALA:HB3  | 1.81                     | 0.62              |
| 6:CF:62:TRP:C      | 6:CF:63:TYR:HD2   | 2.06                     | 0.62              |
| 12:CL:43:VAL:HG23  | 12:CL:44:THR:N    | 2.14                     | 0.62              |
| 13:CM:83:ASP:H     | 13:CM:93:ARG:NH2  | 1.96                     | 0.62              |
| 13:CM:126:LYS:HG3  | 13:CM:126:LYS:O   | 1.99                     | 0.62              |
| 16:CP:20:VAL:HG21  | 16:CP:32:TYR:CG   | 2.35                     | 0.62              |
| 20:CT:97:ALA:O     | 20:CT:99:LEU:N    | 2.31                     | 0.62              |
| 25:DA:956:G:H4'    | 37:DQ:83:MET:HE1  | 1.81                     | 0.62              |
| 36:DP:57:THR:HG23  | 36:DP:59:LEU:HB3  | 1.80                     | 0.62              |
| 41:DU:57:PHE:C     | 41:DU:59:ARG:N    | 2.55                     | 0.62              |
| 45:DY:47:LYS:O     | 45:DY:49:VAL:HG23 | 1.99                     | 0.62              |
| 55:D8:23:VAL:CG1   | 55:D8:46:ARG:HH11 | 2.11                     | 0.62              |
| 1:AA:251:G:N1      | 1:AA:266:G:N1     | 2.47                     | 0.62              |
| 1:AA:1228:C:O2'    | 13:AM:116:THR:O   | 2.15                     | 0.62              |
| 2:AB:115:LEU:HB2   | 2:AB:145:LEU:HD12 | 1.82                     | 0.62              |
| 3:AC:61:ALA:O      | 3:AC:62:ASP:HB2   | 1.97                     | 0.62              |
| 14:AN:9:LYS:HG3    | 14:AN:12:ARG:NH2  | 2.15                     | 0.62              |
| 19:AS:40:ILE:HG21  | 19:AS:62:ILE:HD11 | 1.80                     | 0.62              |
| 20:AT:18:GLN:O     | 20:AT:19:SER:C    | 2.42                     | 0.62              |
| 23:AW:14:A:N1      | 23:AW:15:G:H1'    | 2.14                     | 0.62              |
| 25:BA:804:A:H2'    | 25:BA:806:C:C4    | 2.35                     | 0.62              |
| 25:BA:1251:C:C5'   | 25:BA:1251:C:C6   | 2.79                     | 0.62              |
| 25:BA:2447:G:H1'   | 25:BA:2501:C:C5   | 2.33                     | 0.62              |
| 25:BA:2789:C:H1'   | 25:BA:2892:A:H2   | 1.63                     | 0.62              |
| 30:BF:25:PRO:HG3   | 30:BF:119:ARG:HB2 | 1.80                     | 0.62              |
| 30:BF:101:LEU:O    | 30:BF:106:ARG:NH1 | 2.31                     | 0.62              |
| 31:BG:72:ARG:HD3   | 31:BG:86:MET:CA   | 2.30                     | 0.62              |
| 50:B3:29:ARG:HG3   | 50:B3:29:ARG:NH1  | 2.13                     | 0.62              |
| 2:CB:235:SER:OG    | 2:CB:236:TYR:HD1  | 1.82                     | 0.62              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:CD:33:MET:CE     | 4:CD:37:PRO:HA     | 2.29                     | 0.62              |
| 19:CS:52:TYR:CD1   | 19:CS:57:HIS:CE1   | 2.84                     | 0.62              |
| 20:CT:29:LYS:HD2   | 20:CT:66:ALA:CB    | 2.29                     | 0.62              |
| 28:DD:24:ILE:HG12  | 28:DD:25:THR:N     | 2.10                     | 0.62              |
| 29:DE:101:ARG:HH21 | 29:DE:171:GLU:CA   | 2.11                     | 0.62              |
| 32:DH:147:ASN:N    | 32:DH:147:ASN:HD22 | 1.96                     | 0.62              |
| 35:DO:104:ARG:HH21 | 40:DT:43:GLN:HE22  | 1.47                     | 0.62              |
| 40:DT:27:THR:HA    | 40:DT:87:ASP:HB2   | 1.81                     | 0.62              |
| 1:AA:991:U:O2      | 1:AA:993:G:H8      | 1.81                     | 0.62              |
| 1:AA:1049:U:C2     | 1:AA:1201:A:C4     | 2.86                     | 0.62              |
| 1:AA:1358:U:OP1    | 14:AN:35:ARG:HG2   | 2.00                     | 0.62              |
| 3:AC:7:PRO:O       | 3:AC:11:ARG:HG2    | 1.99                     | 0.62              |
| 5:AE:57:LYS:O      | 5:AE:61:TYR:CD2    | 2.52                     | 0.62              |
| 9:AI:58:HIS:CB     | 9:AI:59:PHE:CE1    | 2.82                     | 0.62              |
| 12:AL:112:ASP:O    | 12:AL:113:ARG:C    | 2.41                     | 0.62              |
| 15:AO:56:LEU:O     | 15:AO:60:VAL:HG23  | 1.99                     | 0.62              |
| 17:AQ:63:ARG:HG2   | 17:AQ:64:PRO:HD2   | 1.81                     | 0.62              |
| 23:AW:34:G:C5      | 24:AX:14:A:C4      | 2.86                     | 0.62              |
| 25:BA:2614:A:C5'   | 25:BA:2615:U:OP1   | 2.48                     | 0.62              |
| 27:BC:78:ALA:HB2   | 27:BC:82:LYS:HD2   | 1.81                     | 0.62              |
| 33:BI:29:TYR:HD2   | 33:BI:30:LEU:CD2   | 2.12                     | 0.62              |
| 33:BI:38:LEU:HD12  | 33:BI:38:LEU:N     | 2.11                     | 0.62              |
| 36:BP:57:THR:HG23  | 36:BP:59:LEU:H     | 1.64                     | 0.62              |
| 38:BR:5:LYS:O      | 38:BR:6:SER:HB3    | 1.99                     | 0.62              |
| 40:BT:26:ASP:OD2   | 40:BT:26:ASP:C     | 2.43                     | 0.62              |
| 42:BV:22:VAL:O     | 42:BV:23:GLU:HB2   | 2.00                     | 0.62              |
| 43:BW:6:ILE:HA     | 43:BW:103:ILE:O    | 2.00                     | 0.62              |
| 47:B0:41:ARG:HD2   | 47:B0:41:ARG:H     | 1.65                     | 0.62              |
| 48:B1:58:ILE:HD11  | 48:B1:60:PHE:CZ    | 2.34                     | 0.62              |
| 13:CM:116:THR:HG22 | 13:CM:117:VAL:H    | 1.65                     | 0.62              |
| 25:DA:250:G:C6     | 25:DA:251:A:C6     | 2.87                     | 0.62              |
| 25:DA:890:A:N6     | 25:DA:892:G:C6     | 2.67                     | 0.62              |
| 26:DB:66:A:H61     | 26:DB:108:U:H2'    | 1.65                     | 0.62              |
| 30:DF:198:ALA:HA   | 30:DF:201:VAL:CG1  | 2.28                     | 0.62              |
| 31:DG:97:ASP:O     | 31:DG:100:TRP:N    | 2.32                     | 0.62              |
| 32:DH:86:GLU:O     | 32:DH:87:LEU:HB2   | 2.00                     | 0.62              |
| 32:DH:143:GLN:C    | 32:DH:143:GLN:HE21 | 2.08                     | 0.62              |
| 33:DI:52:ARG:CB    | 33:DI:52:ARG:NH1   | 2.62                     | 0.62              |
| 34:DN:9:VAL:HG12   | 34:DN:10:GLU:N     | 2.14                     | 0.62              |
| 36:DP:84:ASN:CG    | 36:DP:116:GLY:HA3  | 2.25                     | 0.62              |
| 46:DZ:6:LYS:HD2    | 46:DZ:6:LYS:H      | 1.64                     | 0.62              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 46:DZ:99:TYR:CD2  | 46:DZ:125:LEU:HD13 | 2.35                     | 0.62              |
| 46:DZ:125:LEU:HG  | 46:DZ:164:ALA:HB3  | 1.82                     | 0.62              |
| 52:D5:46:CYS:SG   | 52:D5:47:PRO:HD2   | 2.39                     | 0.62              |
| 1:AA:742:G:OP2    | 15:AO:35:ARG:NH2   | 2.32                     | 0.62              |
| 3:AC:35:GLU:HA    | 3:AC:38:ARG:HD2    | 1.80                     | 0.62              |
| 4:AD:116:GLN:HE22 | 4:AD:157:LEU:HD11  | 1.64                     | 0.62              |
| 7:AG:10:ARG:HG3   | 7:AG:10:ARG:NH1    | 1.99                     | 0.62              |
| 7:AG:16:LEU:HD13  | 9:AI:44:VAL:HG23   | 1.82                     | 0.62              |
| 13:AM:11:ARG:O    | 13:AM:13:LYS:N     | 2.33                     | 0.62              |
| 15:AO:33:THR:HG23 | 15:AO:63:ARG:NH1   | 2.15                     | 0.62              |
| 25:BA:1050:A:H2'  | 25:BA:1051:G:H8    | 1.65                     | 0.62              |
| 25:BA:1453:U:HO2' | 25:BA:1455:G:H8    | 1.43                     | 0.62              |
| 25:BA:2344:U:OP1  | 53:B6:38:LYS:HD2   | 1.99                     | 0.62              |
| 27:BC:49:ILE:HG22 | 27:BC:50:ASP:H     | 1.64                     | 0.62              |
| 30:BF:1:MET:HE2   | 30:BF:26:ALA:O     | 1.99                     | 0.62              |
| 31:BG:44:GLY:H    | 31:BG:88:ILE:CG1   | 2.12                     | 0.62              |
| 34:BN:90:MET:HE2  | 34:BN:90:MET:HA    | 1.80                     | 0.62              |
| 37:BQ:140:ALA:HB1 | 46:BZ:99:TYR:HB2   | 1.82                     | 0.62              |
| 40:BT:91:ARG:HA   | 40:BT:117:ASP:H    | 1.65                     | 0.62              |
| 46:BZ:117:LEU:HA  | 46:BZ:173:ALA:O    | 2.00                     | 0.62              |
| 1:CA:279:A:P      | 1:CA:281:G:H5'     | 2.39                     | 0.62              |
| 17:CQ:5:VAL:C     | 17:CQ:6:LEU:HD12   | 2.25                     | 0.62              |
| 23:CY:35:A:H2'    | 23:CY:36:A:H5''    | 1.82                     | 0.62              |
| 25:DA:2712:U:O2'  | 25:DA:2713:A:C5'   | 2.48                     | 0.62              |
| 26:DB:57:A:H1'    | 31:DG:29:TRP:HB2   | 1.81                     | 0.62              |
| 29:DE:44:TYR:O    | 29:DE:45:THR:HB    | 1.99                     | 0.62              |
| 29:DE:59:VAL:O    | 29:DE:60:ASN:HB3   | 1.99                     | 0.62              |
| 31:DG:181:ARG:HG2 | 31:DG:181:ARG:O    | 1.98                     | 0.62              |
| 36:DP:92:GLU:HA   | 36:DP:123:LEU:HD13 | 1.81                     | 0.62              |
| 41:DU:103:PRO:O   | 41:DU:104:GLN:C    | 2.41                     | 0.62              |
| 43:DW:8:ARG:HA    | 43:DW:102:HIS:CD2  | 2.34                     | 0.62              |
| 46:DZ:99:TYR:HA   | 46:DZ:125:LEU:HA   | 1.80                     | 0.62              |
| 48:D1:45:ASN:ND2  | 48:D1:47:GLN:HE21  | 1.96                     | 0.62              |
| 50:D3:36:VAL:O    | 50:D3:36:VAL:HG23  | 1.99                     | 0.62              |
| 3:AC:14:ILE:HG23  | 3:AC:15:THR:N      | 2.14                     | 0.62              |
| 3:AC:123:GLN:O    | 3:AC:128:PHE:HB2   | 1.99                     | 0.62              |
| 10:AJ:58:ASP:O    | 10:AJ:59:SER:C     | 2.43                     | 0.62              |
| 18:AR:19:LYS:O    | 18:AR:20:ALA:HB2   | 2.00                     | 0.62              |
| 19:AS:6:LYS:HD2   | 19:AS:7:LYS:HD3    | 1.81                     | 0.62              |
| 25:BA:588:U:OP2   | 25:BA:588:U:H5     | 1.83                     | 0.62              |
| 25:BA:704:G:N2    | 25:BA:726:G:C4     | 2.68                     | 0.62              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 30:BF:124:LEU:HG  | 30:BF:126:VAL:HG13 | 1.82                     | 0.62              |
| 31:BG:117:PHE:HE1 | 31:BG:119:GLY:CA   | 2.11                     | 0.62              |
| 32:BH:76:VAL:O    | 32:BH:79:VAL:HG22  | 2.00                     | 0.62              |
| 36:BP:78:PRO:HB2  | 36:BP:111:ARG:HD3  | 1.81                     | 0.62              |
| 38:BR:11:ASN:O    | 38:BR:12:ARG:HB2   | 1.98                     | 0.62              |
| 1:CA:192:U:O3'    | 20:CT:57:ARG:HD2   | 2.00                     | 0.62              |
| 1:CA:365:U:O2'    | 1:CA:366:C:H5      | 1.82                     | 0.62              |
| 3:CC:14:ILE:O     | 3:CC:15:THR:C      | 2.43                     | 0.62              |
| 4:CD:8:VAL:O      | 4:CD:10:ARG:N      | 2.33                     | 0.62              |
| 6:CF:72:VAL:HG12  | 6:CF:73:ASN:N      | 2.13                     | 0.62              |
| 9:CI:10:ARG:HD3   | 9:CI:75:ASP:HB3    | 1.80                     | 0.62              |
| 10:CJ:56:HIS:O    | 10:CJ:58:ASP:N     | 2.33                     | 0.62              |
| 22:CV:48:U:H3'    | 22:CV:49:C:H5''    | 1.81                     | 0.62              |
| 23:CY:33:U:H5''   | 23:CY:34:G:OP2     | 2.00                     | 0.62              |
| 25:DA:481:G:H1'   | 25:DA:506:G:H21    | 1.63                     | 0.62              |
| 40:DT:23:ARG:HG3  | 40:DT:120:ARG:CZ   | 2.29                     | 0.62              |
| 44:DX:54:VAL:HG22 | 44:DX:81:VAL:HG12  | 1.81                     | 0.62              |
| 45:DY:88:LYS:HB3  | 45:DY:90:LEU:CD2   | 2.29                     | 0.62              |
| 50:D3:4:LEU:HD23  | 50:D3:5:LYS:N      | 2.15                     | 0.62              |
| 1:AA:1158:C:O2    | 1:AA:1158:C:C2'    | 2.47                     | 0.62              |
| 9:AI:50:LEU:HA    | 9:AI:53:VAL:HG22   | 1.82                     | 0.62              |
| 22:AV:15:G:N2     | 22:AV:49:C:H41     | 1.98                     | 0.62              |
| 22:AV:19:G:C2     | 22:AV:59:A:C5      | 2.87                     | 0.62              |
| 22:AV:57:C:H1'    | 31:BG:76:SER:O     | 1.99                     | 0.62              |
| 27:BC:36:LYS:HZ3  | 27:BC:36:LYS:HB2   | 1.65                     | 0.62              |
| 29:BE:119:ARG:HD2 | 29:BE:120:TRP:CE2  | 2.34                     | 0.62              |
| 36:BP:102:ARG:O   | 36:BP:102:ARG:HD2  | 2.00                     | 0.62              |
| 45:BY:48:ALA:C    | 45:BY:50:ARG:H     | 2.07                     | 0.62              |
| 48:B1:52:ARG:NH1  | 48:B1:74:VAL:HG12  | 2.14                     | 0.62              |
| 48:B1:86:SER:HB2  | 48:B1:89:GLU:HB2   | 1.80                     | 0.62              |
| 51:B4:36:VAL:HB   | 51:B4:37:PRO:HD2   | 1.82                     | 0.62              |
| 1:CA:1057:G:H5''  | 3:CC:154:SER:HB2   | 1.82                     | 0.62              |
| 13:CM:3:ARG:HG2   | 13:CM:9:ILE:HG12   | 1.82                     | 0.62              |
| 25:DA:1648:C:N4   | 25:DA:2010:G:C6    | 2.68                     | 0.62              |
| 26:DB:109:C:OP2   | 26:DB:109:C:C6     | 2.53                     | 0.62              |
| 31:DG:41:GLN:HB3  | 31:DG:43:LEU:CD1   | 2.30                     | 0.62              |
| 33:DI:74:ASN:ND2  | 33:DI:74:ASN:H     | 1.97                     | 0.62              |
| 34:DN:120:LEU:CD1 | 34:DN:122:VAL:HG23 | 2.29                     | 0.62              |
| 37:DQ:16:ARG:C    | 37:DQ:17:LEU:HD23  | 2.25                     | 0.62              |
| 38:DR:94:TYR:N    | 38:DR:94:TYR:CD1   | 2.68                     | 0.62              |
| 39:DS:56:LEU:O    | 39:DS:58:LEU:HD22  | 1.98                     | 0.62              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 39:DS:70:GLY:O    | 39:DS:73:LEU:HB3   | 1.99                     | 0.62              |
| 53:D6:41:PRO:CD   | 53:D6:46:HIS:C     | 2.73                     | 0.62              |
| 55:D8:14:VAL:HG21 | 55:D8:22:VAL:CG1   | 2.29                     | 0.62              |
| 1:AA:710:G:OP1    | 6:AF:54:LYS:HD2    | 2.00                     | 0.62              |
| 1:AA:1139:G:N3    | 1:AA:1141:C:N4     | 2.47                     | 0.62              |
| 1:AA:1346:A:N1    | 1:AA:1374:A:H5''   | 2.14                     | 0.62              |
| 2:AB:144:ARG:HA   | 2:AB:147:LYS:CB    | 2.28                     | 0.62              |
| 10:AJ:48:THR:HG23 | 10:AJ:62:HIS:HB3   | 1.81                     | 0.62              |
| 13:AM:63:THR:HG22 | 13:AM:64:TRP:N     | 2.14                     | 0.62              |
| 14:AN:15:LYS:O    | 14:AN:16:PHE:O     | 2.17                     | 0.62              |
| 23:AW:51:U:H2'    | 23:AW:52:G:H8      | 1.64                     | 0.62              |
| 25:BA:84:A:H4'    | 25:BA:85:G:O5'     | 1.99                     | 0.62              |
| 25:BA:686:G:N2    | 25:BA:788:A:H61    | 1.97                     | 0.62              |
| 25:BA:1456:G:H2'  | 25:BA:1457:A:H8    | 1.64                     | 0.62              |
| 32:BH:20:ALA:HB3  | 32:BH:23:ARG:O     | 1.99                     | 0.62              |
| 34:BN:34:LEU:O    | 34:BN:49:GLY:HA3   | 2.00                     | 0.62              |
| 34:BN:126:PRO:O   | 34:BN:127:ASP:HB2  | 1.99                     | 0.62              |
| 36:BP:92:GLU:HA   | 36:BP:123:LEU:HD13 | 1.80                     | 0.62              |
| 39:BS:67:ARG:HH11 | 39:BS:67:ARG:HG2   | 1.64                     | 0.62              |
| 1:CA:438:G:H4'    | 1:CA:439:A:OP1     | 1.98                     | 0.62              |
| 1:CA:1224:G:C6    | 1:CA:1322:C:H1'    | 2.34                     | 0.62              |
| 3:CC:62:ASP:O     | 3:CC:98:ASN:HB3    | 1.99                     | 0.62              |
| 18:CR:74:ARG:HH21 | 18:CR:81:PHE:HA    | 1.65                     | 0.62              |
| 23:CY:36:A:H3'    | 23:CY:36:A:C8      | 2.34                     | 0.62              |
| 25:DA:2469:A:O2'  | 37:DQ:56:ARG:HD3   | 2.00                     | 0.62              |
| 25:DA:2729:G:H1'  | 29:DE:187:ALA:HB2  | 1.81                     | 0.62              |
| 31:DG:94:LEU:HD23 | 31:DG:94:LEU:N     | 2.14                     | 0.62              |
| 35:DO:18:LYS:HB2  | 35:DO:45:GLU:HG2   | 1.82                     | 0.62              |
| 42:DV:55:ALA:HB1  | 42:DV:101:GLY:HA2  | 1.82                     | 0.62              |
| 1:AA:324:G:OP1    | 20:AT:70:SER:HB2   | 2.00                     | 0.62              |
| 2:AB:74:LYS:HD2   | 2:AB:74:LYS:N      | 2.12                     | 0.62              |
| 4:AD:105:VAL:HG11 | 4:AD:126:ILE:HD11  | 1.82                     | 0.62              |
| 22:AV:35:C:O2'    | 22:AV:36:A:P       | 2.57                     | 0.62              |
| 23:AW:34:G:N1     | 24:AX:14:A:N3      | 2.47                     | 0.62              |
| 25:BA:311:A:O4'   | 25:BA:332:A:C8     | 2.52                     | 0.62              |
| 25:BA:531:C:OP1   | 25:BA:561:G:N1     | 2.33                     | 0.62              |
| 25:BA:1139:G:O2'  | 25:BA:1143:A:N1    | 2.29                     | 0.62              |
| 25:BA:2477:C:C4   | 56:B9:4:ARG:NH1    | 2.66                     | 0.62              |
| 28:BD:31:LYS:HZ1  | 28:BD:102:LYS:NZ   | 1.98                     | 0.62              |
| 28:BD:49:ILE:HD11 | 28:BD:51:VAL:O     | 1.99                     | 0.62              |
| 29:BE:100:GLU:O   | 29:BE:172:VAL:HG23 | 2.00                     | 0.62              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 30:BF:132:VAL:HG13 | 30:BF:133:ASN:N    | 2.13                     | 0.62              |
| 38:BR:10:LEU:CB    | 38:BR:17:ARG:NE    | 2.54                     | 0.62              |
| 39:BS:96:GLY:O     | 39:BS:98:VAL:N     | 2.29                     | 0.62              |
| 45:BY:42:VAL:CB    | 45:BY:65:ALA:HB3   | 2.26                     | 0.62              |
| 46:BZ:150:LEU:HD21 | 46:BZ:172:ALA:HB3  | 1.82                     | 0.62              |
| 1:CA:324:G:P       | 20:CT:70:SER:HB2   | 2.39                     | 0.62              |
| 1:CA:1372:U:H5''   | 9:CI:71:SER:HB3    | 1.81                     | 0.62              |
| 25:DA:1312:U:OP2   | 44:DX:63:LYS:NZ    | 2.32                     | 0.62              |
| 26:DB:9:G:OP1      | 39:DS:15:ARG:NH1   | 2.32                     | 0.62              |
| 26:DB:14:U:O2'     | 26:DB:108:U:C4'    | 2.46                     | 0.62              |
| 27:DC:196:LEU:C    | 27:DC:198:ALA:H    | 2.08                     | 0.62              |
| 28:DD:28:GLU:N     | 28:DD:29:PRO:HD2   | 2.15                     | 0.62              |
| 28:DD:77:ALA:CB    | 28:DD:97:TYR:HA    | 2.29                     | 0.62              |
| 30:DF:133:ASN:O    | 30:DF:135:LYS:N    | 2.32                     | 0.62              |
| 31:DG:98:ARG:O     | 31:DG:101:ILE:HG12 | 2.00                     | 0.62              |
| 36:DP:57:THR:HG23  | 36:DP:59:LEU:N     | 2.15                     | 0.62              |
| 39:DS:41:ASP:OD2   | 39:DS:44:LYS:HB2   | 2.00                     | 0.62              |
| 39:DS:106:ARG:HB2  | 39:DS:106:ARG:CZ   | 2.28                     | 0.62              |
| 42:DV:66:ARG:NH1   | 42:DV:88:ARG:HD3   | 2.15                     | 0.62              |
| 45:DY:50:ARG:HB3   | 45:DY:53:PRO:HG2   | 1.82                     | 0.62              |
| 49:D2:13:ALA:C     | 49:D2:15:LYS:H     | 2.08                     | 0.62              |
| 56:D9:2:LYS:HD2    | 56:D9:3:VAL:HG23   | 1.81                     | 0.62              |
| 1:AA:547:A:H4'     | 1:AA:548:G:O5'     | 2.00                     | 0.61              |
| 1:AA:1243:C:OP2    | 21:AU:10:ARG:NH2   | 2.33                     | 0.61              |
| 9:AI:96:LEU:HD11   | 9:AI:102:LEU:HD23  | 1.82                     | 0.61              |
| 25:BA:637:A:H4'    | 25:BA:638:G:O5'    | 1.99                     | 0.61              |
| 25:BA:2693:A:H2'   | 25:BA:2694:G:H8    | 1.64                     | 0.61              |
| 33:BI:25:TYR:HE1   | 33:BI:29:TYR:CD2   | 2.18                     | 0.61              |
| 37:BQ:42:ILE:HD12  | 37:BQ:42:ILE:N     | 2.15                     | 0.61              |
| 39:BS:15:ARG:HD3   | 39:BS:15:ARG:H     | 1.61                     | 0.61              |
| 45:BY:28:LYS:CB    | 45:BY:37:VAL:CG2   | 2.78                     | 0.61              |
| 46:BZ:57:ILE:HG22  | 46:BZ:58:VAL:H     | 1.64                     | 0.61              |
| 1:CA:411:A:N7      | 1:CA:429:U:C4      | 2.68                     | 0.61              |
| 2:CB:33:TYR:HB3    | 2:CB:41:ILE:HG22   | 1.82                     | 0.61              |
| 2:CB:63:MET:HG3    | 2:CB:64:ARG:N      | 2.14                     | 0.61              |
| 25:DA:2378:A:H4'   | 39:DS:23:ARG:NH1   | 2.14                     | 0.61              |
| 28:DD:26:LYS:HZ3   | 28:DD:82:ILE:H     | 1.48                     | 0.61              |
| 33:DI:25:TYR:CE2   | 33:DI:29:TYR:HD2   | 2.18                     | 0.61              |
| 45:DY:75:ILE:HD13  | 45:DY:75:ILE:C     | 2.24                     | 0.61              |
| 47:D0:41:ARG:H     | 47:D0:41:ARG:CD    | 2.11                     | 0.61              |
| 48:D1:6:GLU:HG3    | 48:D1:61:ARG:O     | 2.00                     | 0.61              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 53:D6:15:GLU:O     | 53:D6:47:THR:HG21  | 1.99                     | 0.61              |
| 1:AA:1279:A:H2'    | 1:AA:1282:C:H41    | 1.55                     | 0.61              |
| 3:AC:46:GLU:O      | 3:AC:47:LEU:HB2    | 1.99                     | 0.61              |
| 25:BA:27:G:N2      | 25:BA:512:G:H2'    | 2.14                     | 0.61              |
| 25:BA:243:U:OP1    | 55:B8:6:THR:CG2    | 2.46                     | 0.61              |
| 25:BA:660:G:H5'    | 30:BF:99:TYR:CD2   | 2.35                     | 0.61              |
| 25:BA:806:C:OP2    | 36:BP:41:ARG:NH2   | 2.32                     | 0.61              |
| 25:BA:1188:U:H4'   | 42:BV:79:VAL:HG23  | 1.82                     | 0.61              |
| 25:BA:2249:U:H1'   | 25:BA:2275:C:H41   | 1.65                     | 0.61              |
| 29:BE:132:HIS:CG   | 29:BE:135:HIS:NE2  | 2.68                     | 0.61              |
| 30:BF:28:ILE:HG21  | 30:BF:116:ASP:HB2  | 1.82                     | 0.61              |
| 31:BG:72:ARG:CD    | 31:BG:86:MET:HB3   | 2.27                     | 0.61              |
| 36:BP:52:GLU:OE1   | 36:BP:55:ARG:HD3   | 1.99                     | 0.61              |
| 42:BV:79:VAL:HG22  | 42:BV:79:VAL:O     | 1.98                     | 0.61              |
| 46:BZ:128:VAL:HG13 | 46:BZ:129:SER:N    | 2.14                     | 0.61              |
| 10:CJ:61:GLU:OE1   | 14:CN:58:LYS:HD3   | 2.00                     | 0.61              |
| 16:CP:8:ARG:O      | 16:CP:9:PHE:CD2    | 2.53                     | 0.61              |
| 20:CT:33:ILE:CD1   | 20:CT:33:ILE:N     | 2.61                     | 0.61              |
| 20:CT:83:ARG:O     | 20:CT:85:MET:N     | 2.30                     | 0.61              |
| 20:CT:98:PRO:C     | 20:CT:100:ILE:H    | 2.07                     | 0.61              |
| 29:DE:30:PRO:HA    | 29:DE:92:THR:HG22  | 1.83                     | 0.61              |
| 35:DO:9:GLU:O      | 35:DO:83:ALA:HA    | 2.00                     | 0.61              |
| 36:DP:82:GLY:HA2   | 36:DP:113:LYS:O    | 2.00                     | 0.61              |
| 39:DS:99:LYS:O     | 39:DS:102:ALA:HB3  | 2.00                     | 0.61              |
| 46:DZ:17:ALA:HA    | 46:DZ:20:ARG:HG3   | 1.82                     | 0.61              |
| 53:D6:10:LEU:HD12  | 55:D8:34:TRP:CD1   | 2.34                     | 0.61              |
| 1:AA:79:G:H21      | 1:AA:91:C:H41      | 1.48                     | 0.61              |
| 1:AA:971:G:OP1     | 1:AA:972:C:C5'     | 2.49                     | 0.61              |
| 1:AA:1239:A:H1'    | 1:AA:1241:G:C4     | 2.35                     | 0.61              |
| 2:AB:186:ALA:O     | 2:AB:201:ILE:HG12  | 1.99                     | 0.61              |
| 3:AC:141:VAL:HG11  | 3:AC:149:ALA:HB2   | 1.81                     | 0.61              |
| 22:AV:50:G:O6      | 22:AV:66:C:N4      | 2.33                     | 0.61              |
| 25:BA:1266:G:OP2   | 52:B5:19:ARG:NH1   | 2.34                     | 0.61              |
| 25:BA:2123:G:N2    | 27:BC:42:GLU:OE2   | 2.32                     | 0.61              |
| 25:BA:2729:G:H1'   | 29:BE:187:ALA:HB2  | 1.82                     | 0.61              |
| 28:BD:60:ARG:HD3   | 28:BD:86:PRO:O     | 2.01                     | 0.61              |
| 29:BE:179:GLU:HB3  | 29:BE:181:LEU:HD22 | 1.81                     | 0.61              |
| 30:BF:117:ARG:HD3  | 30:BF:120:GLU:OE1  | 2.00                     | 0.61              |
| 52:B5:35:GLU:O     | 52:B5:36:CYS:HB2   | 1.99                     | 0.61              |
| 53:B6:11:LEU:HG    | 53:B6:26:ASN:ND2   | 2.15                     | 0.61              |
| 1:CA:748:C:H6      | 1:CA:748:C:O5'     | 1.82                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:CD:19:LEU:HD23  | 4:CD:21:LEU:HD11  | 1.82                     | 0.61              |
| 16:CP:22:THR:HA   | 16:CP:33:ILE:CG1  | 2.30                     | 0.61              |
| 23:CY:36:A:H8     | 23:CY:36:A:C5'    | 2.13                     | 0.61              |
| 32:DH:6:ARG:NE    | 32:DH:54:ARG:HH12 | 1.99                     | 0.61              |
| 36:DP:102:ARG:O   | 36:DP:102:ARG:HD2 | 2.00                     | 0.61              |
| 45:DY:88:LYS:C    | 45:DY:90:LEU:H    | 2.07                     | 0.61              |
| 51:D4:9:LEU:CA    | 51:D4:26:SER:O    | 2.39                     | 0.61              |
| 3:AC:16:ARG:HB2   | 3:AC:16:ARG:HH11  | 1.61                     | 0.61              |
| 19:AS:40:ILE:CG2  | 19:AS:62:ILE:HD11 | 2.29                     | 0.61              |
| 23:AW:8:U:O2      | 23:AW:21:A:C2     | 2.54                     | 0.61              |
| 25:BA:2578:G:O2'  | 25:BA:2579:C:H5'  | 2.01                     | 0.61              |
| 29:BE:33:VAL:CG1  | 29:BE:69:LYS:HE3  | 2.22                     | 0.61              |
| 31:BG:44:GLY:H    | 31:BG:88:ILE:HG12 | 1.65                     | 0.61              |
| 31:BG:114:ILE:O   | 31:BG:116:ASP:N   | 2.33                     | 0.61              |
| 49:B2:67:LYS:HA   | 49:B2:70:GLN:HE22 | 1.65                     | 0.61              |
| 2:CB:18:GLY:CA    | 2:CB:42:ILE:HG22  | 2.30                     | 0.61              |
| 12:CL:60:LEU:HD21 | 12:CL:66:VAL:HG22 | 1.81                     | 0.61              |
| 13:CM:124:PRO:CB  | 13:CM:125:ARG:CA  | 2.77                     | 0.61              |
| 25:DA:82:G:C6     | 25:DA:83:G:O6     | 2.53                     | 0.61              |
| 25:DA:340:A:H2'   | 25:DA:341:G:H8    | 1.65                     | 0.61              |
| 25:DA:704:G:O2'   | 25:DA:726:G:N2    | 2.34                     | 0.61              |
| 25:DA:995:C:C5    | 41:DU:57:PHE:CE1  | 2.88                     | 0.61              |
| 25:DA:1209:G:O2'  | 25:DA:1237:A:N1   | 2.26                     | 0.61              |
| 25:DA:1272:A:H1'  | 25:DA:1618:A:C8   | 2.35                     | 0.61              |
| 27:DC:36:LYS:HD3  | 27:DC:37:PHE:H    | 1.63                     | 0.61              |
| 30:DF:46:ARG:HG2  | 30:DF:46:ARG:NH1  | 2.10                     | 0.61              |
| 30:DF:132:VAL:O   | 30:DF:133:ASN:C   | 2.44                     | 0.61              |
| 32:DH:127:GLU:HG3 | 32:DH:130:ARG:CZ  | 2.30                     | 0.61              |
| 34:DN:51:PHE:CZ   | 34:DN:119:ARG:HD2 | 2.35                     | 0.61              |
| 1:AA:429:U:OP1    | 4:AD:13:ARG:NH2   | 2.33                     | 0.61              |
| 3:AC:131:ARG:NH1  | 5:AE:50:GLU:HG2   | 2.15                     | 0.61              |
| 23:AY:31:A:C4     | 23:AY:32:U:C6     | 2.88                     | 0.61              |
| 25:BA:1170:G:O6   | 25:BA:1179:C:N4   | 2.33                     | 0.61              |
| 30:BF:20:LEU:O    | 30:BF:24:LEU:HD23 | 2.00                     | 0.61              |
| 31:BG:86:MET:CG   | 31:BG:87:PRO:CD   | 2.75                     | 0.61              |
| 33:BI:18:VAL:HG12 | 33:BI:18:VAL:O    | 2.00                     | 0.61              |
| 36:BP:55:ARG:HG2  | 36:BP:56:SER:N    | 2.15                     | 0.61              |
| 37:BQ:79:LEU:HD22 | 37:BQ:80:GLU:CG   | 2.30                     | 0.61              |
| 55:B8:46:ARG:O    | 55:B8:47:LYS:CB   | 2.49                     | 0.61              |
| 1:CA:280:C:O2     | 17:CQ:38:ARG:HG3  | 2.00                     | 0.61              |
| 1:CA:992:U:O2'    | 1:CA:993:G:P      | 2.59                     | 0.61              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:CB:158:LEU:HD12 | 2:CB:158:LEU:N     | 2.15                     | 0.61              |
| 2:CB:171:ALA:O    | 2:CB:172:ILE:C     | 2.42                     | 0.61              |
| 5:CE:86:ALA:HB3   | 5:CE:130:ASN:HD22  | 1.64                     | 0.61              |
| 7:CG:69:VAL:HG12  | 7:CG:69:VAL:O      | 1.98                     | 0.61              |
| 7:CG:146:GLU:HA   | 7:CG:149:ARG:HB2   | 1.81                     | 0.61              |
| 17:CQ:31:LEU:HD12 | 17:CQ:31:LEU:O     | 2.00                     | 0.61              |
| 23:CY:29:G:N3     | 23:CY:29:G:H2'     | 2.14                     | 0.61              |
| 25:DA:568:U:H5'   | 25:DA:945:A:C6     | 2.35                     | 0.61              |
| 25:DA:913:U:O2'   | 25:DA:914:C:C5     | 2.53                     | 0.61              |
| 25:DA:1826:G:H4'  | 28:DD:242:ARG:HH21 | 1.64                     | 0.61              |
| 25:DA:2406:U:N3   | 36:DP:73:GLY:O     | 2.28                     | 0.61              |
| 29:DE:97:LYS:HE2  | 29:DE:98:PRO:HD2   | 1.80                     | 0.61              |
| 36:DP:9:ASN:CB    | 36:DP:10:PRO:HD2   | 2.30                     | 0.61              |
| 36:DP:79:ARG:CZ   | 36:DP:109:GLY:HA3  | 2.31                     | 0.61              |
| 36:DP:124:LYS:HZ3 | 36:DP:143:GLY:HA3  | 1.64                     | 0.61              |
| 39:DS:108:GLY:H   | 39:DS:110:LEU:HD12 | 1.64                     | 0.61              |
| 39:DS:110:LEU:O   | 39:DS:112:PHE:CE1  | 2.54                     | 0.61              |
| 40:DT:33:LYS:CE   | 40:DT:43:GLN:NE2   | 2.46                     | 0.61              |
| 41:DU:79:PHE:CE2  | 41:DU:83:LEU:HD21  | 2.25                     | 0.61              |
| 42:DV:41:GLY:HA3  | 42:DV:46:VAL:CG1   | 2.31                     | 0.61              |
| 46:DZ:28:MET:HE1  | 46:DZ:59:LEU:HD12  | 1.82                     | 0.61              |
| 50:D3:8:LEU:C     | 50:D3:8:LEU:HD13   | 2.24                     | 0.61              |
| 4:AD:78:LEU:CD2   | 4:AD:96:LEU:HB3    | 2.30                     | 0.61              |
| 6:AF:37:VAL:HG12  | 6:AF:38:GLU:H      | 1.65                     | 0.61              |
| 12:AL:46:LYS:CG   | 12:AL:47:LYS:H     | 2.13                     | 0.61              |
| 23:AY:39:U:H2'    | 23:AY:40:C:H6      | 1.64                     | 0.61              |
| 25:BA:139:G:H1    | 25:BA:142(A):C:H42 | 1.49                     | 0.61              |
| 25:BA:1569:A:O2'  | 28:BD:38:LYS:HG3   | 2.01                     | 0.61              |
| 31:BG:139:LEU:O   | 31:BG:139:LEU:HG   | 1.97                     | 0.61              |
| 38:BR:103:ARG:HB2 | 38:BR:109:ALA:C    | 2.25                     | 0.61              |
| 40:BT:27:THR:O    | 40:BT:28:VAL:HB    | 1.98                     | 0.61              |
| 2:CB:149:LEU:O    | 2:CB:153:ARG:HG3   | 2.00                     | 0.61              |
| 3:CC:70:VAL:O     | 3:CC:106:VAL:N     | 2.33                     | 0.61              |
| 10:CJ:9:ARG:O     | 10:CJ:94:VAL:HG13  | 2.00                     | 0.61              |
| 18:CR:86:VAL:O    | 18:CR:87:ARG:HD3   | 2.01                     | 0.61              |
| 25:DA:602:G:N2    | 25:DA:655:A:N7     | 2.47                     | 0.61              |
| 25:DA:1693:U:H4'  | 25:DA:1694:C:OP1   | 2.01                     | 0.61              |
| 31:DG:88:ILE:C    | 31:DG:88:ILE:HD13  | 2.25                     | 0.61              |
| 35:DO:119:PRO:HB2 | 40:DT:68:TYR:HE1   | 1.60                     | 0.61              |
| 40:DT:80:SER:OG   | 40:DT:81:PRO:HD3   | 2.01                     | 0.61              |
| 46:DZ:169:GLU:HG2 | 46:DZ:170:THR:N    | 2.15                     | 0.61              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 50:D3:5:LYS:HG3    | 50:D3:36:VAL:HG12 | 1.83                     | 0.61              |
| 1:AA:1065:U:H4'    | 1:AA:1066:C:H5'   | 1.82                     | 0.61              |
| 13:AM:65:LYS:HD2   | 13:AM:69:GLU:HB3  | 1.83                     | 0.61              |
| 25:BA:8:A:H2'      | 25:BA:9:U:C6      | 2.35                     | 0.61              |
| 25:BA:2857:G:N2    | 25:BA:2860:A:OP2  | 2.23                     | 0.61              |
| 30:BF:65:TRP:CH2   | 30:BF:72:ARG:CZ   | 2.84                     | 0.61              |
| 33:BI:83:ALA:HB1   | 33:BI:87:LYS:O    | 2.01                     | 0.61              |
| 38:BR:11:ASN:O     | 38:BR:12:ARG:CD   | 2.49                     | 0.61              |
| 3:CC:141:VAL:HG11  | 3:CC:202:ILE:HG23 | 1.83                     | 0.61              |
| 10:CJ:45:ARG:HH12  | 14:CN:36:PHE:HE2  | 1.47                     | 0.61              |
| 18:CR:37:VAL:HG23  | 18:CR:38:GLU:H    | 1.65                     | 0.61              |
| 25:DA:297:C:H5''   | 45:DY:85:VAL:HG21 | 1.82                     | 0.61              |
| 25:DA:568:U:O5'    | 25:DA:945:A:N6    | 2.33                     | 0.61              |
| 25:DA:886:C:C2'    | 25:DA:887:A:H4'   | 2.28                     | 0.61              |
| 25:DA:2125:G:N1    | 25:DA:2172:U:OP2  | 2.31                     | 0.61              |
| 25:DA:2406:U:C4    | 36:DP:72:PRO:HG2  | 2.35                     | 0.61              |
| 27:DC:76:ALA:C     | 27:DC:78:ALA:H    | 2.07                     | 0.61              |
| 28:DD:221:VAL:HG22 | 28:DD:226:MET:HE3 | 1.81                     | 0.61              |
| 31:DG:21:ARG:HG2   | 31:DG:21:ARG:NH1  | 2.15                     | 0.61              |
| 45:DY:81:LYS:HD3   | 45:DY:97:ARG:HE   | 1.63                     | 0.61              |
| 46:DZ:39:VAL:HG23  | 46:DZ:40:ASP:N    | 2.14                     | 0.61              |
| 49:D2:2:LYS:HA     | 49:D2:5:GLU:OE1   | 2.00                     | 0.61              |
| 53:D6:32:ASN:ND2   | 53:D6:33:LYS:H    | 1.99                     | 0.61              |
| 2:AB:24:TRP:HB3    | 2:AB:40:HIS:CD2   | 2.35                     | 0.61              |
| 4:AD:10:ARG:HH11   | 4:AD:10:ARG:HG2   | 1.65                     | 0.61              |
| 9:AI:59:PHE:HD1    | 9:AI:59:PHE:N     | 1.93                     | 0.61              |
| 13:AM:117:VAL:HG12 | 13:AM:118:ALA:N   | 2.12                     | 0.61              |
| 25:BA:196:A:C4     | 25:BA:805:G:O6    | 2.54                     | 0.61              |
| 25:BA:1287:A:C5    | 25:BA:1288:U:C4   | 2.89                     | 0.61              |
| 25:BA:2377:A:H4'   | 39:BS:107:GLU:HG3 | 1.81                     | 0.61              |
| 36:BP:79:ARG:CZ    | 36:BP:109:GLY:HA3 | 2.31                     | 0.61              |
| 36:BP:107:LYS:O    | 36:BP:109:GLY:N   | 2.34                     | 0.61              |
| 43:BW:5:ALA:O      | 43:BW:6:ILE:CB    | 2.49                     | 0.61              |
| 45:BY:8:LYS:HE3    | 45:BY:72:VAL:O    | 2.00                     | 0.61              |
| 1:CA:950:U:H1'     | 1:CA:971:G:C5     | 2.35                     | 0.61              |
| 2:CB:22:LYS:O      | 2:CB:24:TRP:CD1   | 2.45                     | 0.61              |
| 10:CJ:49:VAL:HG22  | 10:CJ:50:ILE:N    | 2.15                     | 0.61              |
| 13:CM:110:ARG:HG2  | 13:CM:110:ARG:O   | 2.01                     | 0.61              |
| 19:CS:4:SER:O      | 19:CS:5:LEU:CB    | 2.47                     | 0.61              |
| 19:CS:7:LYS:HD3    | 19:CS:7:LYS:N     | 2.16                     | 0.61              |
| 23:CW:69:G:C3'     | 23:CW:70:G:H5''   | 2.31                     | 0.61              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 23:CY:28:G:N3     | 23:CY:43:C:N3      | 2.49                     | 0.61              |
| 25:DA:958:U:OP2   | 37:DQ:14:ARG:NH1   | 2.33                     | 0.61              |
| 25:DA:2520:C:H6   | 25:DA:2520:C:O5'   | 1.84                     | 0.61              |
| 32:DH:132:ARG:HB2 | 32:DH:132:ARG:HH11 | 1.64                     | 0.61              |
| 34:DN:22:THR:HB   | 34:DN:25:ARG:HB2   | 1.83                     | 0.61              |
| 36:DP:107:LYS:O   | 36:DP:109:GLY:N    | 2.34                     | 0.61              |
| 39:DS:49:VAL:HG21 | 39:DS:77:ALA:HA    | 1.82                     | 0.61              |
| 40:DT:60:THR:HG22 | 40:DT:77:PRO:HA    | 1.81                     | 0.61              |
| 41:DU:92:ARG:NH1  | 41:DU:92:ARG:HG2   | 2.10                     | 0.61              |
| 44:DX:27:THR:HG22 | 44:DX:80:ILE:HB    | 1.81                     | 0.61              |
| 45:DY:84:ARG:NH1  | 45:DY:97:ARG:HA    | 2.14                     | 0.61              |
| 46:DZ:99:TYR:HD2  | 46:DZ:99:TYR:N     | 1.99                     | 0.61              |
| 5:AE:101:ILE:HD11 | 5:AE:119:LEU:HD23  | 1.83                     | 0.61              |
| 7:AG:150:ALA:O    | 7:AG:153:HIS:CE1   | 2.54                     | 0.61              |
| 18:AR:70:ILE:O    | 18:AR:74:ARG:HG3   | 2.01                     | 0.61              |
| 20:AT:46:GLU:HG2  | 20:AT:46:GLU:O     | 2.00                     | 0.61              |
| 28:BD:139:GLY:H   | 28:BD:165:ILE:HB   | 1.66                     | 0.61              |
| 30:BF:20:LEU:C    | 30:BF:24:LEU:HD23  | 2.26                     | 0.61              |
| 31:BG:45:GLU:N    | 31:BG:88:ILE:HD13  | 2.05                     | 0.61              |
| 31:BG:72:ARG:CD   | 31:BG:86:MET:HA    | 2.30                     | 0.61              |
| 33:BI:5:LEU:C     | 33:BI:6:LEU:HD23   | 2.25                     | 0.61              |
| 34:BN:3:THR:O     | 34:BN:5:VAL:HG12   | 2.00                     | 0.61              |
| 46:BZ:71:VAL:HG22 | 46:BZ:88:PHE:CE2   | 2.35                     | 0.61              |
| 49:B2:25:VAL:O    | 49:B2:29:LYS:HG2   | 2.00                     | 0.61              |
| 54:B7:46:VAL:HG12 | 54:B7:48:LYS:HZ3   | 1.65                     | 0.61              |
| 2:CB:223:ILE:O    | 2:CB:226:ARG:HG2   | 2.00                     | 0.61              |
| 4:CD:33:MET:HE2   | 4:CD:37:PRO:CA     | 2.30                     | 0.61              |
| 4:CD:206:PHE:CD2  | 4:CD:207:TYR:CE2   | 2.89                     | 0.61              |
| 7:CG:23:VAL:CG1   | 7:CG:43:PHE:HE2    | 2.12                     | 0.61              |
| 10:CJ:8:LEU:N     | 10:CJ:70:ARG:O     | 2.33                     | 0.61              |
| 10:CJ:49:VAL:C    | 10:CJ:50:ILE:HD13  | 2.25                     | 0.61              |
| 16:CP:72:ARG:HG2  | 16:CP:73:LEU:HD23  | 1.83                     | 0.61              |
| 20:CT:26:ASN:O    | 20:CT:30:LYS:HB2   | 2.01                     | 0.61              |
| 23:CW:11:C:O5'    | 23:CW:11:C:H6      | 1.84                     | 0.61              |
| 25:DA:598:G:C4'   | 36:DP:11:GLY:CA    | 2.78                     | 0.61              |
| 32:DH:109:PHE:CZ  | 32:DH:152:ARG:HG2  | 2.36                     | 0.61              |
| 37:DQ:140:ALA:HB1 | 46:DZ:99:TYR:HB2   | 1.83                     | 0.61              |
| 40:DT:98:LYS:HB3  | 40:DT:100:TYR:CE1  | 2.36                     | 0.61              |
| 45:DY:97:ARG:HH21 | 45:DY:98:VAL:CB    | 2.08                     | 0.61              |
| 53:D6:15:GLU:HG3  | 53:D6:47:THR:OG1   | 2.01                     | 0.61              |
| 53:D6:40:CYS:SG   | 53:D6:45:LYS:HE2   | 2.41                     | 0.61              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 55:D8:50:LEU:C     | 55:D8:53:PRO:HD2   | 2.25                     | 0.61              |
| 1:AA:840:C:H4'     | 1:AA:841:U:OP1     | 2.01                     | 0.61              |
| 4:AD:88:VAL:HG22   | 5:AE:97:GLY:HA3    | 1.83                     | 0.61              |
| 11:AK:51:LYS:HG2   | 11:AK:52:GLY:N     | 2.16                     | 0.61              |
| 15:AO:50:HIS:O     | 15:AO:53:HIS:HB3   | 2.00                     | 0.61              |
| 18:AR:62:GLU:HA    | 18:AR:65:ILE:HD12  | 1.82                     | 0.61              |
| 22:AV:35:C:C2      | 22:AV:36:A:C8      | 2.89                     | 0.61              |
| 29:BE:111:ARG:C    | 38:BR:2:ARG:HG3    | 2.26                     | 0.61              |
| 31:BG:5:VAL:HG23   | 31:BG:6:ALA:N      | 2.15                     | 0.61              |
| 33:BI:8:PRO:O      | 33:BI:9:LEU:HG     | 2.01                     | 0.61              |
| 36:BP:82:GLY:HA2   | 36:BP:113:LYS:O    | 2.01                     | 0.61              |
| 43:BW:51:LEU:CD1   | 43:BW:52:GLU:N     | 2.64                     | 0.61              |
| 46:BZ:166:SER:OG   | 46:BZ:168:GLU:N    | 2.33                     | 0.61              |
| 2:CB:87:ARG:HE     | 2:CB:233:SER:HB2   | 1.66                     | 0.61              |
| 4:CD:80:GLU:C      | 4:CD:82:ALA:H      | 2.09                     | 0.61              |
| 4:CD:108:LEU:CB    | 4:CD:110:PHE:CE1   | 2.77                     | 0.61              |
| 5:CE:102:ALA:HB1   | 5:CE:106:PRO:HB3   | 1.77                     | 0.61              |
| 25:DA:531:C:OP1    | 25:DA:561:G:N1     | 2.34                     | 0.61              |
| 25:DA:1212:G:H1'   | 25:DA:1237:A:N6    | 2.16                     | 0.61              |
| 27:DC:86:ALA:HB3   | 27:DC:94:VAL:HG21  | 1.83                     | 0.61              |
| 28:DD:132:PRO:HD3  | 28:DD:190:TYR:CZ   | 2.36                     | 0.61              |
| 30:DF:133:ASN:O    | 30:DF:134:GLY:C    | 2.43                     | 0.61              |
| 34:DN:120:LEU:HD11 | 34:DN:122:VAL:HG23 | 1.82                     | 0.61              |
| 35:DO:20:MET:O     | 35:DO:41:ALA:HB1   | 2.01                     | 0.61              |
| 36:DP:59:LEU:C     | 36:DP:61:ARG:NH1   | 2.59                     | 0.61              |
| 39:DS:13:ARG:O     | 39:DS:13:ARG:HD2   | 2.00                     | 0.61              |
| 44:DX:63:LYS:HE3   | 44:DX:72:LYS:CE    | 2.25                     | 0.61              |
| 1:AA:327:A:C2      | 1:AA:329:A:C4      | 2.88                     | 0.60              |
| 1:AA:942:G:N2      | 9:AI:124:GLN:OE1   | 2.33                     | 0.60              |
| 1:AA:1277:C:C2'    | 1:AA:1278:U:H5'    | 2.31                     | 0.60              |
| 3:AC:64:VAL:O      | 3:AC:100:ALA:HB3   | 2.01                     | 0.60              |
| 4:AD:8:VAL:O       | 4:AD:11:LEU:HG     | 2.01                     | 0.60              |
| 5:AE:20:GLN:HG2    | 5:AE:21:ALA:O      | 2.01                     | 0.60              |
| 8:AH:6:ILE:H       | 8:AH:6:ILE:CD1     | 2.11                     | 0.60              |
| 8:AH:122:ARG:NH1   | 8:AH:122:ARG:HB2   | 2.16                     | 0.60              |
| 11:AK:57:THR:HG22  | 11:AK:59:TYR:H     | 1.66                     | 0.60              |
| 30:BF:17:ARG:HH11  | 30:BF:17:ARG:CG    | 2.13                     | 0.60              |
| 30:BF:41:LEU:HA    | 30:BF:44:ARG:HD3   | 1.81                     | 0.60              |
| 30:BF:202:PHE:O    | 30:BF:206:ILE:HG12 | 2.01                     | 0.60              |
| 31:BG:130:ASN:HB3  | 31:BG:160:VAL:HA   | 1.83                     | 0.60              |
| 32:BH:41:MET:HG3   | 32:BH:54:ARG:HA    | 1.83                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 34:BN:57:ALA:O    | 34:BN:58:ASP:O    | 2.19                     | 0.60              |
| 36:BP:84:ASN:CG   | 36:BP:116:GLY:HA3 | 2.25                     | 0.60              |
| 36:BP:101:VAL:HA  | 36:BP:105:LEU:O   | 2.01                     | 0.60              |
| 38:BR:2:ARG:NH2   | 38:BR:5:LYS:NZ    | 2.49                     | 0.60              |
| 1:CA:652:U:H1'    | 1:CA:653:A:C2     | 2.36                     | 0.60              |
| 2:CB:223:ILE:HA   | 2:CB:226:ARG:HG2  | 1.83                     | 0.60              |
| 3:CC:134:ILE:HG23 | 3:CC:151:VAL:HB   | 1.82                     | 0.60              |
| 7:CG:115:ARG:O    | 7:CG:118:VAL:HG22 | 2.01                     | 0.60              |
| 25:DA:607:U:OP1   | 30:DF:102:PRO:HA  | 2.00                     | 0.60              |
| 29:DE:176:ILE:CG2 | 29:DE:178:GLU:HB3 | 2.31                     | 0.60              |
| 30:DF:57:VAL:CG1  | 30:DF:58:ALA:N    | 2.64                     | 0.60              |
| 32:DH:151:ILE:C   | 32:DH:152:ARG:O   | 2.42                     | 0.60              |
| 33:DI:60:GLU:HG3  | 33:DI:61:ARG:CZ   | 2.31                     | 0.60              |
| 39:DS:86:ALA:O    | 39:DS:87:PHE:HB3  | 1.99                     | 0.60              |
| 43:DW:64:MET:CE   | 43:DW:109:GLU:HG2 | 2.30                     | 0.60              |
| 46:DZ:114:GLY:HA3 | 46:DZ:177:PRO:HG3 | 1.83                     | 0.60              |
| 48:D1:45:ASN:HD21 | 48:D1:47:GLN:NE2  | 1.99                     | 0.60              |
| 51:D4:22:ILE:H    | 51:D4:22:ILE:HD12 | 1.65                     | 0.60              |
| 55:D8:43:GLN:O    | 55:D8:44:LYS:HD2  | 2.01                     | 0.60              |
| 1:AA:952:U:H5'    | 1:AA:972:C:N4     | 2.16                     | 0.60              |
| 1:AA:1342:C:H4'   | 9:AI:125:TYR:HB3  | 1.82                     | 0.60              |
| 2:AB:92:TYR:CE2   | 2:AB:151:GLY:HA3  | 2.36                     | 0.60              |
| 2:AB:93:VAL:HG23  | 2:AB:93:VAL:O     | 2.01                     | 0.60              |
| 2:AB:162:ILE:HD11 | 2:AB:184:VAL:HG22 | 1.83                     | 0.60              |
| 3:AC:70:VAL:O     | 3:AC:105:GLU:HA   | 2.01                     | 0.60              |
| 3:AC:156:ARG:HD3  | 3:AC:193:TYR:O    | 2.01                     | 0.60              |
| 5:AE:78:HIS:HE1   | 5:AE:143:ARG:N    | 1.98                     | 0.60              |
| 6:AF:22:GLU:O     | 6:AF:26:ILE:HG13  | 2.01                     | 0.60              |
| 10:AJ:35:SER:O    | 10:AJ:36:GLY:O    | 2.19                     | 0.60              |
| 10:AJ:40:LEU:HB2  | 10:AJ:41:PRO:CD   | 2.22                     | 0.60              |
| 18:AR:44:LEU:CD1  | 18:AR:80:PRO:HD2  | 2.31                     | 0.60              |
| 23:AW:39:U:O2     | 23:AW:39:U:H5'    | 2.01                     | 0.60              |
| 25:BA:311:A:C8    | 25:BA:332:A:C6    | 2.89                     | 0.60              |
| 25:BA:2576:G:N3   | 25:BA:2576:G:C3'  | 2.62                     | 0.60              |
| 25:BA:2779:U:H1'  | 25:BA:2781:A:C5   | 2.35                     | 0.60              |
| 39:BS:49:VAL:HG12 | 39:BS:50:SER:H    | 1.66                     | 0.60              |
| 44:BX:64:LYS:HZ2  | 44:BX:73:ARG:HH21 | 1.49                     | 0.60              |
| 45:BY:76:CYS:SG   | 45:BY:77:PRO:CD   | 2.87                     | 0.60              |
| 1:CA:411:A:C4     | 1:CA:413:G:H1'    | 2.35                     | 0.60              |
| 2:CB:86:GLU:C     | 2:CB:88:ALA:H     | 2.08                     | 0.60              |
| 10:CJ:63:PHE:HA   | 14:CN:59:ALA:H    | 1.65                     | 0.60              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:DA:2847:U:C2'   | 25:DA:2848:G:H5'   | 2.31                     | 0.60              |
| 26:DB:50:G:OP1     | 39:DS:63:THR:HG23  | 2.01                     | 0.60              |
| 28:DD:238:GLY:O    | 28:DD:239:ARG:O    | 2.19                     | 0.60              |
| 36:DP:101:VAL:HA   | 36:DP:105:LEU:O    | 2.01                     | 0.60              |
| 41:DU:58:ARG:O     | 41:DU:62:ILE:HG12  | 2.01                     | 0.60              |
| 45:DY:74:PRO:O     | 45:DY:80:GLY:HA2   | 2.01                     | 0.60              |
| 48:D1:64:ALA:C     | 48:D1:66:HIS:H     | 2.09                     | 0.60              |
| 53:D6:9:LEU:HD23   | 53:D6:9:LEU:C      | 2.26                     | 0.60              |
| 1:AA:279:A:H5''    | 1:AA:281:G:O4'     | 2.01                     | 0.60              |
| 4:AD:13:ARG:HA     | 4:AD:33:MET:SD     | 2.41                     | 0.60              |
| 14:AN:42:ILE:O     | 14:AN:45:ARG:HB3   | 2.01                     | 0.60              |
| 17:AQ:58:GLU:O     | 17:AQ:59:ILE:HD13  | 2.01                     | 0.60              |
| 18:AR:36:ASN:O     | 18:AR:37:VAL:C     | 2.43                     | 0.60              |
| 20:AT:27:LYS:HD3   | 20:AT:27:LYS:C     | 2.26                     | 0.60              |
| 25:BA:1183:G:O3'   | 50:B3:29:ARG:NH1   | 2.35                     | 0.60              |
| 28:BD:97:TYR:CE1   | 28:BD:103:ARG:HG3  | 2.35                     | 0.60              |
| 34:BN:2:LYS:HB3    | 34:BN:4:TYR:CE2    | 2.36                     | 0.60              |
| 37:BQ:137:TYR:OH   | 46:BZ:81:ARG:NH1   | 2.35                     | 0.60              |
| 38:BR:93:GLY:O     | 38:BR:117:VAL:HG21 | 2.01                     | 0.60              |
| 45:BY:17:SER:HB2   | 45:BY:71:LYS:HE2   | 1.81                     | 0.60              |
| 3:CC:130:VAL:O     | 3:CC:134:ILE:HG12  | 2.01                     | 0.60              |
| 4:CD:25:ARG:O      | 4:CD:27:TYR:N      | 2.33                     | 0.60              |
| 10:CJ:33:GLN:O     | 10:CJ:75:ILE:HG23  | 2.01                     | 0.60              |
| 12:CL:31:PRO:O     | 12:CL:32:PHE:CD1   | 2.53                     | 0.60              |
| 12:CL:101:VAL:HG12 | 12:CL:104:VAL:CG2  | 2.31                     | 0.60              |
| 13:CM:23:TYR:HE1   | 13:CM:70:LEU:HD12  | 1.64                     | 0.60              |
| 22:CV:64:G:H2'     | 22:CV:65:G:H5'     | 1.82                     | 0.60              |
| 25:DA:242:G:N2     | 25:DA:255:A:OP2    | 2.31                     | 0.60              |
| 25:DA:598:G:O4'    | 36:DP:11:GLY:HA3   | 2.01                     | 0.60              |
| 25:DA:1272:A:C4    | 25:DA:1618:A:C8    | 2.89                     | 0.60              |
| 25:DA:1558:A:O2'   | 25:DA:1559:G:P     | 2.60                     | 0.60              |
| 25:DA:2330:G:H1'   | 47:D0:41:ARG:HB3   | 1.84                     | 0.60              |
| 33:DI:133:HIS:CB   | 33:DI:134:PRO:HD2  | 2.31                     | 0.60              |
| 34:DN:2:LYS:HZ1    | 41:DU:95:LEU:HD21  | 1.66                     | 0.60              |
| 44:DX:60:ARG:HH22  | 54:D7:47:ARG:HH21  | 1.46                     | 0.60              |
| 53:D6:16:CYS:O     | 53:D6:17:LYS:HB2   | 2.01                     | 0.60              |
| 53:D6:46:HIS:CD2   | 53:D6:47:THR:CA    | 2.75                     | 0.60              |
| 55:D8:51:ALA:HA    | 55:D8:54:GLU:CD    | 2.25                     | 0.60              |
| 4:AD:9:CYS:HB2     | 4:AD:22:LYS:HZ3    | 1.65                     | 0.60              |
| 5:AE:131:ILE:O     | 5:AE:134:ALA:HB3   | 2.02                     | 0.60              |
| 10:AJ:49:VAL:HG23  | 14:AN:41:ARG:CB    | 2.25                     | 0.60              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 12:AL:7:ILE:C      | 12:AL:9:GLN:H      | 2.09                     | 0.60              |
| 19:AS:6:LYS:CD     | 19:AS:7:LYS:HE3    | 2.30                     | 0.60              |
| 25:BA:2520:C:C6    | 25:BA:2567:G:H1'   | 2.36                     | 0.60              |
| 27:BC:187:ASP:C    | 27:BC:189:ILE:H    | 2.09                     | 0.60              |
| 28:BD:206:LEU:HD22 | 28:BD:211:ARG:CG   | 2.31                     | 0.60              |
| 28:BD:248:SER:C    | 28:BD:250:TRP:H    | 2.07                     | 0.60              |
| 31:BG:25:TYR:CE2   | 31:BG:31:VAL:HG23  | 2.36                     | 0.60              |
| 40:BT:28:VAL:HG21  | 40:BT:46:GLU:CG    | 2.08                     | 0.60              |
| 42:BV:35:LEU:O     | 42:BV:37:VAL:N     | 2.35                     | 0.60              |
| 1:CA:624:C:H2'     | 1:CA:625:G:H8      | 1.65                     | 0.60              |
| 1:CA:707:C:OP1     | 11:CK:85:ARG:NH1   | 2.30                     | 0.60              |
| 2:CB:15:VAL:HG21   | 2:CB:209:ARG:NE    | 2.16                     | 0.60              |
| 5:CE:107:ARG:HD3   | 5:CE:111:GLU:OE2   | 2.00                     | 0.60              |
| 6:CF:89:MET:HE1    | 18:CR:75:ILE:HG21  | 1.84                     | 0.60              |
| 9:CI:3:GLN:HA      | 9:CI:19:LEU:O      | 2.01                     | 0.60              |
| 9:CI:19:LEU:CD2    | 9:CI:59:PHE:HB2    | 2.31                     | 0.60              |
| 28:DD:226:MET:HB3  | 28:DD:230:ASP:HB2  | 1.83                     | 0.60              |
| 32:DH:126:PRO:CG   | 32:DH:130:ARG:HH11 | 2.14                     | 0.60              |
| 33:DI:93:THR:O     | 33:DI:96:ASP:HB2   | 2.01                     | 0.60              |
| 34:DN:1:MET:HG2    | 34:DN:2:LYS:N      | 2.15                     | 0.60              |
| 34:DN:15:LEU:HD13  | 34:DN:16:ILE:N     | 2.15                     | 0.60              |
| 34:DN:25:ARG:HH11  | 34:DN:25:ARG:CG    | 2.14                     | 0.60              |
| 35:DO:3:GLN:HB2    | 35:DO:4:PRO:HD2    | 1.84                     | 0.60              |
| 35:DO:24:VAL:HG22  | 35:DO:24:VAL:O     | 2.01                     | 0.60              |
| 38:DR:33:ARG:HD2   | 38:DR:33:ARG:N     | 2.16                     | 0.60              |
| 40:DT:33:LYS:HG2   | 40:DT:43:GLN:HB3   | 1.83                     | 0.60              |
| 25:BA:2405:G:O2'   | 25:BA:2411:A:N6    | 2.34                     | 0.60              |
| 30:BF:103:LYS:HG3  | 30:BF:106:ARG:NH2  | 2.16                     | 0.60              |
| 31:BG:3:LEU:O      | 31:BG:4:ASP:HB3    | 2.01                     | 0.60              |
| 37:BQ:63:LYS:HD3   | 37:BQ:65:PHE:CZ    | 2.37                     | 0.60              |
| 39:BS:26:LEU:HD13  | 39:BS:87:PHE:CD1   | 2.36                     | 0.60              |
| 42:BV:4:ILE:HG22   | 42:BV:4:ILE:O      | 2.01                     | 0.60              |
| 43:BW:38:TYR:CE2   | 52:B5:41:PRO:HD3   | 2.37                     | 0.60              |
| 53:B6:14:THR:O     | 53:B6:49:HIS:HA    | 2.01                     | 0.60              |
| 1:CA:66:G:O4'      | 1:CA:173:U:C4      | 2.54                     | 0.60              |
| 1:CA:67:C:H2'      | 1:CA:68:G:C8       | 2.36                     | 0.60              |
| 1:CA:792:A:H1'     | 1:CA:794:A:N7      | 2.16                     | 0.60              |
| 18:CR:65:ILE:O     | 18:CR:69:THR:HG23  | 2.01                     | 0.60              |
| 30:DF:134:GLY:H    | 30:DF:162:LEU:HD22 | 1.65                     | 0.60              |
| 36:DP:66:GLY:O     | 36:DP:67:MET:HB3   | 2.02                     | 0.60              |
| 38:DR:111:LEU:N    | 38:DR:111:LEU:HD22 | 2.16                     | 0.60              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 41:DU:57:PHE:C    | 41:DU:59:ARG:H     | 2.08                     | 0.60              |
| 41:DU:57:PHE:O    | 41:DU:59:ARG:N     | 2.35                     | 0.60              |
| 46:DZ:28:MET:HE3  | 46:DZ:37:VAL:HG11  | 1.83                     | 0.60              |
| 46:DZ:114:GLY:HA3 | 46:DZ:177:PRO:HB3  | 1.83                     | 0.60              |
| 1:AA:67:C:H2'     | 1:AA:68:G:C8       | 2.37                     | 0.60              |
| 3:AC:40:ARG:HD3   | 3:AC:55:VAL:HB     | 1.84                     | 0.60              |
| 4:AD:94:LEU:HA    | 4:AD:97:LEU:HD12   | 1.81                     | 0.60              |
| 5:AE:48:ALA:HB2   | 5:AE:57:LYS:HD3    | 1.83                     | 0.60              |
| 17:AQ:97:SER:C    | 17:AQ:98:LEU:HD23  | 2.27                     | 0.60              |
| 18:AR:82:THR:CG2  | 18:AR:83:GLU:N     | 2.64                     | 0.60              |
| 25:BA:769:G:C4'   | 25:BA:1379:A:H62   | 2.14                     | 0.60              |
| 25:BA:1300:U:H4'  | 25:BA:1301:A:H5''  | 1.80                     | 0.60              |
| 25:BA:1971:A:C4   | 28:BD:241:PRO:HD3  | 2.36                     | 0.60              |
| 30:BF:51:THR:HG22 | 30:BF:92:PRO:O     | 2.01                     | 0.60              |
| 36:BP:29:LYS:HD2  | 36:BP:30:THR:HG23  | 1.84                     | 0.60              |
| 44:BX:36:LYS:HA   | 44:BX:39:ILE:HG13  | 1.82                     | 0.60              |
| 1:CA:511:C:C2     | 1:CA:512:U:C5      | 2.90                     | 0.60              |
| 1:CA:869:G:H4'    | 1:CA:872:A:C8      | 2.36                     | 0.60              |
| 8:CH:112:LEU:HD12 | 8:CH:113:SER:N     | 2.17                     | 0.60              |
| 16:CP:17:TYR:CE1  | 16:CP:41:PRO:HG3   | 2.36                     | 0.60              |
| 20:CT:82:SER:O    | 20:CT:83:ARG:C     | 2.44                     | 0.60              |
| 25:DA:861:A:N3    | 26:DB:79:C:O2'     | 2.34                     | 0.60              |
| 25:DA:1205:U:C5'  | 25:DA:1206:G:OP2   | 2.50                     | 0.60              |
| 26:DB:44:G:H1'    | 26:DB:47:C:N4      | 2.16                     | 0.60              |
| 28:DD:36:PRO:HB2  | 28:DD:61:LEU:HD12  | 1.84                     | 0.60              |
| 30:DF:167:ALA:HB1 | 30:DF:173:VAL:HG11 | 1.83                     | 0.60              |
| 46:DZ:103:ARG:HG3 | 46:DZ:138:GLU:HG2  | 1.82                     | 0.60              |
| 50:D3:29:ARG:HH11 | 50:D3:29:ARG:HG3   | 1.66                     | 0.60              |
| 54:D7:29:LYS:O    | 54:D7:32:LYS:HB3   | 2.01                     | 0.60              |
| 1:AA:372:C:H4'    | 1:AA:373:A:OP1     | 2.01                     | 0.60              |
| 4:AD:170:VAL:O    | 4:AD:171:GLY:O     | 2.20                     | 0.60              |
| 13:AM:3:ARG:CB    | 31:BG:113:ARG:HH22 | 2.14                     | 0.60              |
| 13:AM:3:ARG:NE    | 31:BG:113:ARG:HH21 | 1.99                     | 0.60              |
| 13:AM:7:VAL:HG21  | 31:BG:115:ARG:HG2  | 1.83                     | 0.60              |
| 25:BA:532:A:N7    | 25:BA:2021:C:H2'   | 2.16                     | 0.60              |
| 25:BA:2172:U:C4'  | 25:BA:2173:A:OP2   | 2.48                     | 0.60              |
| 34:BN:40:PRO:HD3  | 41:BU:67:ALA:O     | 2.01                     | 0.60              |
| 36:BP:57:THR:C    | 36:BP:59:LEU:N     | 2.59                     | 0.60              |
| 36:BP:59:LEU:O    | 55:B8:13:ARG:NH1   | 2.34                     | 0.60              |
| 40:BT:27:THR:HG22 | 40:BT:49:VAL:CG2   | 2.31                     | 0.60              |
| 41:BU:31:SER:OG   | 41:BU:34:LYS:HB2   | 2.02                     | 0.60              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 42:BV:19:LYS:HG3   | 42:BV:20:LEU:C     | 2.26                     | 0.60              |
| 43:BW:9:TYR:HD2    | 43:BW:9:TYR:N      | 1.98                     | 0.60              |
| 3:CC:14:ILE:HG12   | 3:CC:15:THR:N      | 2.15                     | 0.60              |
| 4:CD:148:VAL:HG21  | 4:CD:158:ILE:HG21  | 1.84                     | 0.60              |
| 14:CN:15:LYS:O     | 14:CN:16:PHE:O     | 2.19                     | 0.60              |
| 17:CQ:8:GLY:O      | 17:CQ:56:VAL:HA    | 2.00                     | 0.60              |
| 22:CV:20:G:H1      | 22:CV:57:C:H42     | 1.48                     | 0.60              |
| 25:DA:890:A:C6     | 25:DA:892:G:C6     | 2.89                     | 0.60              |
| 28:DD:176:ARG:HH11 | 28:DD:176:ARG:HG2  | 1.65                     | 0.60              |
| 29:DE:59:VAL:HG22  | 29:DE:60:ASN:N     | 2.03                     | 0.60              |
| 30:DF:65:TRP:HB2   | 30:DF:66:PRO:HD2   | 1.82                     | 0.60              |
| 31:DG:180:PHE:C    | 31:DG:182:LYS:N    | 2.60                     | 0.60              |
| 33:DI:74:ASN:ND2   | 33:DI:75:LEU:N     | 2.46                     | 0.60              |
| 34:DN:24:GLY:HA2   | 34:DN:27:ALA:HB3   | 1.84                     | 0.60              |
| 39:DS:42:ASP:O     | 39:DS:43:GLU:HB2   | 1.99                     | 0.60              |
| 41:DU:103:PRO:O    | 41:DU:106:PHE:N    | 2.34                     | 0.60              |
| 43:DW:27:LYS:O     | 43:DW:70:TYR:HB2   | 2.01                     | 0.60              |
| 44:DX:11:PRO:O     | 44:DX:13:LEU:HG    | 2.02                     | 0.60              |
| 50:D3:1:MET:HE2    | 50:D3:44:ARG:HH22  | 1.67                     | 0.60              |
| 13:AM:39:ILE:CD1   | 13:AM:56:LEU:HD23  | 2.31                     | 0.60              |
| 17:AQ:53:LEU:HD12  | 17:AQ:54:GLY:H     | 1.67                     | 0.60              |
| 19:AS:10:PHE:CD1   | 19:AS:10:PHE:N     | 2.69                     | 0.60              |
| 25:BA:848:G:C4     | 25:BA:933:A:H8     | 2.19                     | 0.60              |
| 25:BA:1602:U:H3'   | 25:BA:1603:A:C5'   | 2.31                     | 0.60              |
| 28:BD:52:ARG:HB2   | 28:BD:53:PHE:CD2   | 2.36                     | 0.60              |
| 29:BE:66:HIS:ND1   | 29:BE:66:HIS:O     | 2.35                     | 0.60              |
| 30:BF:143:ALA:HB1  | 30:BF:148:LEU:HB2  | 1.83                     | 0.60              |
| 30:BF:178:PRO:HB2  | 30:BF:201:VAL:HG11 | 1.82                     | 0.60              |
| 32:BH:65:HIS:CE1   | 32:BH:69:ARG:HD2   | 2.37                     | 0.60              |
| 36:BP:66:GLY:O     | 36:BP:67:MET:HB3   | 2.02                     | 0.60              |
| 42:BV:46:VAL:HG13  | 42:BV:47:VAL:N     | 2.15                     | 0.60              |
| 10:CJ:58:ASP:O     | 10:CJ:59:SER:C     | 2.44                     | 0.60              |
| 25:DA:1250:G:O2'   | 41:DU:13:LYS:NZ    | 2.31                     | 0.60              |
| 25:DA:2725:A:C6    | 25:DA:2727:G:C4    | 2.89                     | 0.60              |
| 25:DA:2847:U:H2'   | 25:DA:2848:G:H5'   | 1.82                     | 0.60              |
| 26:DB:117:G:H4'    | 39:DS:54:LEU:HD12  | 1.84                     | 0.60              |
| 29:DE:61:ARG:HB3   | 29:DE:62:PRO:HD3   | 1.84                     | 0.60              |
| 31:DG:15:VAL:HG13  | 31:DG:175:LEU:HB2  | 1.84                     | 0.60              |
| 36:DP:52:GLU:OE1   | 36:DP:55:ARG:HD3   | 2.01                     | 0.60              |
| 40:DT:25:GLY:CA    | 40:DT:120:ARG:NH2  | 2.54                     | 0.60              |
| 42:DV:35:LEU:C     | 42:DV:37:VAL:N     | 2.59                     | 0.60              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 42:DV:91:TYR:CD1   | 42:DV:91:TYR:C     | 2.80                     | 0.60              |
| 43:DW:61:ASN:HD22  | 43:DW:61:ASN:N     | 1.98                     | 0.60              |
| 46:DZ:150:LEU:HD13 | 46:DZ:150:LEU:O    | 2.01                     | 0.60              |
| 49:D2:42:GLY:O     | 49:D2:44:LEU:N     | 2.34                     | 0.60              |
| 54:D7:1:MET:O      | 54:D7:2:LYS:C      | 2.45                     | 0.60              |
| 55:D8:53:PRO:HA    | 55:D8:56:GLU:HB2   | 1.82                     | 0.60              |
| 1:AA:745:C:OP1     | 1:AA:851:G:O2'     | 2.20                     | 0.60              |
| 5:AE:78:HIS:NE2    | 5:AE:142:LEU:HD23  | 2.15                     | 0.60              |
| 25:BA:196:A:N3     | 25:BA:805:G:O6     | 2.35                     | 0.60              |
| 25:BA:532:A:O2'    | 25:BA:2021:C:N4    | 2.35                     | 0.60              |
| 25:BA:1653:G:O2'   | 25:BA:1654:A:P     | 2.59                     | 0.60              |
| 30:BF:41:LEU:O     | 30:BF:44:ARG:HG2   | 2.01                     | 0.60              |
| 31:BG:44:GLY:H     | 31:BG:88:ILE:HD13  | 1.64                     | 0.60              |
| 33:BI:5:LEU:O      | 33:BI:6:LEU:HD23   | 2.02                     | 0.60              |
| 34:BN:18:ALA:HB1   | 34:BN:21:LYS:CB    | 2.31                     | 0.60              |
| 40:BT:28:VAL:HG13  | 40:BT:45:PHE:C     | 2.25                     | 0.60              |
| 42:BV:39:LEU:CB    | 42:BV:40:LEU:HD23  | 2.31                     | 0.60              |
| 1:CA:523:A:H61     | 12:CL:92:ASP:HB2   | 1.66                     | 0.60              |
| 22:CV:53:G:HO2'    | 22:CV:54:G:P       | 2.25                     | 0.60              |
| 25:DA:222:A:N6     | 25:DA:232:G:H1'    | 2.17                     | 0.60              |
| 25:DA:695:G:C6     | 25:DA:768:G:C6     | 2.90                     | 0.60              |
| 25:DA:974:G:H5'    | 25:DA:975:C:H5'    | 1.84                     | 0.60              |
| 25:DA:1566:A:OP1   | 28:DD:211:ARG:NH1  | 2.34                     | 0.60              |
| 25:DA:1821:A:OP1   | 28:DD:201:HIS:HE1  | 1.83                     | 0.60              |
| 25:DA:2030:A:H4'   | 25:DA:2031:A:H8    | 1.67                     | 0.60              |
| 27:DC:36:LYS:HB2   | 27:DC:36:LYS:HZ3   | 1.67                     | 0.60              |
| 28:DD:130:ALA:C    | 28:DD:131:LEU:HD12 | 2.26                     | 0.60              |
| 31:DG:107:LEU:HD11 | 31:DG:178:PHE:CE1  | 2.37                     | 0.60              |
| 31:DG:131:TYR:HB3  | 31:DG:159:VAL:CG1  | 2.32                     | 0.60              |
| 34:DN:30:ILE:O     | 34:DN:34:LEU:HB2   | 2.02                     | 0.60              |
| 35:DO:104:ARG:NH2  | 40:DT:43:GLN:NE2   | 2.50                     | 0.60              |
| 39:DS:18:ILE:C     | 39:DS:19:LYS:O     | 2.43                     | 0.60              |
| 40:DT:36:GLU:CD    | 40:DT:38:ASN:ND2   | 2.55                     | 0.60              |
| 40:DT:65:LYS:CE    | 40:DT:66:VAL:H     | 2.14                     | 0.60              |
| 41:DU:110:VAL:O    | 41:DU:113:ALA:HB3  | 2.02                     | 0.60              |
| 47:D0:73:GLY:O     | 47:D0:75:LEU:N     | 2.35                     | 0.60              |
| 1:AA:983:A:N6      | 1:AA:1222:G:H22    | 2.00                     | 0.60              |
| 1:AA:1049:U:C2     | 1:AA:1201:A:N9     | 2.70                     | 0.60              |
| 3:AC:19:GLU:O      | 3:AC:20:SER:HB2    | 2.01                     | 0.60              |
| 3:AC:83:ARG:O      | 3:AC:86:VAL:HG22   | 2.02                     | 0.60              |
| 4:AD:4:TYR:O       | 4:AD:5:ILE:HB      | 2.01                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:AN:38:GLY:O    | 14:AN:39:LEU:HD23 | 2.02                     | 0.60              |
| 18:AR:37:VAL:O    | 18:AR:40:LEU:N    | 2.28                     | 0.60              |
| 20:AT:43:LEU:HD12 | 20:AT:52:ALA:HA   | 1.83                     | 0.60              |
| 23:AW:39:U:O2'    | 23:AW:40:C:H5'    | 2.02                     | 0.60              |
| 25:BA:587:C:H6    | 25:BA:587:C:O5'   | 1.85                     | 0.60              |
| 25:BA:1128:A:O2'  | 25:BA:1129:A:O4'  | 2.20                     | 0.60              |
| 25:BA:2127:G:O5'  | 27:BC:36:LYS:HE2  | 2.01                     | 0.60              |
| 28:BD:181:GLU:CA  | 28:BD:272:ALA:HB3 | 2.31                     | 0.60              |
| 28:BD:201:HIS:C   | 28:BD:203:ASN:H   | 2.10                     | 0.60              |
| 28:BD:243:GLY:O   | 28:BD:244:ARG:CB  | 2.50                     | 0.60              |
| 31:BG:47:LYS:NZ   | 31:BG:82:LEU:HD12 | 2.17                     | 0.60              |
| 40:BT:15:VAL:HA   | 40:BT:79:HIS:CD2  | 2.37                     | 0.60              |
| 45:BY:101:LYS:HG2 | 45:BY:102:CYS:N   | 2.17                     | 0.60              |
| 2:CB:101:MET:HA   | 2:CB:108:ILE:HG13 | 1.84                     | 0.60              |
| 6:CF:86:ARG:O     | 6:CF:87:ARG:HG2   | 2.01                     | 0.60              |
| 7:CG:15:ASP:HB2   | 7:CG:20:ASP:O     | 2.02                     | 0.60              |
| 7:CG:76:ARG:HH11  | 7:CG:76:ARG:HG2   | 1.66                     | 0.60              |
| 11:CK:69:ALA:O    | 11:CK:70:LYS:C    | 2.45                     | 0.60              |
| 13:CM:93:ARG:NH1  | 25:DA:888:C:C4'   | 2.64                     | 0.60              |
| 20:CT:45:GLN:C    | 20:CT:47:GLY:N    | 2.59                     | 0.60              |
| 23:CW:60:U:OP2    | 23:CW:61:C:N4     | 2.30                     | 0.60              |
| 25:DA:99:U:H1'    | 25:DA:102:G:C2    | 2.37                     | 0.60              |
| 29:DE:45:THR:HG22 | 29:DE:83:ASP:HA   | 1.82                     | 0.60              |
| 29:DE:55:ASN:O    | 29:DE:57:LYS:N    | 2.35                     | 0.60              |
| 30:DF:66:PRO:O    | 30:DF:67:GLN:CB   | 2.50                     | 0.60              |
| 32:DH:8:PRO:HG2   | 32:DH:69:ARG:HE   | 1.66                     | 0.60              |
| 34:DN:73:THR:HG23 | 34:DN:82:LEU:HD11 | 1.84                     | 0.60              |
| 35:DO:17:ARG:HD3  | 35:DO:47:ILE:HD13 | 1.84                     | 0.60              |
| 50:D3:6:VAL:CG1   | 50:D3:56:VAL:HG13 | 2.32                     | 0.60              |
| 54:D7:24:THR:HG23 | 54:D7:27:GLY:H    | 1.67                     | 0.60              |
| 1:AA:979:C:H3'    | 1:AA:980:C:H5''   | 1.83                     | 0.59              |
| 1:AA:1277:C:O2'   | 1:AA:1279:A:H8    | 1.82                     | 0.59              |
| 2:AB:71:VAL:HG22  | 2:AB:93:VAL:HG21  | 1.83                     | 0.59              |
| 4:AD:4:TYR:HE2    | 4:AD:6:GLY:O      | 1.84                     | 0.59              |
| 14:AN:36:PHE:HD1  | 14:AN:37:PHE:CD2  | 2.20                     | 0.59              |
| 20:AT:63:ILE:HD12 | 20:AT:81:LYS:CG   | 2.29                     | 0.59              |
| 23:AW:38:A:N6     | 23:AW:39:U:C4     | 2.70                     | 0.59              |
| 25:BA:2787:C:H1'  | 29:BE:61:ARG:HG3  | 1.84                     | 0.59              |
| 28:BD:241:PRO:O   | 28:BD:242:ARG:C   | 2.42                     | 0.59              |
| 31:BG:44:GLY:N    | 31:BG:88:ILE:HG12 | 2.17                     | 0.59              |
| 31:BG:76:SER:O    | 31:BG:77:ILE:HD13 | 2.02                     | 0.59              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 40:BT:32:TYR:HB2   | 40:BT:81:PRO:CB    | 2.27                     | 0.59              |
| 52:B5:41:PRO:HG2   | 52:B5:44:THR:CG2   | 2.31                     | 0.59              |
| 1:CA:452:A:H62     | 1:CA:480:U:H3      | 1.49                     | 0.59              |
| 1:CA:870:U:H5''    | 1:CA:871:U:H5'     | 1.82                     | 0.59              |
| 1:CA:873:A:H4'     | 1:CA:874:G:OP1     | 2.00                     | 0.59              |
| 1:CA:1279:A:H61    | 3:CC:26:LYS:NZ     | 2.00                     | 0.59              |
| 13:CM:81:LEU:O     | 13:CM:84:ILE:HG22  | 2.02                     | 0.59              |
| 23:CW:5:G:C2       | 23:CW:69:G:C2      | 2.90                     | 0.59              |
| 25:DA:387:U:H4'    | 25:DA:388:G:O5'    | 2.02                     | 0.59              |
| 25:DA:1846:G:H5'   | 25:DA:1847:A:OP2   | 2.03                     | 0.59              |
| 29:DE:9:VAL:HG13   | 29:DE:25:VAL:O     | 2.02                     | 0.59              |
| 29:DE:116:VAL:O    | 29:DE:117:MET:HB3  | 2.01                     | 0.59              |
| 32:DH:151:ILE:HG22 | 32:DH:151:ILE:O    | 2.02                     | 0.59              |
| 38:DR:81:ASP:O     | 38:DR:82:GLU:HB2   | 2.02                     | 0.59              |
| 50:D3:13:ILE:HG22  | 50:D3:13:ILE:O     | 2.01                     | 0.59              |
| 53:D6:36:LEU:HD13  | 53:D6:50:ARG:HH12  | 1.66                     | 0.59              |
| 5:AE:39:GLY:HA2    | 5:AE:71:LEU:CD1    | 2.32                     | 0.59              |
| 20:AT:87:LYS:HE3   | 20:AT:91:LEU:HD11  | 1.84                     | 0.59              |
| 22:AV:15:G:N1      | 22:AV:49:C:C5      | 2.56                     | 0.59              |
| 25:BA:1140:C:OP2   | 34:BN:66:LYS:NZ    | 2.31                     | 0.59              |
| 25:BA:1678:G:N2    | 25:BA:1989:G:H22   | 2.00                     | 0.59              |
| 25:BA:2503:A:C4'   | 25:BA:2504:U:OP1   | 2.46                     | 0.59              |
| 25:BA:2753:A:O2'   | 56:B9:15:LYS:NZ    | 2.35                     | 0.59              |
| 29:BE:174:ASP:O    | 29:BE:183:LEU:HB2  | 2.01                     | 0.59              |
| 34:BN:16:ILE:HG23  | 34:BN:54:VAL:HG22  | 1.83                     | 0.59              |
| 34:BN:62:VAL:HG22  | 34:BN:66:LYS:CB    | 2.32                     | 0.59              |
| 1:CA:562:C:O2'     | 12:CL:15:ARG:HB3   | 2.02                     | 0.59              |
| 3:CC:155:GLY:O     | 3:CC:156:ARG:HB2   | 2.01                     | 0.59              |
| 4:CD:119:GLN:HG2   | 4:CD:123:HIS:CD2   | 2.37                     | 0.59              |
| 5:CE:41:VAL:CG2    | 5:CE:113:ALA:HA    | 2.33                     | 0.59              |
| 9:CI:19:LEU:HD23   | 9:CI:61:ALA:HA     | 1.83                     | 0.59              |
| 13:CM:3:ARG:CB     | 51:D4:34:GLU:HG2   | 2.32                     | 0.59              |
| 13:CM:82:MET:HE3   | 13:CM:92:HIS:HB3   | 1.84                     | 0.59              |
| 20:CT:56:MET:CG    | 20:CT:84:LEU:CD1   | 2.55                     | 0.59              |
| 25:DA:1139:G:O2'   | 25:DA:1143:A:N1    | 2.32                     | 0.59              |
| 26:DB:15:A:H1'     | 26:DB:110:G:C5     | 2.36                     | 0.59              |
| 28:DD:112:GLN:HB2  | 28:DD:115:GLN:HE21 | 1.67                     | 0.59              |
| 28:DD:118:VAL:HG22 | 28:DD:119:ALA:N    | 2.17                     | 0.59              |
| 30:DF:102:PRO:O    | 30:DF:106:ARG:HG2  | 2.01                     | 0.59              |
| 32:DH:19:VAL:HG12  | 32:DH:20:ALA:H     | 1.64                     | 0.59              |
| 32:DH:98:LEU:HD22  | 32:DH:125:VAL:HG23 | 1.83                     | 0.59              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 44:DX:63:LYS:CE   | 44:DX:72:LYS:HE3   | 2.26                     | 0.59              |
| 45:DY:47:LYS:HA   | 45:DY:60:PHE:HD1   | 1.67                     | 0.59              |
| 46:DZ:154:ASP:C   | 46:DZ:155:LEU:HD12 | 2.26                     | 0.59              |
| 50:D3:4:LEU:HD12  | 50:D3:39:ASP:OD1   | 2.03                     | 0.59              |
| 52:D5:37:LYS:HG3  | 52:D5:38:ALA:N     | 2.17                     | 0.59              |
| 53:D6:35:GLU:HB3  | 53:D6:51:GLU:CG    | 2.30                     | 0.59              |
| 1:AA:1065:U:OP2   | 1:AA:1190:G:N2     | 2.35                     | 0.59              |
| 5:AE:81:GLU:HG2   | 5:AE:90:VAL:CG1    | 2.32                     | 0.59              |
| 7:AG:41:ARG:C     | 7:AG:45:ASP:HB2    | 2.27                     | 0.59              |
| 9:AI:114:TYR:N    | 9:AI:114:TYR:CD2   | 2.67                     | 0.59              |
| 13:AM:35:GLU:HG3  | 13:AM:36:LYS:H     | 1.65                     | 0.59              |
| 20:AT:81:LYS:O    | 20:AT:85:MET:N     | 2.30                     | 0.59              |
| 25:BA:668:G:C5    | 25:BA:670:A:N7     | 2.71                     | 0.59              |
| 25:BA:832:G:N2    | 36:BP:53:GLY:HA3   | 2.16                     | 0.59              |
| 25:BA:1187:G:H5'' | 42:BV:81:TYR:CE2   | 2.38                     | 0.59              |
| 25:BA:2712:U:HO2' | 25:BA:2712(A):A:P  | 2.25                     | 0.59              |
| 28:BD:245:PRO:HB2 | 28:BD:246:PRO:HD2  | 1.83                     | 0.59              |
| 29:BE:101:ARG:NH2 | 29:BE:171:GLU:HB2  | 2.16                     | 0.59              |
| 31:BG:43:LEU:CD2  | 31:BG:88:ILE:HD11  | 2.32                     | 0.59              |
| 39:BS:53:SER:OG   | 39:BS:54:LEU:N     | 2.23                     | 0.59              |
| 42:BV:39:LEU:HA   | 42:BV:47:VAL:HG11  | 1.83                     | 0.59              |
| 45:BY:15:VAL:HG11 | 45:BY:20:TYR:O     | 2.02                     | 0.59              |
| 48:B1:3:LYS:HG3   | 48:B1:4:VAL:N      | 2.16                     | 0.59              |
| 1:CA:1054:C:OP2   | 1:CA:1054:C:H4'    | 2.01                     | 0.59              |
| 8:CH:21:LYS:O     | 8:CH:63:LEU:HD23   | 2.01                     | 0.59              |
| 10:CJ:54:PHE:CE1  | 10:CJ:55:LYS:HE3   | 2.37                     | 0.59              |
| 12:CL:62:SER:O    | 12:CL:64:TYR:HD1   | 1.84                     | 0.59              |
| 28:DD:26:LYS:HD2  | 28:DD:113:VAL:HG11 | 1.84                     | 0.59              |
| 31:DG:67:LYS:O    | 31:DG:67:LYS:HD2   | 2.02                     | 0.59              |
| 38:DR:9:LYS:HG2   | 38:DR:9:LYS:O      | 2.02                     | 0.59              |
| 1:AA:59:A:H3'     | 1:AA:331:G:H22     | 1.68                     | 0.59              |
| 6:AF:60:PHE:CZ    | 18:AR:78:LEU:HD21  | 2.37                     | 0.59              |
| 12:AL:6:THR:H     | 12:AL:9:GLN:HE21   | 1.49                     | 0.59              |
| 18:AR:50:ILE:HD11 | 18:AR:70:ILE:HG21  | 1.82                     | 0.59              |
| 20:AT:93:GLU:HG2  | 20:AT:93:GLU:O     | 2.01                     | 0.59              |
| 23:AW:16:U:H3'    | 23:AW:17:C:C5'     | 2.32                     | 0.59              |
| 25:BA:226:G:HO2'  | 25:BA:227:A:H8     | 1.49                     | 0.59              |
| 25:BA:2343:C:H2'  | 25:BA:2343:C:O2    | 2.02                     | 0.59              |
| 25:BA:2414:G:H21  | 36:BP:67:MET:HE1   | 1.65                     | 0.59              |
| 34:BN:99:LEU:O    | 34:BN:103:VAL:HG23 | 2.03                     | 0.59              |
| 37:BQ:16:ARG:HG2  | 37:BQ:18:LYS:CD    | 2.32                     | 0.59              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 38:BR:104:ARG:HH11 | 38:BR:104:ARG:HB2  | 1.66                     | 0.59              |
| 39:BS:17:ARG:HA    | 39:BS:20:ARG:NH1   | 2.17                     | 0.59              |
| 43:BW:83:LYS:O     | 43:BW:84:ARG:HD3   | 2.02                     | 0.59              |
| 44:BX:30:VAL:HG23  | 44:BX:31:HIS:O     | 2.02                     | 0.59              |
| 45:BY:14:LEU:CG    | 45:BY:15:VAL:N     | 2.65                     | 0.59              |
| 53:B6:19:ARG:HG2   | 53:B6:20:ASN:H     | 1.67                     | 0.59              |
| 1:CA:49:U:C4       | 1:CA:364:A:N6      | 2.71                     | 0.59              |
| 1:CA:624:C:H2'     | 1:CA:625:G:C8      | 2.36                     | 0.59              |
| 1:CA:686:U:H5'     | 1:CA:686:U:H6      | 1.68                     | 0.59              |
| 2:CB:88:ALA:HB2    | 2:CB:219:VAL:HG13  | 1.84                     | 0.59              |
| 2:CB:109:SER:HA    | 2:CB:112:VAL:HG23  | 1.84                     | 0.59              |
| 3:CC:101:LEU:HD23  | 3:CC:102:ASN:O     | 2.01                     | 0.59              |
| 9:CI:26:VAL:HG13   | 9:CI:61:ALA:HB3    | 1.84                     | 0.59              |
| 22:CV:3:C:N4       | 22:CV:71:G:H1      | 1.99                     | 0.59              |
| 25:DA:443:A:C5     | 30:DF:45:ARG:HD2   | 2.37                     | 0.59              |
| 25:DA:532:A:OP1    | 25:DA:561:G:N2     | 2.34                     | 0.59              |
| 25:DA:2347:C:H4'   | 53:D6:39:TYR:HE1   | 1.66                     | 0.59              |
| 25:DA:2477:C:C4    | 56:D9:4:ARG:NH1    | 2.71                     | 0.59              |
| 30:DF:9:ILE:HD12   | 30:DF:123:LEU:CD2  | 2.32                     | 0.59              |
| 30:DF:155:LEU:CD1  | 30:DF:174:VAL:HG22 | 2.33                     | 0.59              |
| 31:DG:38:VAL:HG22  | 31:DG:93:THR:HG23  | 1.84                     | 0.59              |
| 32:DH:42:ARG:HH11  | 32:DH:42:ARG:HG2   | 1.67                     | 0.59              |
| 40:DT:93:ARG:NH1   | 40:DT:93:ARG:HG3   | 2.18                     | 0.59              |
| 41:DU:92:ARG:CZ    | 42:DV:11:GLN:CB    | 2.69                     | 0.59              |
| 42:DV:41:GLY:N     | 42:DV:46:VAL:HG13  | 2.17                     | 0.59              |
| 45:DY:81:LYS:NZ    | 45:DY:98:VAL:HG11  | 2.17                     | 0.59              |
| 20:AT:89:ARG:NH2   | 20:AT:104:LEU:HD21 | 2.18                     | 0.59              |
| 22:AV:56:U:C4      | 22:AV:58:A:OP2     | 2.56                     | 0.59              |
| 25:BA:8:A:H2'      | 25:BA:9:U:H6       | 1.67                     | 0.59              |
| 29:BE:3:GLY:O      | 29:BE:4:ILE:HB     | 2.00                     | 0.59              |
| 29:BE:86:PRO:O     | 29:BE:88:GLY:N     | 2.35                     | 0.59              |
| 31:BG:141:PHE:O    | 31:BG:144:ILE:CG2  | 2.50                     | 0.59              |
| 34:BN:62:VAL:CG2   | 34:BN:66:LYS:CB    | 2.80                     | 0.59              |
| 35:BO:7:TYR:C      | 35:BO:8:LEU:HD22   | 2.27                     | 0.59              |
| 35:BO:7:TYR:OH     | 35:BO:44:LYS:HD2   | 2.02                     | 0.59              |
| 40:BT:35:LYS:O     | 40:BT:37:GLY:N     | 2.35                     | 0.59              |
| 40:BT:80:SER:CB    | 40:BT:81:PRO:HD3   | 2.31                     | 0.59              |
| 42:BV:38:LEU:O     | 42:BV:39:LEU:HD13  | 2.03                     | 0.59              |
| 55:B8:5:LYS:O      | 55:B8:61:LEU:HD11  | 2.03                     | 0.59              |
| 55:B8:6:THR:HB     | 55:B8:63:PRO:HG3   | 1.83                     | 0.59              |
| 1:CA:1491:G:N7     | 58:CA:1741:PAR:O53 | 2.34                     | 0.59              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 5:CE:16:THR:O      | 5:CE:17:ALA:HB2   | 2.01                     | 0.59              |
| 5:CE:146:ALA:HB1   | 5:CE:150:ARG:HH22 | 1.67                     | 0.59              |
| 13:CM:90:LEU:C     | 13:CM:90:LEU:HD12 | 2.26                     | 0.59              |
| 20:CT:45:GLN:C     | 20:CT:47:GLY:H    | 2.11                     | 0.59              |
| 25:DA:458:G:H1'    | 25:DA:459:U:H5    | 1.66                     | 0.59              |
| 27:DC:78:ALA:CB    | 27:DC:82:LYS:HB2  | 2.33                     | 0.59              |
| 27:DC:100:ILE:HG22 | 27:DC:101:GLN:HG3 | 1.85                     | 0.59              |
| 31:DG:161:THR:HG22 | 31:DG:162:THR:N   | 2.17                     | 0.59              |
| 33:DI:2:LYS:HB3    | 33:DI:20:ASP:HB3  | 1.83                     | 0.59              |
| 36:DP:55:ARG:O     | 36:DP:56:SER:C    | 2.45                     | 0.59              |
| 38:DR:45:ARG:HG3   | 38:DR:46:GLY:N    | 2.16                     | 0.59              |
| 51:D4:36:CYS:SG    | 51:D4:37:SER:N    | 2.75                     | 0.59              |
| 53:D6:41:PRO:HD3   | 53:D6:46:HIS:CA   | 2.33                     | 0.59              |
| 1:AA:575:G:H4'     | 1:AA:576:G:O5'    | 2.01                     | 0.59              |
| 1:AA:1291:G:H4'    | 9:AI:39:GLY:HA3   | 1.85                     | 0.59              |
| 1:AA:1378:C:O2     | 7:AG:76:ARG:NH2   | 2.35                     | 0.59              |
| 6:AF:6:VAL:HG13    | 6:AF:90:VAL:HG22  | 1.84                     | 0.59              |
| 10:AJ:78:ASN:OD1   | 10:AJ:80:LYS:HB2  | 2.03                     | 0.59              |
| 11:AK:33:THR:OG1   | 11:AK:37:GLY:HA2  | 2.02                     | 0.59              |
| 19:AS:9:VAL:CG1    | 19:AS:11:VAL:HG11 | 2.17                     | 0.59              |
| 25:BA:50:U:H4'     | 25:BA:51:G:OP2    | 2.03                     | 0.59              |
| 25:BA:997:G:OP1    | 41:BU:93:LYS:HD3  | 2.03                     | 0.59              |
| 25:BA:2406:U:H5''  | 25:BA:2408:U:OP2  | 2.03                     | 0.59              |
| 25:BA:2866:U:C4'   | 25:BA:2867:G:OP1  | 2.49                     | 0.59              |
| 29:BE:31:CYS:HB3   | 29:BE:49:LEU:HB3  | 1.84                     | 0.59              |
| 31:BG:76:SER:C     | 31:BG:77:ILE:HD13 | 2.28                     | 0.59              |
| 32:BH:156:ALA:HB3  | 32:BH:159:GLU:HB3 | 1.85                     | 0.59              |
| 34:BN:58:ASP:O     | 34:BN:60:ILE:N    | 2.36                     | 0.59              |
| 35:BO:104:ARG:CZ   | 35:BO:104:ARG:HB3 | 2.32                     | 0.59              |
| 39:BS:56:LEU:O     | 39:BS:57:LYS:HB2  | 2.01                     | 0.59              |
| 40:BT:55:ASN:N     | 40:BT:59:THR:HB   | 2.17                     | 0.59              |
| 1:CA:1101:A:H4'    | 1:CA:1102:A:O5'   | 2.02                     | 0.59              |
| 1:CA:1286:A:H2'    | 1:CA:1287:A:C4'   | 2.31                     | 0.59              |
| 4:CD:92:VAL:HG12   | 4:CD:96:LEU:HD11  | 1.83                     | 0.59              |
| 8:CH:83:ILE:HG13   | 8:CH:137:VAL:HG22 | 1.84                     | 0.59              |
| 17:CQ:76:LEU:HD11  | 17:CQ:78:GLU:O    | 2.01                     | 0.59              |
| 18:CR:43:PHE:O     | 18:CR:44:LEU:HD23 | 2.03                     | 0.59              |
| 19:CS:16:LEU:O     | 19:CS:17:GLU:C    | 2.45                     | 0.59              |
| 25:DA:84:A:C5'     | 45:DY:8:LYS:CD    | 2.81                     | 0.59              |
| 25:DA:1929:G:H4'   | 25:DA:1930:G:OP1  | 2.03                     | 0.59              |
| 25:DA:2287:A:OP1   | 53:D6:31:PRO:HG2  | 2.02                     | 0.59              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:DA:2505:G:O2'   | 25:DA:2506:U:H5'   | 2.03                     | 0.59              |
| 25:DA:2725:A:N6    | 25:DA:2727:G:C4    | 2.71                     | 0.59              |
| 27:DC:41:VAL:HG23  | 27:DC:178:ALA:HB3  | 1.84                     | 0.59              |
| 31:DG:10:LYS:O     | 31:DG:15:VAL:HG23  | 2.02                     | 0.59              |
| 34:DN:67:LEU:HD12  | 34:DN:67:LEU:N     | 2.17                     | 0.59              |
| 44:DX:35:THR:HB    | 44:DX:38:GLU:H     | 1.67                     | 0.59              |
| 47:D0:3:HIS:ND1    | 47:D0:3:HIS:N      | 2.51                     | 0.59              |
| 47:D0:49:LYS:H     | 47:D0:80:HIS:HB3   | 1.67                     | 0.59              |
| 1:AA:1095:U:OP1    | 1:AA:1108:G:N2     | 2.35                     | 0.59              |
| 4:AD:30:LYS:HA     | 4:AD:35:ARG:HD2    | 1.84                     | 0.59              |
| 4:AD:187:ARG:HH11  | 4:AD:187:ARG:HG2   | 1.67                     | 0.59              |
| 23:AW:43:C:C2'     | 23:AW:44:G:H5'     | 2.33                     | 0.59              |
| 25:BA:2563:U:O2'   | 35:BO:28:SER:HB3   | 2.02                     | 0.59              |
| 28:BD:44:ASN:HB3   | 28:BD:49:ILE:CA    | 2.26                     | 0.59              |
| 28:BD:147:LEU:HD13 | 28:BD:155:LEU:HD11 | 1.83                     | 0.59              |
| 38:BR:45:ARG:HG3   | 38:BR:46:GLY:H     | 1.68                     | 0.59              |
| 40:BT:31:SER:HB3   | 40:BT:43:GLN:N     | 2.18                     | 0.59              |
| 45:BY:54:LYS:O     | 45:BY:54:LYS:HG2   | 2.01                     | 0.59              |
| 45:BY:66:PRO:O     | 45:BY:67:LEU:CD2   | 2.50                     | 0.59              |
| 47:B0:49:LYS:O     | 47:B0:50:ASN:HB2   | 2.02                     | 0.59              |
| 1:CA:243:A:N6      | 1:CA:246:A:H62     | 2.00                     | 0.59              |
| 2:CB:18:GLY:HA2    | 2:CB:42:ILE:HG22   | 1.85                     | 0.59              |
| 11:CK:92:GLU:HG3   | 11:CK:96:ARG:HD3   | 1.83                     | 0.59              |
| 16:CP:2:VAL:HG22   | 16:CP:64:ALA:CB    | 2.33                     | 0.59              |
| 21:CU:5:ASP:HB3    | 21:CU:8:THR:CG2    | 2.33                     | 0.59              |
| 22:CV:54:G:O2'     | 22:CV:55:U:P       | 2.60                     | 0.59              |
| 23:CW:34:G:C5      | 24:CX:14:A:N6      | 2.71                     | 0.59              |
| 25:DA:593:G:H1'    | 55:D8:4:MET:HE1    | 1.84                     | 0.59              |
| 25:DA:614(A):U:O2' | 25:DA:614(B):G:P   | 2.61                     | 0.59              |
| 25:DA:1012:U:O4    | 34:DN:28:THR:HG21  | 2.03                     | 0.59              |
| 28:DD:45:ASN:CG    | 28:DD:46:GLN:N     | 2.59                     | 0.59              |
| 29:DE:184:VAL:HG12 | 29:DE:185:LYS:H    | 1.67                     | 0.59              |
| 30:DF:126:VAL:O    | 30:DF:195:ASP:HA   | 2.03                     | 0.59              |
| 32:DH:24:VAL:O     | 32:DH:24:VAL:HG23  | 2.02                     | 0.59              |
| 32:DH:152:ARG:HE   | 32:DH:153:LYS:HE3  | 1.65                     | 0.59              |
| 53:D6:16:CYS:SG    | 53:D6:47:THR:CG2   | 2.91                     | 0.59              |
| 1:AA:242:C:C2'     | 1:AA:243:A:O5'     | 2.51                     | 0.59              |
| 1:AA:538:G:P       | 12:AL:115:LYS:HG3  | 2.43                     | 0.59              |
| 1:AA:1279:A:P      | 1:AA:1279:A:C2     | 2.96                     | 0.59              |
| 3:AC:66:VAL:HG12   | 3:AC:66:VAL:O      | 2.03                     | 0.59              |
| 5:AE:11:ILE:HD12   | 5:AE:31:LEU:CD1    | 2.32                     | 0.59              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 7:AG:113:GLU:HG3   | 7:AG:119:ARG:HG2  | 1.84                     | 0.59              |
| 9:AI:18:PHE:HB2    | 9:AI:62:TYR:HB3   | 1.84                     | 0.59              |
| 22:AV:53:G:O2'     | 22:AV:54:G:C5'    | 2.50                     | 0.59              |
| 25:BA:331:A:N6     | 25:BA:1210:A:OP2  | 2.36                     | 0.59              |
| 25:BA:805:G:H5'    | 25:BA:806:C:H5    | 1.66                     | 0.59              |
| 25:BA:2447:G:C4    | 25:BA:2501:C:C4   | 2.91                     | 0.59              |
| 25:BA:2520:C:O5'   | 25:BA:2520:C:H6   | 1.86                     | 0.59              |
| 28:BD:53:PHE:CE2   | 28:BD:220:HIS:CD2 | 2.90                     | 0.59              |
| 29:BE:12:THR:O     | 29:BE:23:VAL:HG22 | 2.02                     | 0.59              |
| 37:BQ:47:ILE:HG22  | 37:BQ:48:GLU:N    | 2.17                     | 0.59              |
| 38:BR:81:ASP:O     | 38:BR:82:GLU:HB2  | 2.02                     | 0.59              |
| 52:B5:56:LYS:HG3   | 52:B5:59:GLU:HG3  | 1.84                     | 0.59              |
| 1:CA:1211:U:H4'    | 1:CA:1212:U:OP1   | 2.02                     | 0.59              |
| 2:CB:57:PHE:O      | 2:CB:61:LEU:HB3   | 2.03                     | 0.59              |
| 6:CF:52:ILE:O      | 6:CF:53:ALA:HB3   | 2.03                     | 0.59              |
| 6:CF:70:ASP:N      | 6:CF:70:ASP:OD1   | 2.34                     | 0.59              |
| 13:CM:3:ARG:NE     | 13:CM:7:VAL:HG13  | 2.17                     | 0.59              |
| 13:CM:12:ASN:HA    | 13:CM:46:LYS:HB2  | 1.85                     | 0.59              |
| 16:CP:19:ILE:HB    | 16:CP:37:GLY:C    | 2.28                     | 0.59              |
| 25:DA:301:G:OP1    | 25:DA:301:G:H4'   | 2.03                     | 0.59              |
| 25:DA:800:A:H4'    | 25:DA:801:G:O5'   | 2.03                     | 0.59              |
| 25:DA:914:C:H2'    | 25:DA:915:C:O5'   | 2.03                     | 0.59              |
| 25:DA:1648:C:N4    | 25:DA:2010:G:N1   | 2.50                     | 0.59              |
| 25:DA:2285:C:OP2   | 53:D6:27:LYS:HD2  | 2.01                     | 0.59              |
| 25:DA:2751:G:H8    | 25:DA:2751:G:P    | 2.25                     | 0.59              |
| 26:DB:66:A:C6      | 26:DB:108:U:C2    | 2.91                     | 0.59              |
| 28:DD:101:GLU:OE1  | 28:DD:103:ARG:HD3 | 2.02                     | 0.59              |
| 28:DD:145:VAL:HG12 | 28:DD:146:GLU:O   | 2.03                     | 0.59              |
| 29:DE:137:HIS:HB3  | 29:DE:138:PRO:HD2 | 1.84                     | 0.59              |
| 33:DI:3:VAL:O      | 33:DI:18:VAL:HA   | 2.03                     | 0.59              |
| 33:DI:57:ARG:HB2   | 33:DI:57:ARG:HH11 | 1.68                     | 0.59              |
| 40:DT:93:ARG:HG3   | 40:DT:93:ARG:HH11 | 1.68                     | 0.59              |
| 44:DX:63:LYS:HB3   | 44:DX:72:LYS:HG3  | 1.84                     | 0.59              |
| 1:AA:1199:U:H4'    | 10:AJ:54:PHE:CE2  | 2.37                     | 0.59              |
| 1:AA:1301:U:O4     | 1:AA:1303:C:H1'   | 2.03                     | 0.59              |
| 15:AO:82:ILE:O     | 15:AO:82:ILE:HD13 | 2.02                     | 0.59              |
| 15:AO:87:ILE:HG22  | 15:AO:88:ARG:N    | 2.17                     | 0.59              |
| 18:AR:82:THR:O     | 18:AR:83:GLU:HG2  | 2.03                     | 0.59              |
| 25:BA:1963:U:O2'   | 25:BA:1964:G:OP1  | 2.20                     | 0.59              |
| 28:BD:11:PRO:C     | 28:BD:13:ARG:N    | 2.61                     | 0.59              |
| 29:BE:46:ALA:HA    | 29:BE:82:ARG:O    | 2.03                     | 0.59              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 30:BF:7:TYR:CE2    | 30:BF:10:PRO:HG3   | 2.37                     | 0.59              |
| 31:BG:106:LEU:HA   | 31:BG:110:ALA:HB3  | 1.84                     | 0.59              |
| 32:BH:107:VAL:O    | 32:BH:109:PHE:CD1  | 2.55                     | 0.59              |
| 34:BN:133:GLN:C    | 34:BN:134:ARG:HG3  | 2.27                     | 0.59              |
| 37:BQ:103:MET:HE1  | 37:BQ:125:LEU:HD13 | 1.85                     | 0.59              |
| 41:BU:98:LEU:O     | 41:BU:101:ARG:O    | 2.21                     | 0.59              |
| 45:BY:17:SER:HA    | 45:BY:71:LYS:HD2   | 1.85                     | 0.59              |
| 46:BZ:3:TYR:N      | 46:BZ:3:TYR:HD1    | 1.99                     | 0.59              |
| 10:CJ:16:LEU:HD13  | 10:CJ:70:ARG:HD2   | 1.83                     | 0.59              |
| 11:CK:21:ILE:CB    | 11:CK:30:VAL:HG12  | 2.32                     | 0.59              |
| 12:CL:25:PRO:O     | 12:CL:27:LEU:HD22  | 2.03                     | 0.59              |
| 18:CR:85:LEU:HD12  | 18:CR:86:VAL:N     | 2.17                     | 0.59              |
| 20:CT:24:LEU:HD22  | 20:CT:24:LEU:C     | 2.28                     | 0.59              |
| 25:DA:2056:G:N2    | 52:D5:4:HIS:O      | 2.36                     | 0.59              |
| 25:DA:2172:U:H4'   | 25:DA:2173:A:OP2   | 1.99                     | 0.59              |
| 26:DB:109:C:OP2    | 26:DB:109:C:H6     | 1.84                     | 0.59              |
| 31:DG:34:LEU:HD13  | 31:DG:34:LEU:O     | 2.03                     | 0.59              |
| 35:DO:53:LYS:N     | 35:DO:53:LYS:HD2   | 2.18                     | 0.59              |
| 39:DS:83:LYS:HG2   | 39:DS:109:GLY:N    | 2.17                     | 0.59              |
| 41:DU:92:ARG:HG3   | 42:DV:11:GLN:OE1   | 2.02                     | 0.59              |
| 41:DU:95:LEU:CD1   | 42:DV:4:ILE:HG23   | 2.31                     | 0.59              |
| 44:DX:30:VAL:HG21  | 44:DX:39:ILE:HD11  | 1.84                     | 0.59              |
| 50:D3:15:TYR:O     | 50:D3:20:LYS:HE2   | 2.03                     | 0.59              |
| 51:D4:20:ASN:HD22  | 51:D4:21:VAL:H     | 1.48                     | 0.59              |
| 1:AA:301:G:H2'     | 1:AA:302:G:H8      | 1.68                     | 0.59              |
| 2:AB:204:ASN:HD21  | 2:AB:206:ASP:H     | 1.49                     | 0.59              |
| 4:AD:2:GLY:O       | 4:AD:4:TYR:N       | 2.36                     | 0.59              |
| 9:AI:95:LYS:HD3    | 9:AI:96:LEU:H      | 1.68                     | 0.59              |
| 9:AI:95:LYS:HZ3    | 9:AI:96:LEU:HD13   | 1.68                     | 0.59              |
| 12:AL:104:VAL:HG12 | 12:AL:105:TYR:CD1  | 2.38                     | 0.59              |
| 14:AN:59:ALA:O     | 14:AN:60:SER:HB2   | 2.02                     | 0.59              |
| 15:AO:74:ASP:OD2   | 15:AO:77:ARG:HG2   | 2.02                     | 0.59              |
| 25:BA:71:A:H62     | 25:BA:114:U:H1'    | 1.68                     | 0.59              |
| 25:BA:2078:C:C2    | 25:BA:2079:U:C5    | 2.91                     | 0.59              |
| 26:BB:14:U:C4'     | 26:BB:15:A:OP2     | 2.48                     | 0.59              |
| 28:BD:6:PHE:HE1    | 28:BD:18:VAL:HG22  | 1.68                     | 0.59              |
| 28:BD:267:SER:HA   | 28:BD:270:ILE:HD11 | 1.85                     | 0.59              |
| 29:BE:132:HIS:CD2  | 29:BE:135:HIS:HE1  | 2.20                     | 0.59              |
| 31:BG:113:ARG:NH1  | 51:B4:60:GLU:HB2   | 2.18                     | 0.59              |
| 32:BH:97:ARG:O     | 32:BH:125:VAL:HG21 | 2.03                     | 0.59              |
| 32:BH:109:PHE:CD1  | 32:BH:109:PHE:N    | 2.71                     | 0.59              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 34:BN:40:PRO:HG3   | 41:BU:68:ALA:HB2   | 1.83                     | 0.59              |
| 40:BT:30:VAL:CG2   | 40:BT:84:GLN:CD    | 2.76                     | 0.59              |
| 48:B1:34:THR:HG22  | 48:B1:34:THR:O     | 2.02                     | 0.59              |
| 51:B4:44:CYS:SG    | 51:B4:64:LYS:HB2   | 2.43                     | 0.59              |
| 1:CA:66:G:H4'      | 1:CA:173:U:C4      | 2.38                     | 0.59              |
| 4:CD:206:PHE:CE2   | 4:CD:207:TYR:HE2   | 2.21                     | 0.59              |
| 5:CE:26:PHE:N      | 5:CE:26:PHE:CD1    | 2.70                     | 0.59              |
| 8:CH:74:PRO:O      | 8:CH:75:ARG:C      | 2.46                     | 0.59              |
| 10:CJ:5:ARG:HD2    | 10:CJ:71:LEU:HD11  | 1.83                     | 0.59              |
| 15:CO:15:PHE:CE2   | 15:CO:84:LYS:HD2   | 2.38                     | 0.59              |
| 16:CP:70:ALA:O     | 16:CP:74:LEU:HD12  | 2.02                     | 0.59              |
| 20:CT:29:LYS:CD    | 20:CT:66:ALA:HA    | 2.33                     | 0.59              |
| 20:CT:53:LEU:N     | 20:CT:53:LEU:CD1   | 2.63                     | 0.59              |
| 29:DE:26:ILE:HG22  | 29:DE:27:LEU:N     | 2.18                     | 0.59              |
| 32:DH:60:ARG:HH11  | 32:DH:60:ARG:HG2   | 1.68                     | 0.59              |
| 33:DI:52:ARG:HH11  | 33:DI:52:ARG:CB    | 2.15                     | 0.59              |
| 33:DI:57:ARG:HA    | 33:DI:60:GLU:HB3   | 1.84                     | 0.59              |
| 33:DI:95:LYS:CA    | 33:DI:111:PRO:HG3  | 2.27                     | 0.59              |
| 33:DI:142:VAL:O    | 33:DI:142:VAL:HG23 | 2.03                     | 0.59              |
| 35:DO:50:GLY:C     | 35:DO:52:VAL:H     | 2.09                     | 0.59              |
| 40:DT:89:VAL:CG1   | 40:DT:91:ARG:NE    | 2.65                     | 0.59              |
| 41:DU:61:TRP:CH2   | 41:DU:94:ASN:HB2   | 2.37                     | 0.59              |
| 42:DV:49:THR:OG1   | 42:DV:50:PRO:CD    | 2.51                     | 0.59              |
| 2:AB:83:MET:HE2    | 2:AB:83:MET:HA     | 1.85                     | 0.58              |
| 2:AB:103:THR:OG1   | 2:AB:176:GLU:HG3   | 2.03                     | 0.58              |
| 3:AC:14:ILE:HG12   | 3:AC:15:THR:N      | 2.15                     | 0.58              |
| 3:AC:172:ARG:O     | 3:AC:173:VAL:CG2   | 2.51                     | 0.58              |
| 11:AK:12:ARG:HG2   | 11:AK:13:GLN:N     | 2.18                     | 0.58              |
| 11:AK:84:VAL:HG11  | 11:AK:95:ILE:HD11  | 1.84                     | 0.58              |
| 28:BD:43:ARG:NH1   | 28:BD:44:ASN:ND2   | 2.50                     | 0.58              |
| 30:BF:132:VAL:HG22 | 30:BF:133:ASN:H    | 1.67                     | 0.58              |
| 36:BP:21:ARG:O     | 36:BP:28:GLY:HA2   | 2.03                     | 0.58              |
| 39:BS:106:ARG:HD2  | 39:BS:106:ARG:C    | 2.28                     | 0.58              |
| 40:BT:55:ASN:H     | 40:BT:59:THR:HB    | 1.67                     | 0.58              |
| 43:BW:9:TYR:N      | 43:BW:9:TYR:CD2    | 2.68                     | 0.58              |
| 45:BY:84:ARG:HH12  | 45:BY:97:ARG:HD2   | 1.68                     | 0.58              |
| 45:BY:99:CYS:O     | 45:BY:100:ALA:HB2  | 2.03                     | 0.58              |
| 46:BZ:61:LEU:HB2   | 46:BZ:65:GLN:HB2   | 1.84                     | 0.58              |
| 49:B2:5:GLU:O      | 49:B2:8:LYS:HB2    | 2.01                     | 0.58              |
| 52:B5:57:VAL:HG23  | 52:B5:58:LEU:H     | 1.68                     | 0.58              |
| 53:B6:10:LEU:CD1   | 55:B8:34:TRP:CD1   | 2.85                     | 0.58              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:329:A:H4'     | 1:CA:330:C:OP1     | 2.02                     | 0.58              |
| 1:CA:686:U:O2'     | 1:CA:687:A:H5''    | 2.02                     | 0.58              |
| 1:CA:872:A:H2'     | 1:CA:872:A:N3      | 2.18                     | 0.58              |
| 1:CA:877:C:H5''    | 8:CH:88:LYS:HD3    | 1.85                     | 0.58              |
| 4:CD:162:LEU:HD13  | 4:CD:181:MET:HG2   | 1.85                     | 0.58              |
| 7:CG:27:ILE:HD12   | 7:CG:40:ALA:HA     | 1.84                     | 0.58              |
| 13:CM:116:THR:CG2  | 13:CM:117:VAL:H    | 2.15                     | 0.58              |
| 25:DA:83:G:N2      | 25:DA:84:A:N6      | 2.51                     | 0.58              |
| 28:DD:33:LEU:O     | 28:DD:35:LYS:HG2   | 2.03                     | 0.58              |
| 37:DQ:51:ARG:HH11  | 37:DQ:51:ARG:HG2   | 1.65                     | 0.58              |
| 38:DR:1:MET:O      | 38:DR:2:ARG:HB2    | 2.02                     | 0.58              |
| 39:DS:107:GLU:H    | 39:DS:110:LEU:HD12 | 1.64                     | 0.58              |
| 44:DX:35:THR:O     | 44:DX:39:ILE:HG12  | 2.03                     | 0.58              |
| 48:D1:83:GLU:CD    | 48:D1:83:GLU:N     | 2.61                     | 0.58              |
| 52:D5:20:ARG:HA    | 52:D5:23:HIS:ND1   | 2.18                     | 0.58              |
| 1:AA:243:A:H4'     | 1:AA:244:U:C5'     | 2.32                     | 0.58              |
| 1:AA:406:G:H21     | 4:AD:119:GLN:HE22  | 1.51                     | 0.58              |
| 1:AA:792:A:C5      | 1:AA:794:A:N6      | 2.71                     | 0.58              |
| 6:AF:45:LEU:O      | 6:AF:46:ARG:HG3    | 2.03                     | 0.58              |
| 12:AL:18:VAL:O     | 12:AL:19:ARG:HB3   | 2.01                     | 0.58              |
| 12:AL:38:THR:HG23  | 12:AL:57:LYS:O     | 2.03                     | 0.58              |
| 25:BA:890:A:N6     | 25:BA:892:G:O6     | 2.36                     | 0.58              |
| 27:BC:41:VAL:O     | 27:BC:178:ALA:HB3  | 2.03                     | 0.58              |
| 28:BD:105:ILE:HD12 | 28:BD:106:ILE:H    | 1.68                     | 0.58              |
| 29:BE:110:GLY:O    | 38:BR:2:ARG:NE     | 2.37                     | 0.58              |
| 31:BG:107:LEU:HD23 | 31:BG:111:LEU:HD12 | 1.84                     | 0.58              |
| 31:BG:152:LEU:HG   | 31:BG:153:ARG:N    | 2.18                     | 0.58              |
| 36:BP:75:ILE:H     | 36:BP:75:ILE:CD1   | 1.82                     | 0.58              |
| 41:BU:106:PHE:O    | 41:BU:109:LEU:HB2  | 2.02                     | 0.58              |
| 43:BW:18:ARG:NH1   | 43:BW:76:VAL:O     | 2.35                     | 0.58              |
| 5:CE:33:VAL:HG22   | 5:CE:43:LEU:HD13   | 1.85                     | 0.58              |
| 9:CI:4:TYR:N       | 9:CI:4:TYR:HD1     | 2.00                     | 0.58              |
| 17:CQ:5:VAL:HG13   | 17:CQ:59:ILE:O     | 2.03                     | 0.58              |
| 30:DF:184:TYR:CE2  | 30:DF:188:ARG:HD2  | 2.38                     | 0.58              |
| 33:DI:17:GLN:O     | 33:DI:18:VAL:HB    | 2.02                     | 0.58              |
| 42:DV:43:GLU:OE2   | 42:DV:43:GLU:HA    | 2.03                     | 0.58              |
| 1:AA:952:U:H5'     | 1:AA:972:C:H41     | 1.68                     | 0.58              |
| 3:AC:14:ILE:O      | 3:AC:15:THR:C      | 2.45                     | 0.58              |
| 11:AK:124:LYS:HB3  | 11:AK:125:PHE:CD1  | 2.38                     | 0.58              |
| 11:AK:126:ARG:C    | 11:AK:128:ALA:H    | 2.12                     | 0.58              |
| 17:AQ:53:LEU:HG    | 17:AQ:82:MET:HE1   | 1.84                     | 0.58              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 17:AQ:74:LEU:HD13 | 17:AQ:75:ARG:HG2   | 1.85                     | 0.58              |
| 20:AT:30:LYS:HD2  | 20:AT:34:LYS:HE3   | 1.85                     | 0.58              |
| 25:BA:1024:G:H3'  | 25:BA:1025:G:H5''  | 1.84                     | 0.58              |
| 25:BA:1966:A:H2'  | 25:BA:2592:G:O2'   | 2.02                     | 0.58              |
| 40:BT:48:ILE:HG22 | 40:BT:49:VAL:O     | 2.04                     | 0.58              |
| 49:B2:3:LEU:O     | 49:B2:3:LEU:HD23   | 2.04                     | 0.58              |
| 50:B3:13:ILE:HG22 | 50:B3:13:ILE:O     | 2.01                     | 0.58              |
| 2:CB:118:LEU:HB2  | 2:CB:142:LEU:HD13  | 1.86                     | 0.58              |
| 9:CI:58:HIS:CB    | 9:CI:59:PHE:HE1    | 2.14                     | 0.58              |
| 25:DA:1212:G:O2'  | 25:DA:1236:G:N2    | 2.36                     | 0.58              |
| 25:DA:1722:A:C2   | 25:DA:1740:G:H2'   | 2.38                     | 0.58              |
| 25:DA:2789:C:H1'  | 25:DA:2892:A:H2    | 1.67                     | 0.58              |
| 28:DD:27:THR:CG2  | 28:DD:83:GLU:HG2   | 2.34                     | 0.58              |
| 28:DD:27:THR:HG21 | 28:DD:83:GLU:HG2   | 1.85                     | 0.58              |
| 30:DF:195:ASP:O   | 30:DF:197:ASP:O    | 2.21                     | 0.58              |
| 30:DF:197:ASP:O   | 30:DF:198:ALA:HB3  | 2.03                     | 0.58              |
| 33:DI:11:ASN:O    | 33:DI:12:LEU:CB    | 2.51                     | 0.58              |
| 45:DY:94:LYS:CE   | 45:DY:101:LYS:HZ3  | 2.16                     | 0.58              |
| 1:AA:247:G:OP2    | 17:AQ:100:LYS:N    | 2.37                     | 0.58              |
| 1:AA:985:C:H2'    | 1:AA:986:A:H8      | 1.67                     | 0.58              |
| 3:AC:52:LEU:H     | 3:AC:52:LEU:HD23   | 1.68                     | 0.58              |
| 11:AK:32:ILE:CD1  | 11:AK:72:ALA:HB2   | 2.33                     | 0.58              |
| 11:AK:111:ASP:OD2 | 18:AR:84:LYS:HE3   | 2.04                     | 0.58              |
| 12:AL:11:VAL:HG12 | 12:AL:12:ARG:N     | 2.18                     | 0.58              |
| 16:AP:70:ALA:O    | 16:AP:74:LEU:HD12  | 2.03                     | 0.58              |
| 25:BA:434:U:H2'   | 25:BA:436:C:N4     | 2.18                     | 0.58              |
| 25:BA:1434:A:H61  | 25:BA:1558:A:N6    | 2.02                     | 0.58              |
| 28:BD:53:PHE:CD2  | 28:BD:220:HIS:CD2  | 2.92                     | 0.58              |
| 28:BD:125:ILE:N   | 28:BD:125:ILE:HD13 | 2.19                     | 0.58              |
| 30:BF:46:ARG:CG   | 30:BF:46:ARG:NH1   | 2.66                     | 0.58              |
| 30:BF:177:ALA:HB1 | 30:BF:178:PRO:HD2  | 1.86                     | 0.58              |
| 36:BP:86:LYS:HG3  | 36:BP:87:ASP:N     | 2.17                     | 0.58              |
| 39:BS:89:ARG:HD3  | 39:BS:92:TYR:CA    | 2.33                     | 0.58              |
| 40:BT:67:SER:O    | 40:BT:68:TYR:HB2   | 2.03                     | 0.58              |
| 45:BY:28:LYS:HB2  | 45:BY:37:VAL:HB    | 0.69                     | 0.58              |
| 46:BZ:143:GLY:C   | 46:BZ:144:LEU:HD22 | 2.29                     | 0.58              |
| 1:CA:61:G:C6      | 1:CA:107:G:C2      | 2.90                     | 0.58              |
| 1:CA:1295:G:O2'   | 13:CM:14:ARG:NH1   | 2.36                     | 0.58              |
| 5:CE:53:LEU:H     | 5:CE:53:LEU:HD12   | 1.69                     | 0.58              |
| 17:CQ:78:GLU:OE1  | 17:CQ:81:ARG:HD2   | 2.02                     | 0.58              |
| 25:DA:271(D):G:H1 | 25:DA:271(T):C:H42 | 1.51                     | 0.58              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:DA:1819:A:OP1   | 28:DD:158:ALA:HB2  | 2.02                     | 0.58              |
| 32:DH:109:PHE:C    | 32:DH:111:HIS:N    | 2.62                     | 0.58              |
| 34:DN:103:VAL:O    | 34:DN:104:LYS:C    | 2.46                     | 0.58              |
| 36:DP:29:LYS:HD2   | 36:DP:30:THR:HG23  | 1.84                     | 0.58              |
| 39:DS:108:GLY:O    | 39:DS:110:LEU:N    | 2.36                     | 0.58              |
| 46:DZ:25:PRO:HA    | 46:DZ:38:TYR:HB2   | 1.86                     | 0.58              |
| 1:AA:242:C:H2'     | 1:AA:243:A:O5'     | 2.03                     | 0.58              |
| 1:AA:448:A:P       | 1:AA:485:G:H22     | 2.26                     | 0.58              |
| 1:AA:872:A:O2'     | 1:AA:873:A:H3'     | 2.04                     | 0.58              |
| 1:AA:992:U:O2'     | 1:AA:993:G:H5''    | 2.03                     | 0.58              |
| 2:AB:28:PHE:CE2    | 2:AB:31:TYR:HB2    | 2.39                     | 0.58              |
| 7:AG:71:PRO:O      | 7:AG:91:VAL:HG21   | 2.04                     | 0.58              |
| 7:AG:156:TRP:OXT   | 7:AG:156:TRP:CG    | 2.56                     | 0.58              |
| 14:AN:26:ARG:HG3   | 14:AN:27:CYS:N     | 2.19                     | 0.58              |
| 20:AT:43:LEU:CB    | 20:AT:52:ALA:HB2   | 2.33                     | 0.58              |
| 25:BA:560:C:H5'    | 41:BU:52:ARG:HH22  | 1.67                     | 0.58              |
| 29:BE:103:ASP:OD1  | 29:BE:201:THR:HA   | 2.03                     | 0.58              |
| 31:BG:10:LYS:O     | 31:BG:15:VAL:HG23  | 2.04                     | 0.58              |
| 32:BH:125:VAL:HG22 | 32:BH:131:VAL:HG22 | 1.85                     | 0.58              |
| 34:BN:14:VAL:HG13  | 34:BN:137:LYS:CG   | 2.27                     | 0.58              |
| 34:BN:32:THR:O     | 34:BN:35:ARG:O     | 2.21                     | 0.58              |
| 39:BS:61:ASN:O     | 39:BS:62:LYS:HG2   | 2.03                     | 0.58              |
| 45:BY:67:LEU:CD1   | 45:BY:71:LYS:HB2   | 2.32                     | 0.58              |
| 1:CA:15:G:H4'      | 5:CE:24:ARG:HH12   | 1.69                     | 0.58              |
| 1:CA:243:A:N6      | 1:CA:246:A:N6      | 2.51                     | 0.58              |
| 1:CA:344:A:H4'     | 1:CA:345:C:OP1     | 2.04                     | 0.58              |
| 1:CA:818:G:O2'     | 1:CA:820:U:O4      | 2.22                     | 0.58              |
| 2:CB:168:THR:HG23  | 2:CB:192:SER:OG    | 2.04                     | 0.58              |
| 3:CC:58:GLU:N      | 3:CC:65:ALA:HB3    | 2.15                     | 0.58              |
| 5:CE:43:LEU:N      | 5:CE:136:MET:HE2   | 2.18                     | 0.58              |
| 9:CI:43:ALA:HA     | 9:CI:74:ILE:HD13   | 1.84                     | 0.58              |
| 10:CJ:30:SER:HB2   | 10:CJ:81:THR:N     | 2.18                     | 0.58              |
| 19:CS:53:ASN:OD1   | 19:CS:55:LYS:N     | 2.34                     | 0.58              |
| 22:CV:3:C:H2'      | 22:CV:3:C:O2       | 2.03                     | 0.58              |
| 25:DA:1707:G:H1    | 25:DA:1751:C:H42   | 1.49                     | 0.58              |
| 25:DA:2311:A:H1'   | 31:DG:82:LEU:CD1   | 2.33                     | 0.58              |
| 28:DD:129:ASN:O    | 28:DD:193:VAL:HG12 | 2.03                     | 0.58              |
| 32:DH:106:THR:HG22 | 32:DH:112:PRO:CB   | 2.30                     | 0.58              |
| 38:DR:2:ARG:HA     | 38:DR:5:LYS:HD2    | 1.84                     | 0.58              |
| 40:DT:113:LYS:O    | 40:DT:114:LEU:HD23 | 2.03                     | 0.58              |
| 43:DW:88:ARG:HB2   | 43:DW:92:ARG:HB3   | 1.85                     | 0.58              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 50:D3:35:ARG:HH11  | 50:D3:35:ARG:HG3   | 1.69                     | 0.58              |
| 56:D9:24:TYR:O     | 56:D9:25:VAL:HG23  | 2.03                     | 0.58              |
| 1:AA:1226:C:HO2'   | 1:AA:1227:A:H5'    | 1.67                     | 0.58              |
| 1:AA:1363(A):A:H4' | 1:AA:1364:U:O5'    | 2.02                     | 0.58              |
| 2:AB:48:MET:HA     | 2:AB:51:LEU:HD12   | 1.86                     | 0.58              |
| 2:AB:96:ARG:HD2    | 2:AB:96:ARG:N      | 2.16                     | 0.58              |
| 8:AH:104:ARG:CZ    | 8:AH:138:TRP:CH2   | 2.87                     | 0.58              |
| 12:AL:69:TYR:HE2   | 12:AL:71:PRO:HA    | 1.68                     | 0.58              |
| 19:AS:9:VAL:CG1    | 19:AS:9:VAL:O      | 2.51                     | 0.58              |
| 25:BA:84:A:N1      | 25:BA:98:G:O2'     | 2.29                     | 0.58              |
| 27:BC:196:LEU:C    | 27:BC:198:ALA:N    | 2.54                     | 0.58              |
| 30:BF:66:PRO:O     | 30:BF:67:GLN:HG2   | 2.02                     | 0.58              |
| 31:BG:39:ILE:HB    | 31:BG:157:ILE:HG22 | 1.83                     | 0.58              |
| 31:BG:129:GLY:O    | 31:BG:161:THR:HB   | 2.03                     | 0.58              |
| 35:BO:24:VAL:HG22  | 35:BO:24:VAL:O     | 2.02                     | 0.58              |
| 38:BR:9:LYS:O      | 38:BR:10:LEU:HG    | 2.02                     | 0.58              |
| 40:BT:28:VAL:CG2   | 40:BT:46:GLU:HA    | 2.33                     | 0.58              |
| 40:BT:128:GLU:C    | 40:BT:128:GLU:OE1  | 2.47                     | 0.58              |
| 53:B6:12:GLU:HB2   | 53:B6:23:THR:N     | 2.15                     | 0.58              |
| 1:CA:429:U:HO2'    | 1:CA:430:A:P       | 2.24                     | 0.58              |
| 1:CA:1492:A:N6     | 1:CA:1493:A:H61    | 2.02                     | 0.58              |
| 4:CD:31:CYS:O      | 4:CD:31:CYS:SG     | 2.62                     | 0.58              |
| 8:CH:44:PHE:O      | 8:CH:45:ILE:HG23   | 2.04                     | 0.58              |
| 9:CI:8:GLY:HA2     | 9:CI:79:LEU:HD12   | 1.85                     | 0.58              |
| 12:CL:22:SER:C     | 12:CL:24:VAL:H     | 2.12                     | 0.58              |
| 13:CM:14:ARG:N     | 13:CM:44:ARG:HD2   | 2.19                     | 0.58              |
| 14:CN:27:CYS:SG    | 14:CN:29:ARG:HB2   | 2.43                     | 0.58              |
| 17:CQ:21:VAL:HG11  | 17:CQ:59:ILE:HD11  | 1.84                     | 0.58              |
| 25:DA:592:G:N3     | 55:D8:4:MET:HE2    | 2.19                     | 0.58              |
| 25:DA:767:U:H2'    | 25:DA:768:G:H8     | 1.68                     | 0.58              |
| 25:DA:1342:A:C6    | 25:DA:1397:U:C5    | 2.91                     | 0.58              |
| 25:DA:2092:U:H4'   | 25:DA:2093:G:O5'   | 2.04                     | 0.58              |
| 29:DE:116:VAL:CG2  | 29:DE:122:PHE:CG   | 2.87                     | 0.58              |
| 30:DF:63:LYS:HE2   | 30:DF:67:GLN:HB3   | 1.86                     | 0.58              |
| 33:DI:47:LEU:HA    | 33:DI:50:ARG:HD3   | 1.86                     | 0.58              |
| 36:DP:59:LEU:CA    | 36:DP:61:ARG:CZ    | 2.66                     | 0.58              |
| 37:DQ:66:ILE:HG22  | 37:DQ:104:PHE:CE2  | 2.39                     | 0.58              |
| 41:DU:15:LYS:O     | 41:DU:19:LYS:HG3   | 2.04                     | 0.58              |
| 42:DV:45:THR:HG22  | 42:DV:45:THR:O     | 2.02                     | 0.58              |
| 47:D0:40:GLN:HE21  | 47:D0:43:THR:HA    | 1.67                     | 0.58              |
| 1:AA:76:C:N4       | 1:AA:93:G:H1       | 2.01                     | 0.58              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AA:839:U:O2     | 1:AA:839:U:C2'     | 2.50                     | 0.58              |
| 1:AA:1405:G:OP2   | 58:AA:7111:PAR:O34 | 2.21                     | 0.58              |
| 2:AB:150:SER:O    | 2:AB:153:ARG:HG3   | 2.03                     | 0.58              |
| 3:AC:15:THR:HG22  | 3:AC:16:ARG:N      | 2.18                     | 0.58              |
| 4:AD:108:LEU:HB3  | 4:AD:110:PHE:CE1   | 2.38                     | 0.58              |
| 6:AF:58:GLY:O     | 6:AF:60:PHE:CD1    | 2.56                     | 0.58              |
| 8:AH:33:GLU:O     | 8:AH:34:GLU:C      | 2.46                     | 0.58              |
| 8:AH:39:LEU:O     | 8:AH:44:PHE:HB2    | 2.03                     | 0.58              |
| 9:AI:15:ALA:CB    | 9:AI:65:VAL:HG23   | 2.30                     | 0.58              |
| 13:AM:86:CYS:O    | 13:AM:89:GLY:N     | 2.35                     | 0.58              |
| 14:AN:24:CYS:HB3  | 14:AN:27:CYS:O     | 2.03                     | 0.58              |
| 18:AR:65:ILE:O    | 18:AR:69:THR:HG23  | 2.03                     | 0.58              |
| 25:BA:17:G:H4'    | 41:BU:25:TRP:CH2   | 2.39                     | 0.58              |
| 25:BA:49:A:H1'    | 25:BA:51:G:C4      | 2.39                     | 0.58              |
| 25:BA:2426:A:H4'  | 25:BA:2427:C:OP2   | 2.02                     | 0.58              |
| 28:BD:268:ARG:H   | 28:BD:270:ILE:HD11 | 1.68                     | 0.58              |
| 40:BT:31:SER:CB   | 40:BT:43:GLN:N     | 2.64                     | 0.58              |
| 42:BV:39:LEU:O    | 42:BV:40:LEU:HB2   | 2.03                     | 0.58              |
| 44:BX:84:ALA:HB3  | 44:BX:87:GLN:OE1   | 2.04                     | 0.58              |
| 45:BY:67:LEU:CG   | 45:BY:68:HIS:N     | 2.63                     | 0.58              |
| 2:CB:72:GLY:HA2   | 2:CB:165:VAL:HG22  | 1.86                     | 0.58              |
| 9:CI:48:GLU:N     | 9:CI:49:PRO:HD2    | 2.19                     | 0.58              |
| 13:CM:50:GLU:O    | 13:CM:54:VAL:HG23  | 2.02                     | 0.58              |
| 19:CS:45:VAL:HA   | 19:CS:62:ILE:HG23  | 1.86                     | 0.58              |
| 22:CV:20:G:H3'    | 22:CV:21:U:C2      | 2.38                     | 0.58              |
| 25:DA:9272:G:H5'  | 25:DA:9273:G:OP2   | 2.04                     | 0.58              |
| 25:DA:483:A:H4'   | 45:DY:49:VAL:CA    | 2.31                     | 0.58              |
| 25:DA:819:A:N6    | 25:DA:1189:A:H1'   | 2.18                     | 0.58              |
| 25:DA:1251:C:O2'  | 25:DA:1252:G:H3'   | 2.03                     | 0.58              |
| 25:DA:2646:C:OP2  | 25:DA:2732:G:O2'   | 2.20                     | 0.58              |
| 30:DF:128:ALA:C   | 30:DF:129:PHE:CD2  | 2.81                     | 0.58              |
| 31:DG:109:VAL:C   | 31:DG:112:PRO:HD2  | 2.28                     | 0.58              |
| 42:DV:37:VAL:O    | 42:DV:37:VAL:HG23  | 2.03                     | 0.58              |
| 44:DX:31:HIS:ND1  | 44:DX:32:PRO:HD2   | 2.18                     | 0.58              |
| 45:DY:50:ARG:HB3  | 45:DY:53:PRO:CD    | 2.32                     | 0.58              |
| 52:D5:56:LYS:HB3  | 52:D5:56:LYS:NZ    | 2.18                     | 0.58              |
| 1:AA:1225:A:O2'   | 19:AS:78:ARG:HD3   | 2.03                     | 0.58              |
| 2:AB:75:LYS:O     | 2:AB:75:LYS:CD     | 2.47                     | 0.58              |
| 3:AC:44:GLU:HA    | 3:AC:52:LEU:HD11   | 1.86                     | 0.58              |
| 3:AC:116:VAL:HG21 | 3:AC:202:ILE:HD11  | 1.85                     | 0.58              |
| 4:AD:8:VAL:CG1    | 4:AD:21:LEU:HD13   | 2.34                     | 0.58              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:AH:18:ARG:HA     | 8:AH:78:GLN:HE22   | 1.68                     | 0.58              |
| 9:AI:48:GLU:N      | 9:AI:49:PRO:CD     | 2.65                     | 0.58              |
| 10:AJ:8:LEU:CD1    | 10:AJ:20:ALA:HA    | 2.33                     | 0.58              |
| 14:AN:23:ARG:O     | 14:AN:23:ARG:HG3   | 2.04                     | 0.58              |
| 15:AO:61:GLY:O     | 15:AO:65:ARG:HD3   | 2.04                     | 0.58              |
| 15:AO:65:ARG:HH11  | 15:AO:65:ARG:CG    | 2.16                     | 0.58              |
| 22:AV:16:C:O2'     | 22:AV:62:C:OP1     | 2.22                     | 0.58              |
| 25:BA:1541:G:O6    | 25:BA:1542:A:N6    | 2.37                     | 0.58              |
| 26:BB:52:A:N6      | 39:BS:33:LYS:HE2   | 2.19                     | 0.58              |
| 29:BE:173:VAL:HG12 | 29:BE:174:ASP:H    | 1.68                     | 0.58              |
| 31:BG:39:ILE:HD13  | 31:BG:157:ILE:CG2  | 2.33                     | 0.58              |
| 31:BG:64:THR:HG23  | 31:BG:65:GLY:N     | 2.18                     | 0.58              |
| 31:BG:128:ARG:C    | 31:BG:130:ASN:N    | 2.59                     | 0.58              |
| 31:BG:133:LEU:HG   | 31:BG:157:ILE:HG13 | 1.85                     | 0.58              |
| 32:BH:158:HIS:HE2  | 32:BH:170:ARG:C    | 2.11                     | 0.58              |
| 36:BP:85:LEU:CA    | 36:BP:88:LEU:HB3   | 2.32                     | 0.58              |
| 43:BW:60:ASN:O     | 43:BW:61:ASN:ND2   | 2.36                     | 0.58              |
| 49:B2:70:GLN:HG2   | 49:B2:71:ASN:N     | 2.18                     | 0.58              |
| 1:CA:1157:A:H1'    | 1:CA:1181:G:N2     | 2.18                     | 0.58              |
| 9:CI:9:ARG:HG2     | 9:CI:104:ARG:NH1   | 2.18                     | 0.58              |
| 12:CL:27:LEU:HG    | 12:CL:62:SER:HB2   | 1.85                     | 0.58              |
| 16:CP:53:VAL:O     | 16:CP:57:ARG:HG2   | 2.04                     | 0.58              |
| 20:CT:13:LEU:O     | 20:CT:16:HIS:HB3   | 2.03                     | 0.58              |
| 25:DA:483:A:C4'    | 45:DY:49:VAL:HG13  | 2.33                     | 0.58              |
| 25:DA:579:G:O2'    | 25:DA:2019:A:OP1   | 2.22                     | 0.58              |
| 25:DA:708:C:H42    | 25:DA:723:G:H1     | 1.52                     | 0.58              |
| 31:DG:106:LEU:HA   | 31:DG:110:ALA:HB3  | 1.85                     | 0.58              |
| 33:DI:1:MET:HE3    | 33:DI:26:ALA:HB3   | 1.85                     | 0.58              |
| 40:DT:65:LYS:NZ    | 40:DT:66:VAL:N     | 2.48                     | 0.58              |
| 41:DU:83:LEU:CD1   | 41:DU:113:ALA:HB2  | 2.33                     | 0.58              |
| 45:DY:54:LYS:O     | 45:DY:55:TYR:HB2   | 2.02                     | 0.58              |
| 46:DZ:18:LEU:HB3   | 46:DZ:23:LYS:HB2   | 1.84                     | 0.58              |
| 46:DZ:39:VAL:HG21  | 46:DZ:44:PHE:CD2   | 2.38                     | 0.58              |
| 47:D0:60:PHE:CD1   | 47:D0:60:PHE:C     | 2.81                     | 0.58              |
| 1:AA:652:U:H1'     | 1:AA:653:A:H2      | 1.69                     | 0.58              |
| 1:AA:802:A:H3'     | 1:AA:803:G:H8      | 1.68                     | 0.58              |
| 1:AA:1224:G:C6     | 1:AA:1322:C:H1'    | 2.38                     | 0.58              |
| 5:AE:105:VAL:HG12  | 5:AE:106:PRO:HD3   | 1.84                     | 0.58              |
| 6:AF:91:VAL:HG13   | 18:AR:72:ARG:NH1   | 2.19                     | 0.58              |
| 8:AH:35:ILE:HG23   | 8:AH:111:ILE:HD13  | 1.86                     | 0.58              |
| 9:AI:25:LYS:O      | 9:AI:25:LYS:HG3    | 2.02                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 12:AL:30:ALA:O    | 12:AL:31:PRO:C    | 2.47                     | 0.58              |
| 13:AM:8:GLU:OE2   | 13:AM:22:ILE:HA   | 2.04                     | 0.58              |
| 18:AR:82:THR:C    | 18:AR:83:GLU:HG2  | 2.28                     | 0.58              |
| 20:AT:64:ASP:O    | 20:AT:67:ALA:HB3  | 2.04                     | 0.58              |
| 22:AV:64:G:C2     | 22:AV:65:G:C8     | 2.91                     | 0.58              |
| 25:BA:221:A:C4    | 25:BA:266:G:N7    | 2.72                     | 0.58              |
| 25:BA:684:G:O2'   | 25:BA:788:A:N7    | 2.37                     | 0.58              |
| 25:BA:2330:G:H4'  | 47:B0:44:ARG:HH12 | 1.68                     | 0.58              |
| 25:BA:2680:C:H5'  | 29:BE:189:PRO:HA  | 1.85                     | 0.58              |
| 26:BB:66:A:N6     | 26:BB:108:U:C6    | 2.72                     | 0.58              |
| 29:BE:201:THR:OG1 | 29:BE:202:LYS:N   | 2.37                     | 0.58              |
| 30:BF:199:TRP:CZ3 | 30:BF:203:GLN:HG2 | 2.39                     | 0.58              |
| 31:BG:148:MET:HA  | 31:BG:148:MET:HE3 | 1.86                     | 0.58              |
| 33:BI:110:ASP:N   | 33:BI:130:TYR:OH  | 2.33                     | 0.58              |
| 44:BX:55:ASN:HB2  | 44:BX:80:ILE:CD1  | 2.33                     | 0.58              |
| 45:BY:67:LEU:HG   | 45:BY:68:HIS:N    | 2.19                     | 0.58              |
| 1:CA:274:A:O2'    | 1:CA:275:G:C5'    | 2.51                     | 0.58              |
| 1:CA:1223:C:P     | 19:CS:78:ARG:HH21 | 2.27                     | 0.58              |
| 3:CC:116:VAL:O    | 3:CC:119:ARG:HB3  | 2.04                     | 0.58              |
| 6:CF:44:GLY:HA2   | 6:CF:59:TYR:CE2   | 2.38                     | 0.58              |
| 10:CJ:24:VAL:O    | 10:CJ:28:ARG:HG3  | 2.03                     | 0.58              |
| 10:CJ:82:ILE:HD12 | 10:CJ:86:MET:HE1  | 1.86                     | 0.58              |
| 13:CM:97:PRO:HA   | 13:CM:110:ARG:HD3 | 1.84                     | 0.58              |
| 20:CT:51:GLU:O    | 20:CT:52:ALA:C    | 2.47                     | 0.58              |
| 22:CV:42:C:H2'    | 22:CV:43:G:O5'    | 2.04                     | 0.58              |
| 25:DA:1721:G:N1   | 25:DA:1739:U:OP2  | 2.37                     | 0.58              |
| 25:DA:2134:A:N6   | 25:DA:2157:G:H1'  | 2.19                     | 0.58              |
| 29:DE:63:LEU:HD23 | 29:DE:65:GLY:N    | 2.19                     | 0.58              |
| 29:DE:161:GLY:O   | 29:DE:162:ALA:C   | 2.46                     | 0.58              |
| 32:DH:92:ILE:HD12 | 32:DH:92:ILE:N    | 2.13                     | 0.58              |
| 33:DI:21:VAL:HG21 | 33:DI:25:TYR:CD1  | 2.39                     | 0.58              |
| 37:DQ:85:LYS:HG3  | 47:D0:7:LEU:HD13  | 1.85                     | 0.58              |
| 39:DS:110:LEU:O   | 39:DS:112:PHE:CD1 | 2.57                     | 0.58              |
| 42:DV:81:TYR:C    | 42:DV:82:ARG:HG3  | 2.27                     | 0.58              |
| 49:D2:63:VAL:O    | 49:D2:66:GLU:HG2  | 2.04                     | 0.58              |
| 50:D3:4:LEU:HD21  | 50:D3:56:VAL:CG1  | 2.33                     | 0.58              |
| 1:AA:972:C:O2'    | 1:AA:973:G:H5'    | 2.04                     | 0.58              |
| 1:AA:1206:G:H4'   | 3:AC:192:THR:O    | 2.03                     | 0.58              |
| 2:AB:96:ARG:HH12  | 2:AB:147:LYS:HE2  | 1.69                     | 0.58              |
| 5:AE:43:LEU:HD12  | 5:AE:44:GLY:H     | 1.69                     | 0.58              |
| 7:AG:14:PRO:CD    | 7:AG:21:VAL:HG12  | 2.34                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:AH:35:ILE:HG22  | 8:AH:39:LEU:HD21  | 1.86                     | 0.58              |
| 25:BA:94(A):G:H21 | 49:B2:47:ASN:HD22 | 1.51                     | 0.58              |
| 25:BA:994:C:H3'   | 41:BU:54:LYS:HE3  | 1.86                     | 0.58              |
| 25:BA:1827:C:O4'  | 25:BA:1970:A:O2'  | 2.22                     | 0.58              |
| 25:BA:2503:A:H5'  | 25:BA:2503:A:N3   | 2.18                     | 0.58              |
| 28:BD:45:ASN:CG   | 28:BD:46:GLN:N    | 2.59                     | 0.58              |
| 28:BD:69:ARG:HH22 | 28:BD:192:THR:CB  | 2.17                     | 0.58              |
| 31:BG:115:ARG:NH1 | 31:BG:136:ARG:HD3 | 2.18                     | 0.58              |
| 33:BI:88:ILE:HG12 | 33:BI:122:GLU:H   | 1.69                     | 0.58              |
| 34:BN:46:VAL:O    | 34:BN:47:ALA:CB   | 2.51                     | 0.58              |
| 36:BP:107:LYS:C   | 36:BP:109:GLY:H   | 2.12                     | 0.58              |
| 37:BQ:27:VAL:HG23 | 37:BQ:137:TYR:CE1 | 2.39                     | 0.58              |
| 37:BQ:78:PRO:HB2  | 37:BQ:81:VAL:HG11 | 1.86                     | 0.58              |
| 45:BY:20:TYR:HE1  | 45:BY:42:VAL:HA   | 1.69                     | 0.58              |
| 1:CA:250:A:O2'    | 1:CA:251:G:P      | 2.62                     | 0.58              |
| 1:CA:547:A:H4'    | 1:CA:548:G:O5'    | 2.04                     | 0.58              |
| 1:CA:925:G:O2'    | 1:CA:927:G:OP1    | 2.21                     | 0.58              |
| 1:CA:979:C:H42    | 14:CN:18:VAL:HG12 | 1.69                     | 0.58              |
| 2:CB:114:ARG:NH1  | 2:CB:118:LEU:HD21 | 2.19                     | 0.58              |
| 13:CM:11:ARG:HH11 | 13:CM:11:ARG:HB3  | 1.69                     | 0.58              |
| 14:CN:24:CYS:HB2  | 14:CN:40:CYS:HB3  | 1.85                     | 0.58              |
| 15:CO:25:THR:O    | 15:CO:28:GLN:N    | 2.36                     | 0.58              |
| 20:CT:75:ASN:O    | 20:CT:79:ARG:N    | 2.36                     | 0.58              |
| 25:DA:614:U:O2    | 25:DA:614:U:C5'   | 2.51                     | 0.58              |
| 25:DA:1542:A:O2'  | 25:DA:1543:C:O5'  | 2.22                     | 0.58              |
| 25:DA:2377:A:H4'  | 39:DS:112:PHE:HA  | 1.86                     | 0.58              |
| 25:DA:2879:C:H5'  | 25:DA:2880:C:OP1  | 2.04                     | 0.58              |
| 28:DD:16:MET:HG3  | 28:DD:206:LEU:O   | 2.04                     | 0.58              |
| 28:DD:210:GLY:O   | 28:DD:211:ARG:HB3 | 2.02                     | 0.58              |
| 34:DN:43:THR:HB   | 34:DN:46:VAL:HG12 | 1.86                     | 0.58              |
| 37:DQ:55:VAL:O    | 37:DQ:59:ARG:HA   | 2.03                     | 0.58              |
| 40:DT:128:GLU:OE1 | 40:DT:128:GLU:C   | 2.47                     | 0.58              |
| 41:DU:79:PHE:CE2  | 41:DU:83:LEU:CD2  | 2.86                     | 0.58              |
| 44:DX:12:VAL:HG22 | 44:DX:17:ALA:CB   | 2.33                     | 0.58              |
| 46:DZ:57:ILE:HG22 | 46:DZ:58:VAL:N    | 2.18                     | 0.58              |
| 52:D5:48:GLU:HA   | 52:D5:57:VAL:HG22 | 1.86                     | 0.58              |
| 1:AA:241:C:C2'    | 1:AA:242:C:H5'    | 2.33                     | 0.57              |
| 1:AA:243:A:C6     | 1:AA:281:G:N3     | 2.72                     | 0.57              |
| 1:AA:533:A:C4'    | 1:AA:534:U:OP1    | 2.52                     | 0.57              |
| 1:AA:1301:U:O2'   | 1:AA:1302:U:OP1   | 2.22                     | 0.57              |
| 5:AE:138:ALA:O    | 5:AE:141:GLN:HB2  | 2.03                     | 0.57              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:AV:3:C:C2'      | 22:AV:4:G:H5'      | 2.33                     | 0.57              |
| 25:BA:181:A:N1     | 25:BA:435:C:C5     | 2.72                     | 0.57              |
| 25:BA:574:C:N4     | 25:BA:2034:U:OP2   | 2.36                     | 0.57              |
| 25:BA:2526:G:H21   | 56:B9:2:LYS:HG3    | 1.67                     | 0.57              |
| 28:BD:201:HIS:O    | 28:BD:203:ASN:N    | 2.36                     | 0.57              |
| 29:BE:176:ILE:HG22 | 29:BE:179:GLU:H    | 1.67                     | 0.57              |
| 41:BU:83:LEU:HG    | 41:BU:88:ILE:HG13  | 1.84                     | 0.57              |
| 46:BZ:53:ILE:HG23  | 46:BZ:71:VAL:HB    | 1.86                     | 0.57              |
| 46:BZ:116:VAL:O    | 46:BZ:175:VAL:HG22 | 2.04                     | 0.57              |
| 48:B1:52:ARG:NH2   | 48:B1:53:VAL:HA    | 2.19                     | 0.57              |
| 1:CA:46:G:H2'      | 1:CA:366:C:N4      | 2.19                     | 0.57              |
| 1:CA:751:U:H2'     | 1:CA:752:G:H5'     | 1.85                     | 0.57              |
| 5:CE:12:LEU:HD22   | 5:CE:13:ILE:N      | 2.18                     | 0.57              |
| 5:CE:53:LEU:O      | 5:CE:54:ALA:C      | 2.47                     | 0.57              |
| 6:CF:1:MET:HE1     | 6:CF:66:GLU:O      | 2.03                     | 0.57              |
| 8:CH:97:VAL:HG23   | 8:CH:129:VAL:O     | 2.03                     | 0.57              |
| 13:CM:66:LEU:O     | 13:CM:67:GLU:C     | 2.47                     | 0.57              |
| 20:CT:40:ALA:CA    | 20:CT:55:ILE:HG21  | 2.34                     | 0.57              |
| 25:DA:265:A:C8     | 25:DA:266:G:H1'    | 2.39                     | 0.57              |
| 25:DA:2001:A:C5'   | 25:DA:2689:U:H2'   | 2.34                     | 0.57              |
| 28:DD:145:VAL:HB   | 28:DD:155:LEU:HB2  | 1.85                     | 0.57              |
| 37:DQ:34:LEU:HD11  | 37:DQ:129:THR:CB   | 2.33                     | 0.57              |
| 39:DS:89:ARG:O     | 39:DS:89:ARG:HG3   | 2.04                     | 0.57              |
| 46:DZ:151:HIS:CB   | 46:DZ:170:THR:HA   | 2.33                     | 0.57              |
| 1:AA:652:U:H1'     | 1:AA:653:A:C2      | 2.39                     | 0.57              |
| 13:AM:102:ARG:HH11 | 13:AM:102:ARG:HG3  | 1.67                     | 0.57              |
| 13:AM:108:ARG:HG3  | 13:AM:108:ARG:NH1  | 2.09                     | 0.57              |
| 25:BA:1721:G:OP2   | 25:BA:1721:G:N2    | 2.30                     | 0.57              |
| 28:BD:33:LEU:O     | 28:BD:34:VAL:C     | 2.47                     | 0.57              |
| 31:BG:47:LYS:N     | 31:BG:51:ARG:HG3   | 2.19                     | 0.57              |
| 36:BP:124:LYS:HZ3  | 36:BP:143:GLY:HA3  | 1.69                     | 0.57              |
| 41:BU:92:ARG:HD2   | 42:BV:11:GLN:NE2   | 2.18                     | 0.57              |
| 1:CA:129(A):G:H5'' | 1:CA:130:A:OP1     | 2.04                     | 0.57              |
| 3:CC:20:SER:CB     | 3:CC:40:ARG:HH22   | 2.09                     | 0.57              |
| 5:CE:76:ILE:CD1    | 5:CE:142:LEU:HD21  | 2.32                     | 0.57              |
| 7:CG:115:ARG:O     | 7:CG:116:ALA:C     | 2.47                     | 0.57              |
| 8:CH:84:ARG:O      | 8:CH:135:CYS:HB2   | 2.04                     | 0.57              |
| 8:CH:119:LEU:HD12  | 8:CH:124:ALA:HA    | 1.86                     | 0.57              |
| 9:CI:58:HIS:C      | 9:CI:59:PHE:CD1    | 2.82                     | 0.57              |
| 12:CL:84:LEU:HG    | 12:CL:105:TYR:CE1  | 2.36                     | 0.57              |
| 17:CQ:88:TYR:C     | 17:CQ:88:TYR:CD2   | 2.82                     | 0.57              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:CW:3:C:H2'      | 23:CW:4:C:C6       | 2.39                     | 0.57              |
| 23:CY:37:A:O2'     | 25:DA:1913:A:N1    | 2.37                     | 0.57              |
| 25:DA:215:G:H4'    | 25:DA:216:A:O5'    | 2.02                     | 0.57              |
| 25:DA:483:A:C4'    | 45:DY:49:VAL:HA    | 2.34                     | 0.57              |
| 26:DB:13:A:O2'     | 26:DB:14:U:H5'     | 2.04                     | 0.57              |
| 33:DI:38:LEU:H     | 33:DI:38:LEU:CD1   | 2.04                     | 0.57              |
| 33:DI:144:VAL:HG22 | 33:DI:145:VAL:N    | 2.18                     | 0.57              |
| 36:DP:86:LYS:HG3   | 36:DP:87:ASP:N     | 2.17                     | 0.57              |
| 38:DR:77:ARG:O     | 38:DR:79:LEU:N     | 2.37                     | 0.57              |
| 40:DT:35:LYS:O     | 40:DT:36:GLU:HB3   | 2.05                     | 0.57              |
| 42:DV:41:GLY:H     | 42:DV:46:VAL:HG13  | 1.69                     | 0.57              |
| 52:D5:35:GLU:O     | 52:D5:36:CYS:HB2   | 2.04                     | 0.57              |
| 1:AA:47:C:H4'      | 1:AA:48:C:O5'      | 2.04                     | 0.57              |
| 10:AJ:94:VAL:CG1   | 10:AJ:95:GLU:N     | 2.67                     | 0.57              |
| 11:AK:126:ARG:C    | 11:AK:128:ALA:N    | 2.59                     | 0.57              |
| 13:AM:40:ASN:HB3   | 13:AM:43:THR:CG2   | 2.33                     | 0.57              |
| 25:BA:614(A):U:H2' | 25:BA:614(B):G:OP1 | 2.03                     | 0.57              |
| 25:BA:1266:G:HO2'  | 25:BA:2012:G:H1    | 1.52                     | 0.57              |
| 25:BA:2345:G:O2'   | 25:BA:2382:G:O4'   | 2.22                     | 0.57              |
| 33:BI:79:ILE:CG1   | 33:BI:140:LEU:HD11 | 2.34                     | 0.57              |
| 34:BN:27:ALA:HA    | 34:BN:30:ILE:HG13  | 1.87                     | 0.57              |
| 46:BZ:40:ASP:HB3   | 46:BZ:43:GLU:HB2   | 1.85                     | 0.57              |
| 46:BZ:52:SER:O     | 46:BZ:53:ILE:HG23  | 2.03                     | 0.57              |
| 1:CA:251:G:O4'     | 1:CA:252:U:H6      | 1.86                     | 0.57              |
| 1:CA:429:U:C4'     | 1:CA:430:A:O5'     | 2.52                     | 0.57              |
| 1:CA:1067:A:C4'    | 1:CA:1068:G:O5'    | 2.43                     | 0.57              |
| 2:CB:16:HIS:HB3    | 2:CB:210:SER:OG    | 2.04                     | 0.57              |
| 2:CB:114:ARG:O     | 2:CB:114:ARG:HG3   | 2.04                     | 0.57              |
| 4:CD:19:LEU:HB3    | 4:CD:21:LEU:CD1    | 2.34                     | 0.57              |
| 6:CF:6:VAL:O       | 6:CF:62:TRP:HA     | 2.04                     | 0.57              |
| 12:CL:54:LYS:C     | 12:CL:70:ILE:HG13  | 2.29                     | 0.57              |
| 12:CL:69:TYR:HB2   | 12:CL:90:VAL:CG2   | 2.34                     | 0.57              |
| 13:CM:87:TYR:HA    | 13:CM:90:LEU:HG    | 1.86                     | 0.57              |
| 14:CN:6:LEU:HD13   | 14:CN:23:ARG:HH22  | 1.69                     | 0.57              |
| 20:CT:29:LYS:CG    | 20:CT:66:ALA:HB2   | 2.33                     | 0.57              |
| 20:CT:81:LYS:O     | 20:CT:85:MET:SD    | 2.63                     | 0.57              |
| 22:CV:54:G:N3      | 22:CV:55:U:C6      | 2.71                     | 0.57              |
| 23:CW:55:U:C5      | 23:CW:57:G:H5'     | 2.39                     | 0.57              |
| 25:DA:301:G:H1     | 25:DA:316:C:H42    | 1.53                     | 0.57              |
| 25:DA:811:U:C4     | 36:DP:21:ARG:NH2   | 2.73                     | 0.57              |
| 25:DA:1329:U:H5''  | 25:DA:1330:C:H5    | 1.67                     | 0.57              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:DA:1396:U:H5''  | 25:DA:1397:U:OP2   | 2.04                     | 0.57              |
| 28:DD:242:ARG:N    | 28:DD:242:ARG:HD2  | 2.18                     | 0.57              |
| 29:DE:48:GLN:HG2   | 29:DE:48:GLN:O     | 2.04                     | 0.57              |
| 39:DS:101:LEU:HD13 | 39:DS:101:LEU:O    | 2.04                     | 0.57              |
| 52:D5:41:PRO:HG2   | 52:D5:44:THR:HG21  | 1.86                     | 0.57              |
| 55:D8:52:LYS:N     | 55:D8:53:PRO:CD    | 2.65                     | 0.57              |
| 1:AA:1306:A:N6     | 1:AA:1331:G:O2'    | 2.37                     | 0.57              |
| 1:AA:1422:G:O2'    | 35:BO:49:ARG:NH2   | 2.37                     | 0.57              |
| 10:AJ:37:PRO:HA    | 10:AJ:72:VAL:HG21  | 1.87                     | 0.57              |
| 15:AO:16:ALA:CB    | 15:AO:21:ASP:HB3   | 2.33                     | 0.57              |
| 25:BA:249:C:OP2    | 25:BA:2394:C:O2'   | 2.21                     | 0.57              |
| 25:BA:910:A:C5     | 37:BQ:13:GLN:HG3   | 2.40                     | 0.57              |
| 26:BB:107:G:O2'    | 26:BB:108:U:H5''   | 2.04                     | 0.57              |
| 28:BD:71:ASP:N     | 28:BD:71:ASP:OD1   | 2.36                     | 0.57              |
| 29:BE:11:MET:HE3   | 29:BE:23:VAL:O     | 2.05                     | 0.57              |
| 35:BO:115:VAL:O    | 35:BO:117:LEU:N    | 2.37                     | 0.57              |
| 36:BP:19:VAL:CG2   | 36:BP:21:ARG:HD2   | 2.34                     | 0.57              |
| 36:BP:106:LEU:O    | 36:BP:107:LYS:HB2  | 2.05                     | 0.57              |
| 42:BV:34:GLU:HG2   | 42:BV:56:SER:HB2   | 1.85                     | 0.57              |
| 53:B6:10:LEU:HD12  | 55:B8:34:TRP:CD1   | 2.40                     | 0.57              |
| 1:CA:657:G:N2      | 1:CA:749:C:O2      | 2.30                     | 0.57              |
| 3:CC:59:ARG:HG2    | 3:CC:63:ASN:O      | 2.03                     | 0.57              |
| 4:CD:114:ARG:HG3   | 4:CD:114:ARG:NH1   | 2.12                     | 0.57              |
| 5:CE:101:ILE:N     | 5:CE:101:ILE:HD13  | 2.19                     | 0.57              |
| 10:CJ:43:ARG:O     | 10:CJ:67:THR:HG23  | 2.03                     | 0.57              |
| 23:CW:21:A:N6      | 23:CW:46:G:N3      | 2.52                     | 0.57              |
| 25:DA:974:G:O2'    | 25:DA:975(A):G:N7  | 2.30                     | 0.57              |
| 33:DI:77:LEU:HD13  | 33:DI:78:THR:N     | 2.18                     | 0.57              |
| 33:DI:101:LEU:C    | 33:DI:101:LEU:HD23 | 2.30                     | 0.57              |
| 34:DN:43:THR:HB    | 34:DN:46:VAL:CG1   | 2.34                     | 0.57              |
| 44:DX:47:PHE:N     | 44:DX:47:PHE:CD1   | 2.71                     | 0.57              |
| 48:D1:12:PRO:HB3   | 48:D1:43:TYR:CD2   | 2.39                     | 0.57              |
| 51:D4:34:GLU:O     | 51:D4:35:VAL:HB    | 2.04                     | 0.57              |
| 1:AA:1029:C:O2'    | 1:AA:1032:G:N2     | 2.29                     | 0.57              |
| 2:AB:71:VAL:HA     | 2:AB:93:VAL:CG2    | 2.33                     | 0.57              |
| 5:AE:144:THR:O     | 5:AE:148:VAL:HG23  | 2.03                     | 0.57              |
| 7:AG:15:ASP:HB3    | 7:AG:24:THR:CG2    | 2.35                     | 0.57              |
| 15:AO:17:ARG:HD3   | 15:AO:26:GLU:CG    | 2.34                     | 0.57              |
| 23:AW:25:C:H2'     | 23:AW:26:A:H8      | 1.70                     | 0.57              |
| 25:BA:333:G:C6     | 25:BA:334:C:C4     | 2.92                     | 0.57              |
| 25:BA:1203:G:O6    | 25:BA:1204:A:N6    | 2.37                     | 0.57              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:BA:2847:U:C5    | 25:BA:2848:G:C5    | 2.92                     | 0.57              |
| 29:BE:67:PHE:O     | 29:BE:70:ALA:HB2   | 2.03                     | 0.57              |
| 29:BE:177:PRO:O    | 29:BE:178:GLU:C    | 2.47                     | 0.57              |
| 30:BF:72:ARG:NH1   | 30:BF:72:ARG:HB3   | 2.19                     | 0.57              |
| 30:BF:108:LYS:HB3  | 30:BF:112:MET:CE   | 2.35                     | 0.57              |
| 31:BG:110:ALA:HA   | 31:BG:140:ILE:CG2  | 2.34                     | 0.57              |
| 40:BT:29:ARG:HG2   | 40:BT:85:LYS:O     | 2.03                     | 0.57              |
| 40:BT:83:ILE:CD1   | 40:BT:84:GLN:HG3   | 2.34                     | 0.57              |
| 42:BV:38:LEU:O     | 42:BV:52:VAL:HG12  | 2.03                     | 0.57              |
| 42:BV:46:VAL:HG22  | 42:BV:47:VAL:H     | 1.69                     | 0.57              |
| 48:B1:52:ARG:HH11  | 48:B1:74:VAL:HG12  | 1.68                     | 0.57              |
| 54:B7:18:PHE:O     | 54:B7:19:ARG:C     | 2.45                     | 0.57              |
| 1:CA:470:C:H5''    | 1:CA:471:G:OP2     | 2.04                     | 0.57              |
| 1:CA:737:A:H2'     | 1:CA:738:C:C6      | 2.39                     | 0.57              |
| 10:CJ:12:ASP:OD1   | 10:CJ:15:THR:HG23  | 2.04                     | 0.57              |
| 13:CM:11:ARG:HH11  | 13:CM:11:ARG:CB    | 2.16                     | 0.57              |
| 16:CP:32:TYR:C     | 16:CP:32:TYR:CD2   | 2.81                     | 0.57              |
| 16:CP:32:TYR:C     | 16:CP:32:TYR:HD2   | 2.13                     | 0.57              |
| 17:CQ:22:LEU:HD13  | 17:CQ:41:LYS:HG2   | 1.86                     | 0.57              |
| 25:DA:791:C:H4'    | 25:DA:792:G:OP1    | 2.05                     | 0.57              |
| 25:DA:1694:C:OP2   | 25:DA:1694:C:C6    | 2.56                     | 0.57              |
| 25:DA:1818:U:O2'   | 28:DD:157:ARG:HG3  | 2.03                     | 0.57              |
| 25:DA:2198:A:O2'   | 25:DA:2199:A:O4'   | 2.22                     | 0.57              |
| 26:DB:22:U:H3      | 26:DB:61:G:H1      | 1.52                     | 0.57              |
| 30:DF:124:LEU:HG   | 30:DF:126:VAL:CG1  | 2.34                     | 0.57              |
| 31:DG:137:GLU:HB3  | 31:DG:152:LEU:HD13 | 1.86                     | 0.57              |
| 34:DN:87:LEU:O     | 34:DN:90:MET:HB2   | 2.05                     | 0.57              |
| 36:DP:106:LEU:O    | 36:DP:107:LYS:HB2  | 2.05                     | 0.57              |
| 40:DT:67:SER:O     | 40:DT:68:TYR:HB2   | 2.04                     | 0.57              |
| 2:AB:178:ARG:HH22  | 2:AB:196:LEU:C     | 2.12                     | 0.57              |
| 3:AC:44:GLU:HG2    | 3:AC:52:LEU:HD11   | 1.85                     | 0.57              |
| 4:AD:61:LYS:HD2    | 4:AD:206:PHE:CE2   | 2.40                     | 0.57              |
| 9:AI:125:TYR:HD2   | 9:AI:126:SER:H     | 1.53                     | 0.57              |
| 10:AJ:44:VAL:HG12  | 10:AJ:45:ARG:N     | 2.17                     | 0.57              |
| 25:BA:390:A:C6     | 36:BP:71:VAL:HG11  | 2.39                     | 0.57              |
| 25:BA:865:C:C5'    | 25:BA:866:A:OP1    | 2.53                     | 0.57              |
| 25:BA:1336:A:H2'   | 25:BA:1337:G:C8    | 2.40                     | 0.57              |
| 25:BA:1819:A:H4'   | 25:BA:1820:U:O5'   | 2.04                     | 0.57              |
| 25:BA:2346:A:O2'   | 25:BA:2347:C:OP2   | 2.22                     | 0.57              |
| 25:BA:2577:A:H5''  | 25:BA:2578:G:H5'   | 1.86                     | 0.57              |
| 29:BE:176:ILE:HG22 | 29:BE:178:GLU:HB3  | 1.85                     | 0.57              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:BG:86:MET:HG3   | 31:BG:87:PRO:HD3   | 1.82                     | 0.57              |
| 32:BH:35:VAL:HG11  | 32:BH:72:ILE:HG13  | 1.87                     | 0.57              |
| 32:BH:84:SER:O     | 32:BH:85:LYS:HB3   | 2.04                     | 0.57              |
| 33:BI:56:LYS:HG3   | 33:BI:57:ARG:N     | 2.19                     | 0.57              |
| 33:BI:77:LEU:HD11  | 33:BI:104:GLN:CD   | 2.29                     | 0.57              |
| 36:BP:94:GLU:O     | 36:BP:96:THR:HG23  | 2.05                     | 0.57              |
| 38:BR:41:ALA:C     | 38:BR:43:GLU:H     | 2.11                     | 0.57              |
| 43:BW:12:ILE:HD13  | 43:BW:46:PHE:CD2   | 2.39                     | 0.57              |
| 44:BX:65:ARG:HH11  | 44:BX:65:ARG:HG2   | 1.69                     | 0.57              |
| 1:CA:173:U:H1'     | 1:CA:197:A:C5      | 2.39                     | 0.57              |
| 1:CA:458:C:H2'     | 1:CA:460:G:H8      | 1.69                     | 0.57              |
| 1:CA:656:C:H4'     | 15:CO:62:GLN:HE22  | 1.70                     | 0.57              |
| 1:CA:686:U:O2'     | 1:CA:687:A:P       | 2.62                     | 0.57              |
| 3:CC:29:TYR:HA     | 3:CC:32:LEU:HB2    | 1.84                     | 0.57              |
| 9:CI:89:ASN:C      | 9:CI:91:ASP:H      | 2.13                     | 0.57              |
| 19:CS:63:THR:CG2   | 19:CS:66:MET:CE    | 2.74                     | 0.57              |
| 23:CY:36:A:C8      | 23:CY:36:A:C3'     | 2.87                     | 0.57              |
| 25:DA:788:A:OP1    | 25:DA:791:C:N4     | 2.35                     | 0.57              |
| 28:DD:133:LEU:HD22 | 28:DD:165:ILE:HD11 | 1.86                     | 0.57              |
| 28:DD:147:LEU:HD13 | 28:DD:155:LEU:HD11 | 1.85                     | 0.57              |
| 30:DF:110:LEU:HD11 | 30:DF:181:LEU:CD1  | 2.35                     | 0.57              |
| 32:DH:6:ARG:C      | 32:DH:8:PRO:HD2    | 2.30                     | 0.57              |
| 32:DH:37:VAL:CG1   | 32:DH:38:SER:H     | 2.16                     | 0.57              |
| 32:DH:50:VAL:HG22  | 32:DH:50:VAL:O     | 2.05                     | 0.57              |
| 41:DU:17:ILE:HG23  | 41:DU:39:LEU:HD12  | 1.86                     | 0.57              |
| 46:DZ:81:ARG:O     | 46:DZ:81:ARG:HG3   | 2.03                     | 0.57              |
| 46:DZ:102:LEU:O    | 46:DZ:103:ARG:HG2  | 2.04                     | 0.57              |
| 52:D5:32:PRO:O     | 52:D5:33:CYS:CB    | 2.52                     | 0.57              |
| 1:AA:79:G:N2       | 1:AA:91:C:H41      | 2.03                     | 0.57              |
| 1:AA:411:A:C4      | 1:AA:413:G:H1'     | 2.40                     | 0.57              |
| 1:AA:1191:A:OP1    | 3:AC:3:ASN:ND2     | 2.34                     | 0.57              |
| 3:AC:6:HIS:CD2     | 3:AC:7:PRO:HD2     | 2.38                     | 0.57              |
| 13:AM:102:ARG:HG3  | 13:AM:102:ARG:NH1  | 2.19                     | 0.57              |
| 19:AS:61:TYR:O     | 19:AS:62:ILE:HB    | 2.05                     | 0.57              |
| 20:AT:50:GLU:HG3   | 20:AT:51:GLU:N     | 2.19                     | 0.57              |
| 22:AV:48:U:H3'     | 22:AV:49:C:C5'     | 2.35                     | 0.57              |
| 25:BA:242:G:N2     | 25:BA:254:G:N7     | 2.52                     | 0.57              |
| 25:BA:242:G:N3     | 25:BA:254:G:C6     | 2.73                     | 0.57              |
| 25:BA:727:A:C6     | 25:BA:728:G:C6     | 2.93                     | 0.57              |
| 25:BA:2222:G:H5''  | 28:BD:186:HIS:CD2  | 2.40                     | 0.57              |
| 25:BA:2318:G:H3'   | 25:BA:2318:G:N3    | 2.19                     | 0.57              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 27:BC:77:ILE:O     | 27:BC:77:ILE:HG23 | 2.03                     | 0.57              |
| 27:BC:122:ALA:HB1  | 27:BC:129:ARG:CB  | 2.34                     | 0.57              |
| 29:BE:37:ARG:O     | 29:BE:38:THR:C    | 2.48                     | 0.57              |
| 30:BF:7:TYR:HB3    | 30:BF:16:GLY:N    | 2.20                     | 0.57              |
| 30:BF:9:ILE:HG12   | 30:BF:14:PRO:HA   | 1.86                     | 0.57              |
| 30:BF:107:LYS:HE3  | 30:BF:205:ARG:O   | 2.04                     | 0.57              |
| 31:BG:72:ARG:CG    | 31:BG:86:MET:CA   | 2.80                     | 0.57              |
| 34:BN:7:LYS:O      | 34:BN:8:GLN:C     | 2.47                     | 0.57              |
| 35:BO:48:PRO:HB3   | 35:BO:49:ARG:HH11 | 1.68                     | 0.57              |
| 41:BU:101:ARG:O    | 41:BU:102:GLU:HG2 | 2.05                     | 0.57              |
| 46:BZ:158:PRO:HB2  | 46:BZ:159:PRO:CD  | 2.34                     | 0.57              |
| 49:B2:16:LEU:O     | 49:B2:20:GLU:HB3  | 2.05                     | 0.57              |
| 51:B4:42:CYS:SG    | 51:B4:62:CYS:HB3  | 2.45                     | 0.57              |
| 1:CA:351:G:H4'     | 1:CA:352:C:OP1    | 2.03                     | 0.57              |
| 2:CB:15:VAL:HG21   | 2:CB:209:ARG:HH21 | 1.69                     | 0.57              |
| 2:CB:210:SER:O     | 2:CB:214:ILE:HB   | 2.04                     | 0.57              |
| 3:CC:64:VAL:HG22   | 3:CC:97:LYS:HZ2   | 1.69                     | 0.57              |
| 10:CJ:47:PHE:CZ    | 14:CN:37:PHE:CZ   | 2.93                     | 0.57              |
| 12:CL:10:LEU:HB3   | 17:CQ:32:TYR:CE2  | 2.39                     | 0.57              |
| 14:CN:24:CYS:N     | 14:CN:33:VAL:HG11 | 2.19                     | 0.57              |
| 17:CQ:29:HIS:C     | 17:CQ:31:LEU:H    | 2.11                     | 0.57              |
| 18:CR:36:ASN:HB2   | 18:CR:39:VAL:HG23 | 1.87                     | 0.57              |
| 25:DA:660:G:O3'    | 30:DF:38:ARG:NH2  | 2.37                     | 0.57              |
| 25:DA:2330:G:O2'   | 47:D0:41:ARG:HB2  | 2.05                     | 0.57              |
| 30:DF:174:VAL:HG22 | 30:DF:174:VAL:O   | 2.03                     | 0.57              |
| 32:DH:12:PRO:HG3   | 32:DH:48:GLY:O    | 2.05                     | 0.57              |
| 32:DH:169:VAL:HG22 | 32:DH:170:ARG:H   | 1.69                     | 0.57              |
| 32:DH:169:VAL:HG22 | 32:DH:170:ARG:N   | 2.18                     | 0.57              |
| 35:DO:26:LYS:HB2   | 35:DO:30:ALA:HB2  | 1.87                     | 0.57              |
| 35:DO:87:ILE:HG21  | 35:DO:91:LEU:HD13 | 1.85                     | 0.57              |
| 36:DP:94:GLU:O     | 36:DP:96:THR:HG23 | 2.05                     | 0.57              |
| 36:DP:107:LYS:C    | 36:DP:109:GLY:N   | 2.63                     | 0.57              |
| 38:DR:63:ARG:NH1   | 38:DR:80:PHE:HD2  | 2.03                     | 0.57              |
| 41:DU:34:LYS:HA    | 41:DU:34:LYS:HE2  | 1.87                     | 0.57              |
| 42:DV:76:LYS:HB2   | 42:DV:81:TYR:HB3  | 1.84                     | 0.57              |
| 46:DZ:82:ARG:CG    | 46:DZ:83:PRO:HD2  | 2.30                     | 0.57              |
| 54:D7:8:ASN:OD1    | 54:D7:8:ASN:C     | 2.48                     | 0.57              |
| 55:D8:33:ASN:HA    | 55:D8:36:LYS:HD2  | 1.86                     | 0.57              |
| 1:AA:1049:U:N1     | 1:AA:1201:A:C8    | 2.73                     | 0.57              |
| 2:AB:108:ILE:HG22  | 2:AB:152:PHE:CE1  | 2.40                     | 0.57              |
| 6:AF:22:GLU:OE2    | 6:AF:82:ARG:HG3   | 2.04                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:AH:103:VAL:HB   | 8:AH:108:GLY:HA3  | 1.86                     | 0.57              |
| 9:AI:2:GLU:N      | 9:AI:88:TYR:HH    | 2.02                     | 0.57              |
| 25:BA:242:G:C2    | 25:BA:254:G:C5    | 2.93                     | 0.57              |
| 25:BA:534:U:HO2'  | 41:BU:49:HIS:CG   | 2.23                     | 0.57              |
| 25:BA:2078:C:N3   | 25:BA:2079:U:C4   | 2.72                     | 0.57              |
| 28:BD:11:PRO:O    | 28:BD:12:SER:OG   | 2.19                     | 0.57              |
| 28:BD:43:ARG:HD2  | 28:BD:44:ASN:OD1  | 2.05                     | 0.57              |
| 28:BD:83:GLU:O    | 28:BD:92:ILE:HD13 | 2.04                     | 0.57              |
| 31:BG:20:ILE:O    | 31:BG:24:GLY:N    | 2.38                     | 0.57              |
| 31:BG:150:ASP:O   | 31:BG:151:ALA:HB2 | 2.04                     | 0.57              |
| 34:BN:91:LEU:HA   | 34:BN:95:PRO:HB3  | 1.87                     | 0.57              |
| 36:BP:19:VAL:HG21 | 36:BP:21:ARG:HD2  | 1.87                     | 0.57              |
| 37:BQ:55:VAL:HG12 | 37:BQ:64:ILE:HD12 | 1.87                     | 0.57              |
| 38:BR:12:ARG:O    | 38:BR:17:ARG:NH2  | 2.38                     | 0.57              |
| 40:BT:66:VAL:HA   | 40:BT:71:GLY:HA2  | 1.85                     | 0.57              |
| 44:BX:31:HIS:ND1  | 44:BX:32:PRO:HD2  | 2.19                     | 0.57              |
| 45:BY:13:VAL:HG21 | 45:BY:28:LYS:HD3  | 1.86                     | 0.57              |
| 45:BY:19:LYS:HB2  | 45:BY:19:LYS:NZ   | 2.19                     | 0.57              |
| 45:BY:55:TYR:CB   | 45:BY:56:PRO:CD   | 2.76                     | 0.57              |
| 49:B2:37:PHE:O    | 49:B2:41:ILE:HG12 | 2.05                     | 0.57              |
| 1:CA:251:G:C4'    | 1:CA:252:U:O5'    | 2.46                     | 0.57              |
| 1:CA:484:G:O2'    | 1:CA:485:G:P      | 2.63                     | 0.57              |
| 1:CA:527:G:O2'    | 1:CA:535:A:N1     | 2.34                     | 0.57              |
| 2:CB:167:PRO:HG2  | 2:CB:192:SER:CB   | 2.34                     | 0.57              |
| 4:CD:96:LEU:HD12  | 4:CD:96:LEU:H     | 1.69                     | 0.57              |
| 4:CD:138:TYR:CD2  | 4:CD:138:TYR:C    | 2.83                     | 0.57              |
| 7:CG:23:VAL:CG1   | 7:CG:43:PHE:CE2   | 2.84                     | 0.57              |
| 17:CQ:67:LYS:O    | 17:CQ:69:LYS:N    | 2.36                     | 0.57              |
| 18:CR:59:SER:H    | 18:CR:62:GLU:HB2  | 1.70                     | 0.57              |
| 19:CS:9:VAL:HG12  | 19:CS:11:VAL:HG12 | 1.87                     | 0.57              |
| 25:DA:670:A:H5'   | 36:DP:42:SER:OG   | 2.04                     | 0.57              |
| 25:DA:1697:G:H3'  | 25:DA:1698:A:H5'  | 1.83                     | 0.57              |
| 32:DH:28:GLY:HA3  | 32:DH:79:VAL:HB   | 1.85                     | 0.57              |
| 33:DI:78:THR:O    | 33:DI:79:ILE:HG12 | 2.04                     | 0.57              |
| 38:DR:17:ARG:O    | 38:DR:20:LEU:HB3  | 2.04                     | 0.57              |
| 1:AA:448:A:OP2    | 1:AA:485:G:N2     | 2.30                     | 0.57              |
| 1:AA:1321:C:H4'   | 13:AM:87:TYR:CZ   | 2.40                     | 0.57              |
| 2:AB:30:ARG:HH21  | 2:AB:194:PRO:HB2  | 1.69                     | 0.57              |
| 3:AC:9:GLY:HA2    | 3:AC:12:LEU:HD23  | 1.87                     | 0.57              |
| 3:AC:27:LYS:O     | 3:AC:28:GLN:HG3   | 2.04                     | 0.57              |
| 4:AD:31:CYS:C     | 4:AD:33:MET:N     | 2.63                     | 0.57              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 16:AP:1:MET:HG2    | 16:AP:2:VAL:N     | 2.20                     | 0.57              |
| 16:AP:19:ILE:HG22  | 16:AP:36:ILE:HG13 | 1.86                     | 0.57              |
| 25:BA:581:C:P      | 41:BU:33:ARG:HG3  | 2.45                     | 0.57              |
| 25:BA:892:G:O2'    | 25:BA:893:C:H5'   | 2.04                     | 0.57              |
| 25:BA:1820:U:C5'   | 25:BA:1821:A:OP2  | 2.53                     | 0.57              |
| 32:BH:109:PHE:CE1  | 32:BH:152:ARG:CZ  | 2.82                     | 0.57              |
| 36:BP:47:ASP:HB3   | 36:BP:48:PRO:HA   | 1.86                     | 0.57              |
| 37:BQ:141:GLN:OE1  | 46:BZ:72:ARG:HA   | 2.04                     | 0.57              |
| 38:BR:28:LEU:HD23  | 38:BR:34:ILE:HG12 | 1.85                     | 0.57              |
| 40:BT:15:VAL:HA    | 40:BT:79:HIS:HD2  | 1.70                     | 0.57              |
| 41:BU:25:TRP:HD1   | 41:BU:26:GLY:N    | 2.01                     | 0.57              |
| 45:BY:7:VAL:HB     | 45:BY:8:LYS:NZ    | 2.20                     | 0.57              |
| 1:CA:946:A:H2'     | 1:CA:947:G:C8     | 2.40                     | 0.57              |
| 3:CC:47:LEU:HG     | 3:CC:50:ALA:HB3   | 1.87                     | 0.57              |
| 5:CE:148:VAL:HG21  | 8:CH:107:LEU:CD2  | 2.33                     | 0.57              |
| 10:CJ:32:ALA:HB3   | 10:CJ:76:ASN:HB3  | 1.85                     | 0.57              |
| 12:CL:50:SER:O     | 12:CL:51:ALA:HB2  | 2.05                     | 0.57              |
| 25:DA:9272:G:C5'   | 25:DA:9273:G:OP2  | 2.52                     | 0.57              |
| 25:DA:695:G:H4'    | 25:DA:1380:G:H5'  | 1.87                     | 0.57              |
| 25:DA:790:C:OP1    | 25:DA:1781:C:N4   | 2.38                     | 0.57              |
| 25:DA:1416:G:HO2'  | 25:DA:1417:C:H6   | 1.52                     | 0.57              |
| 25:DA:1819:A:C4'   | 25:DA:1820:U:OP2  | 2.53                     | 0.57              |
| 25:DA:1826:G:H4'   | 28:DD:242:ARG:NH2 | 2.19                     | 0.57              |
| 25:DA:2347:C:H4'   | 53:D6:39:TYR:CE1  | 2.40                     | 0.57              |
| 28:DD:31:LYS:HZ2   | 28:DD:102:LYS:HZ2 | 1.52                     | 0.57              |
| 29:DE:47:VAL:HG12  | 29:DE:49:LEU:HD12 | 1.86                     | 0.57              |
| 32:DH:152:ARG:HG3  | 32:DH:153:LYS:HE3 | 1.84                     | 0.57              |
| 35:DO:7:TYR:HE1    | 35:DO:20:MET:HE3  | 1.70                     | 0.57              |
| 36:DP:146:VAL:HG22 | 36:DP:147:LEU:N   | 2.15                     | 0.57              |
| 37:DQ:43:THR:OG1   | 37:DQ:46:GLN:HG3  | 2.05                     | 0.57              |
| 41:DU:91:ASP:OD2   | 41:DU:96:ALA:CB   | 2.53                     | 0.57              |
| 50:D3:8:LEU:HA     | 50:D3:54:VAL:HG22 | 1.87                     | 0.57              |
| 2:AB:98:LEU:N      | 2:AB:98:LEU:HD23  | 2.20                     | 0.57              |
| 5:AE:127:ASN:OD1   | 5:AE:127:ASN:C    | 2.47                     | 0.57              |
| 7:AG:73:MET:HA     | 7:AG:91:VAL:HG23  | 1.86                     | 0.57              |
| 9:AI:16:ARG:CZ     | 9:AI:64:THR:HG21  | 2.33                     | 0.57              |
| 11:AK:34:ASP:O     | 11:AK:36:ASP:N    | 2.38                     | 0.57              |
| 25:BA:125:G:C4'    | 25:BA:126:A:OP2   | 2.53                     | 0.57              |
| 25:BA:435:C:H2'    | 25:BA:436:C:H5'   | 1.85                     | 0.57              |
| 25:BA:775:G:H4'    | 25:BA:776:G:O5'   | 2.04                     | 0.57              |
| 25:BA:1301:A:O2'   | 25:BA:1302:A:P    | 2.63                     | 0.57              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 25:BA:2780:G:OP2    | 34:BN:118:LYS:HD3  | 2.05                     | 0.57              |
| 30:BF:124:LEU:HD12  | 30:BF:125:LEU:N    | 2.20                     | 0.57              |
| 31:BG:102:PHE:HE2   | 31:BG:141:PHE:HE1  | 1.50                     | 0.57              |
| 36:BP:59:LEU:HD11   | 55:B8:13:ARG:NH2   | 2.20                     | 0.57              |
| 39:BS:21:THR:C      | 39:BS:23:ARG:H     | 2.12                     | 0.57              |
| 46:BZ:149:SER:C     | 46:BZ:150:LEU:HD13 | 2.30                     | 0.57              |
| 1:CA:708:C:OP1      | 11:CK:85:ARG:NH2   | 2.29                     | 0.57              |
| 1:CA:1442(B):A:H5'' | 40:DT:122:ASP:OD1  | 2.04                     | 0.57              |
| 1:CA:1457:G:H2'     | 1:CA:1458:G:H8     | 1.68                     | 0.57              |
| 8:CH:85:ARG:HD3     | 8:CH:85:ARG:C      | 2.30                     | 0.57              |
| 17:CQ:83:ASP:O      | 17:CQ:86:GLU:HB2   | 2.04                     | 0.57              |
| 19:CS:45:VAL:C      | 19:CS:62:ILE:CG2   | 2.78                     | 0.57              |
| 20:CT:22:ARG:O      | 20:CT:26:ASN:ND2   | 2.38                     | 0.57              |
| 20:CT:37:SER:O      | 20:CT:41:ILE:HG12  | 2.04                     | 0.57              |
| 23:CW:34:G:C6       | 24:CX:14:A:N1      | 2.72                     | 0.57              |
| 25:DA:1820:U:O2'    | 25:DA:1821:A:P     | 2.63                     | 0.57              |
| 29:DE:57:LYS:HB3    | 29:DE:57:LYS:HZ3   | 1.68                     | 0.57              |
| 32:DH:40:GLU:O      | 32:DH:41:MET:HB2   | 2.05                     | 0.57              |
| 34:DN:42:TRP:HA     | 34:DN:42:TRP:CE3   | 2.40                     | 0.57              |
| 35:DO:111:PHE:O     | 35:DO:115:VAL:HG23 | 2.05                     | 0.57              |
| 36:DP:147:LEU:HD23  | 36:DP:148:LEU:O    | 2.05                     | 0.57              |
| 41:DU:104:GLN:HE22  | 41:DU:105:VAL:H    | 1.50                     | 0.57              |
| 42:DV:35:LEU:HD22   | 42:DV:35:LEU:N     | 2.12                     | 0.57              |
| 1:AA:522:C:H41      | 12:AL:53:ARG:HH22  | 1.53                     | 0.56              |
| 1:AA:1412:C:H2'     | 1:AA:1413:A:C8     | 2.40                     | 0.56              |
| 2:AB:11:LEU:CD1     | 2:AB:217:ARG:HH21  | 2.17                     | 0.56              |
| 3:AC:18:TRP:HE1     | 14:AN:55:GLY:N     | 2.03                     | 0.56              |
| 7:AG:40:ALA:HB1     | 9:AI:41:VAL:HG11   | 1.86                     | 0.56              |
| 20:AT:97:ALA:O      | 20:AT:99:LEU:N     | 2.34                     | 0.56              |
| 21:AU:18:TYR:HD1    | 21:AU:24:ARG:CZ    | 2.18                     | 0.56              |
| 22:AV:18:U:C4'      | 22:AV:19:G:OP2     | 2.41                     | 0.56              |
| 25:BA:2394:C:OP1    | 36:BP:63:PRO:HD2   | 2.04                     | 0.56              |
| 25:BA:2614:A:H5''   | 25:BA:2615:U:OP1   | 2.05                     | 0.56              |
| 28:BD:25:THR:C      | 28:BD:27:THR:H     | 2.12                     | 0.56              |
| 28:BD:131:LEU:HB2   | 28:BD:136:ILE:HD11 | 1.87                     | 0.56              |
| 28:BD:223:GLY:O     | 28:BD:226:MET:HB2  | 2.05                     | 0.56              |
| 29:BE:101:ARG:HD3   | 29:BE:169:ASN:OD1  | 2.04                     | 0.56              |
| 30:BF:64:ILE:CG2    | 30:BF:65:TRP:CG    | 2.82                     | 0.56              |
| 34:BN:62:VAL:CG1    | 34:BN:66:LYS:HB2   | 2.34                     | 0.56              |
| 34:BN:67:LEU:HA     | 34:BN:87:LEU:HB3   | 1.87                     | 0.56              |
| 38:BR:11:ASN:O      | 38:BR:12:ARG:HG3   | 2.05                     | 0.56              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 51:B4:64:LYS:O     | 51:B4:65:CYS:SG   | 2.60                     | 0.56              |
| 1:CA:66:G:H5'      | 1:CA:173:U:O4     | 2.04                     | 0.56              |
| 4:CD:101:LEU:O     | 4:CD:104:VAL:N    | 2.38                     | 0.56              |
| 4:CD:148:VAL:HG12  | 4:CD:149:ALA:O    | 2.05                     | 0.56              |
| 10:CJ:49:VAL:HG22  | 10:CJ:50:ILE:H    | 1.70                     | 0.56              |
| 12:CL:39:VAL:HG12  | 12:CL:40:VAL:N    | 2.18                     | 0.56              |
| 13:CM:88:ARG:HB3   | 13:CM:88:ARG:NH1  | 2.04                     | 0.56              |
| 16:CP:13:HIS:C     | 16:CP:15:PRO:HD3  | 2.29                     | 0.56              |
| 17:CQ:67:LYS:CA    | 17:CQ:70:ARG:HH12 | 2.10                     | 0.56              |
| 19:CS:28:LYS:HD2   | 19:CS:29:ARG:CZ   | 2.35                     | 0.56              |
| 20:CT:84:LEU:CD1   | 20:CT:84:LEU:O    | 2.52                     | 0.56              |
| 23:CW:31:A:C2      | 23:CW:40:C:C2     | 2.94                     | 0.56              |
| 25:DA:1251:C:H4'   | 25:DA:1252:G:OP1  | 2.03                     | 0.56              |
| 25:DA:1455:G:O6    | 25:DA:2705:A:C2   | 2.58                     | 0.56              |
| 28:DD:27:THR:HG21  | 28:DD:81:ALA:HB1  | 1.86                     | 0.56              |
| 29:DE:111:ARG:CA   | 38:DR:1:MET:SD    | 2.93                     | 0.56              |
| 32:DH:13:LYS:HE2   | 32:DH:13:LYS:CA   | 2.30                     | 0.56              |
| 33:DI:40:THR:O     | 33:DI:44:LEU:HB2  | 2.04                     | 0.56              |
| 43:DW:40:ASN:O     | 43:DW:41:LYS:HG2  | 2.04                     | 0.56              |
| 48:D1:3:LYS:O      | 48:D1:12:PRO:HD3  | 2.04                     | 0.56              |
| 1:AA:401:C:H2'     | 1:AA:402:G:C8     | 2.40                     | 0.56              |
| 4:AD:98:GLU:OE2    | 4:AD:103:ASN:ND2  | 2.36                     | 0.56              |
| 4:AD:127:THR:OG1   | 4:AD:147:ALA:HB3  | 2.05                     | 0.56              |
| 5:AE:68:GLU:CD     | 5:AE:68:GLU:C     | 2.73                     | 0.56              |
| 12:AL:59:ARG:HD3   | 12:AL:65:GLU:OE1  | 2.05                     | 0.56              |
| 13:AM:39:ILE:HD12  | 13:AM:56:LEU:HD23 | 1.85                     | 0.56              |
| 17:AQ:3:LYS:HG2    | 17:AQ:60:ILE:HD11 | 1.87                     | 0.56              |
| 25:BA:1012:U:C4    | 34:BN:25:ARG:HD3  | 2.40                     | 0.56              |
| 25:BA:1639:U:H2'   | 25:BA:1640:C:H5'' | 1.87                     | 0.56              |
| 25:BA:1653:G:OP1   | 25:BA:2822:G:N1   | 2.30                     | 0.56              |
| 25:BA:1791:A:N6    | 25:BA:1828:G:O2'  | 2.34                     | 0.56              |
| 25:BA:2000:G:O2'   | 25:BA:2689:U:H5   | 1.86                     | 0.56              |
| 25:BA:2145:C:H4'   | 25:BA:2146:C:OP2  | 2.04                     | 0.56              |
| 28:BD:31:LYS:NZ    | 28:BD:102:LYS:NZ  | 2.53                     | 0.56              |
| 30:BF:114:VAL:HG21 | 30:BF:202:PHE:CZ  | 2.40                     | 0.56              |
| 30:BF:164:ARG:HG3  | 30:BF:175:THR:OG1 | 2.05                     | 0.56              |
| 32:BH:87:LEU:HD23  | 32:BH:164:TYR:HA  | 1.87                     | 0.56              |
| 39:BS:46:VAL:CG1   | 39:BS:47:THR:N    | 2.67                     | 0.56              |
| 41:BU:62:ILE:HG22  | 41:BU:63:VAL:N    | 2.19                     | 0.56              |
| 42:BV:3:ALA:HB1    | 42:BV:38:LEU:HD21 | 1.86                     | 0.56              |
| 46:BZ:96:VAL:HG12  | 46:BZ:97:GLU:N    | 2.19                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 46:BZ:158:PRO:HB2 | 46:BZ:159:PRO:HD2 | 1.86                     | 0.56              |
| 2:CB:16:HIS:NE2   | 2:CB:213:LEU:HD13 | 2.20                     | 0.56              |
| 2:CB:31:TYR:CD2   | 2:CB:31:TYR:N     | 2.72                     | 0.56              |
| 11:CK:95:ILE:HG22 | 11:CK:96:ARG:N    | 2.19                     | 0.56              |
| 14:CN:4:LYS:O     | 14:CN:7:ILE:HG12  | 2.05                     | 0.56              |
| 25:DA:498:G:H21   | 45:DY:47:LYS:HZ2  | 1.53                     | 0.56              |
| 25:DA:1190:G:OP1  | 36:DP:30:THR:OG1  | 2.12                     | 0.56              |
| 25:DA:1819:A:C4'  | 25:DA:1820:U:H5'  | 2.31                     | 0.56              |
| 34:DN:18:ALA:HB1  | 34:DN:21:LYS:CB   | 2.35                     | 0.56              |
| 36:DP:46:LYS:HG2  | 36:DP:51:PHE:CD2  | 2.40                     | 0.56              |
| 36:DP:111:ARG:HG3 | 36:DP:128:HIS:ND1 | 2.20                     | 0.56              |
| 47:D0:53:MET:HA   | 47:D0:58:THR:O    | 2.05                     | 0.56              |
| 48:D1:64:ALA:HA   | 48:D1:67:ILE:HG13 | 1.87                     | 0.56              |
| 1:AA:428:G:O2'    | 1:AA:429:U:OP2    | 2.24                     | 0.56              |
| 1:AA:453:A:C5     | 1:AA:454:C:C4     | 2.93                     | 0.56              |
| 1:AA:529:G:H4'    | 1:AA:533:A:C2     | 2.40                     | 0.56              |
| 1:AA:1275:A:C2'   | 1:AA:1276:G:H8    | 2.14                     | 0.56              |
| 2:AB:210:SER:O    | 2:AB:214:ILE:HG12 | 2.05                     | 0.56              |
| 3:AC:138:VAL:HG22 | 3:AC:151:VAL:HG23 | 1.86                     | 0.56              |
| 7:AG:118:VAL:CG2  | 7:AG:119:ARG:N    | 2.69                     | 0.56              |
| 10:AJ:6:ILE:HG22  | 10:AJ:98:ILE:HG13 | 1.86                     | 0.56              |
| 17:AQ:56:VAL:HB   | 17:AQ:78:GLU:CG   | 2.35                     | 0.56              |
| 19:AS:28:LYS:HD2  | 19:AS:29:ARG:CZ   | 2.35                     | 0.56              |
| 23:AW:16:U:C3'    | 23:AW:17:C:H5'    | 2.36                     | 0.56              |
| 25:BA:581:C:OP1   | 41:BU:33:ARG:CG   | 2.53                     | 0.56              |
| 25:BA:746:A:C6    | 25:BA:2611:U:H5'' | 2.40                     | 0.56              |
| 25:BA:1452:A:N6   | 25:BA:2703:C:H41  | 1.99                     | 0.56              |
| 25:BA:1819:A:O2'  | 25:BA:1820:U:OP2  | 2.22                     | 0.56              |
| 25:BA:1837:C:H2'  | 25:BA:1838:C:H5'' | 1.88                     | 0.56              |
| 25:BA:2282:G:O2'  | 25:BA:2390:U:O4   | 2.22                     | 0.56              |
| 27:BC:49:ILE:HG22 | 27:BC:50:ASP:OD1  | 2.05                     | 0.56              |
| 28:BD:43:ARG:HH11 | 28:BD:44:ASN:ND2  | 2.03                     | 0.56              |
| 29:BE:119:ARG:HD2 | 29:BE:120:TRP:NE1 | 2.20                     | 0.56              |
| 30:BF:7:TYR:CZ    | 30:BF:10:PRO:HG3  | 2.40                     | 0.56              |
| 31:BG:110:ALA:O   | 31:BG:111:LEU:C   | 2.49                     | 0.56              |
| 31:BG:116:ASP:O   | 31:BG:117:PHE:CB  | 2.53                     | 0.56              |
| 36:BP:46:LYS:HG2  | 36:BP:51:PHE:CD2  | 2.40                     | 0.56              |
| 37:BQ:29:PHE:HD2  | 37:BQ:65:PHE:HE1  | 1.53                     | 0.56              |
| 39:BS:26:LEU:HD13 | 39:BS:87:PHE:HD1  | 1.70                     | 0.56              |
| 40:BT:16:ARG:NH1  | 40:BT:18:ASP:OD2  | 2.39                     | 0.56              |
| 40:BT:29:ARG:HG3  | 40:BT:85:LYS:HA   | 0.68                     | 0.56              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 41:BU:61:TRP:CZ2    | 41:BU:94:ASN:CG    | 2.83                     | 0.56              |
| 41:BU:92:ARG:HH11   | 41:BU:92:ARG:HG2   | 1.71                     | 0.56              |
| 41:BU:108:GLU:O     | 41:BU:111:GLU:HB2  | 2.05                     | 0.56              |
| 42:BV:38:LEU:HD23   | 42:BV:39:LEU:N     | 2.21                     | 0.56              |
| 47:B0:10:THR:HG22   | 47:B0:12:ASN:HB2   | 1.88                     | 0.56              |
| 47:B0:25:ARG:HD2    | 47:B0:29:GLN:NE2   | 2.20                     | 0.56              |
| 48:B1:52:ARG:CG     | 48:B1:53:VAL:H     | 2.18                     | 0.56              |
| 49:B2:70:GLN:HG2    | 49:B2:71:ASN:H     | 1.71                     | 0.56              |
| 52:B5:20:ARG:HA     | 52:B5:23:HIS:ND1   | 2.20                     | 0.56              |
| 1:CA:706:A:H1'      | 11:CK:29:ILE:HD11  | 1.87                     | 0.56              |
| 1:CA:968:A:H5''     | 1:CA:969:A:OP2     | 2.04                     | 0.56              |
| 1:CA:1316:G:N1      | 1:CA:1319:A:OP2    | 2.38                     | 0.56              |
| 2:CB:25:ASN:ND2     | 2:CB:193:ASP:HB3   | 2.21                     | 0.56              |
| 4:CD:189:PRO:HB2    | 4:CD:194:LEU:CD2   | 2.35                     | 0.56              |
| 5:CE:131:ILE:O      | 5:CE:134:ALA:HB3   | 2.05                     | 0.56              |
| 9:CI:8:GLY:HA2      | 9:CI:79:LEU:CD1    | 2.35                     | 0.56              |
| 9:CI:19:LEU:HD22    | 9:CI:59:PHE:HB2    | 1.76                     | 0.56              |
| 13:CM:116:THR:O     | 13:CM:117:VAL:CG1  | 2.54                     | 0.56              |
| 13:CM:121:LYS:O     | 13:CM:122:LYS:HB2  | 2.06                     | 0.56              |
| 20:CT:53:LEU:HD13   | 20:CT:53:LEU:H     | 1.68                     | 0.56              |
| 23:CW:38:A:H2'      | 23:CW:39:U:H5''    | 1.88                     | 0.56              |
| 23:CY:29:G:N2       | 23:CY:30:G:H1'     | 2.20                     | 0.56              |
| 25:DA:51:G:O2'      | 25:DA:119:A:N1     | 2.35                     | 0.56              |
| 25:DA:265:A:H61     | 25:DA:428:A:H1'    | 1.69                     | 0.56              |
| 25:DA:362(F):A:HO2' | 25:DA:364:C:H5     | 1.52                     | 0.56              |
| 25:DA:568:U:P       | 25:DA:945:A:H61    | 2.28                     | 0.56              |
| 29:DE:16:ARG:O      | 29:DE:17:ASP:HB3   | 2.04                     | 0.56              |
| 29:DE:91:VAL:HG13   | 29:DE:95:ILE:HG12  | 1.88                     | 0.56              |
| 29:DE:101:ARG:HB2   | 29:DE:201:THR:CG2  | 2.36                     | 0.56              |
| 30:DF:9:ILE:HG23    | 30:DF:20:LEU:O     | 2.05                     | 0.56              |
| 30:DF:206:ILE:HD12  | 30:DF:207:GLY:N    | 2.21                     | 0.56              |
| 31:DG:22:ARG:HH12   | 31:DG:175:LEU:HD21 | 1.70                     | 0.56              |
| 31:DG:136:ARG:O     | 31:DG:137:GLU:C    | 2.47                     | 0.56              |
| 32:DH:154:PRO:HD3   | 32:DH:161:GLY:CA   | 2.35                     | 0.56              |
| 33:DI:76:THR:HG22   | 33:DI:77:LEU:N     | 2.19                     | 0.56              |
| 36:DP:105:LEU:O     | 36:DP:106:LEU:HB2  | 2.05                     | 0.56              |
| 37:DQ:54:MET:HB3    | 37:DQ:64:ILE:CD1   | 2.30                     | 0.56              |
| 38:DR:18:LEU:HD11   | 38:DR:22:ARG:CZ    | 2.35                     | 0.56              |
| 38:DR:28:LEU:HD13   | 38:DR:28:LEU:C     | 2.30                     | 0.56              |
| 41:DU:91:ASP:CG     | 41:DU:96:ALA:HB2   | 2.30                     | 0.56              |
| 42:DV:49:THR:HB     | 42:DV:50:PRO:HD2   | 1.84                     | 0.56              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 46:DZ:37:VAL:O     | 46:DZ:38:TYR:HB3   | 2.03                     | 0.56              |
| 47:D0:25:ARG:HD2   | 47:D0:29:GLN:HE22  | 1.68                     | 0.56              |
| 48:D1:14:VAL:HG12  | 48:D1:14:VAL:O     | 2.05                     | 0.56              |
| 1:AA:6:G:H2'       | 5:AE:119:LEU:HD11  | 1.88                     | 0.56              |
| 1:AA:625:G:H4'     | 16:AP:16:HIS:CD2   | 2.41                     | 0.56              |
| 6:AF:7:ASN:OD1     | 6:AF:7:ASN:N       | 2.36                     | 0.56              |
| 8:AH:127:LEU:HB3   | 8:AH:129:VAL:HG13  | 1.87                     | 0.56              |
| 15:AO:17:ARG:HG2   | 15:AO:21:ASP:OD1   | 2.06                     | 0.56              |
| 17:AQ:78:GLU:OE1   | 17:AQ:81:ARG:HD2   | 2.05                     | 0.56              |
| 20:AT:29:LYS:O     | 20:AT:33:ILE:HG12  | 2.04                     | 0.56              |
| 23:AW:39:U:O2      | 23:AW:39:U:H3'     | 2.05                     | 0.56              |
| 25:BA:34:C:C2'     | 25:BA:35:G:O5'     | 2.51                     | 0.56              |
| 25:BA:221:A:C8     | 25:BA:266:G:C6     | 2.93                     | 0.56              |
| 25:BA:660:G:H21    | 36:BP:12:ALA:HA    | 1.69                     | 0.56              |
| 25:BA:1668:A:H61   | 25:BA:1676:A:H61   | 1.54                     | 0.56              |
| 26:BB:14:U:H3'     | 26:BB:14:U:H6      | 1.69                     | 0.56              |
| 28:BD:127:VAL:HA   | 28:BD:193:VAL:HG22 | 1.86                     | 0.56              |
| 29:BE:3:GLY:HA3    | 29:BE:81:ILE:HD12  | 1.88                     | 0.56              |
| 29:BE:116:VAL:HG23 | 29:BE:120:TRP:HD1  | 1.70                     | 0.56              |
| 30:BF:9:ILE:HG23   | 30:BF:11:VAL:O     | 2.06                     | 0.56              |
| 38:BR:37:THR:HG21  | 38:BR:40:LYS:HE3   | 1.87                     | 0.56              |
| 41:BU:14:HIS:C     | 41:BU:16:LYS:N     | 2.62                     | 0.56              |
| 41:BU:82:GLY:O     | 41:BU:86:ALA:N     | 2.27                     | 0.56              |
| 45:BY:74:PRO:O     | 45:BY:75:ILE:HB    | 2.05                     | 0.56              |
| 50:B3:4:LEU:HD12   | 50:B3:39:ASP:HB2   | 1.88                     | 0.56              |
| 53:B6:11:LEU:HG    | 53:B6:26:ASN:HD22  | 1.69                     | 0.56              |
| 1:CA:31:G:H2'      | 1:CA:48:C:N4       | 2.20                     | 0.56              |
| 1:CA:265:G:H4'     | 17:CQ:66:SER:HA    | 1.86                     | 0.56              |
| 2:CB:68:ILE:CD1    | 2:CB:161:ALA:HB3   | 2.36                     | 0.56              |
| 5:CE:11:ILE:HD11   | 5:CE:31:LEU:HD12   | 1.88                     | 0.56              |
| 7:CG:153:HIS:HE1   | 11:CK:57:THR:HG23  | 1.71                     | 0.56              |
| 8:CH:2:LEU:HD13    | 8:CH:3:THR:N       | 2.20                     | 0.56              |
| 8:CH:39:LEU:HD13   | 8:CH:111:ILE:HD11  | 1.86                     | 0.56              |
| 9:CI:126:SER:O     | 9:CI:127:LYS:CB    | 2.51                     | 0.56              |
| 10:CJ:33:GLN:H     | 10:CJ:75:ILE:HG12  | 1.69                     | 0.56              |
| 13:CM:23:TYR:CE1   | 13:CM:70:LEU:HD12  | 2.40                     | 0.56              |
| 20:CT:97:ALA:O     | 20:CT:99:LEU:HG    | 2.05                     | 0.56              |
| 22:CV:35:C:H2'     | 22:CV:36:A:H8      | 1.70                     | 0.56              |
| 23:CW:14:A:N3      | 23:CW:14:A:H2'     | 2.18                     | 0.56              |
| 25:DA:28:A:N6      | 25:DA:512:G:H1'    | 2.20                     | 0.56              |
| 25:DA:1694:C:H4'   | 25:DA:1695:G:N3    | 2.19                     | 0.56              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:DA:1854:A:H62  | 25:DA:1888:G:H8    | 1.54                     | 0.56              |
| 25:DA:2712:U:HO2' | 25:DA:2712(A):A:P  | 2.28                     | 0.56              |
| 30:DF:65:TRP:HZ3  | 30:DF:73:ALA:O     | 1.88                     | 0.56              |
| 30:DF:153:SER:OG  | 30:DF:189:THR:HA   | 2.04                     | 0.56              |
| 32:DH:94:TYR:CD2  | 32:DH:107:VAL:HG12 | 2.41                     | 0.56              |
| 32:DH:152:ARG:O   | 32:DH:153:LYS:CD   | 2.51                     | 0.56              |
| 38:DR:17:ARG:HH11 | 38:DR:17:ARG:CG    | 2.13                     | 0.56              |
| 40:DT:128:GLU:C   | 40:DT:128:GLU:CD   | 2.73                     | 0.56              |
| 46:DZ:136:PHE:O   | 46:DZ:137:ILE:HD13 | 2.05                     | 0.56              |
| 46:DZ:166:SER:HB2 | 46:DZ:168:GLU:N    | 2.19                     | 0.56              |
| 8:AH:95:VAL:HB    | 8:AH:99:GLU:CB     | 2.35                     | 0.56              |
| 9:AI:4:TYR:HB2    | 9:AI:19:LEU:HB2    | 1.86                     | 0.56              |
| 11:AK:32:ILE:HG12 | 11:AK:41:THR:O     | 2.06                     | 0.56              |
| 17:AQ:82:MET:O    | 17:AQ:86:GLU:HG2   | 2.06                     | 0.56              |
| 22:AV:34:U:C2     | 22:AV:36:A:H5''    | 2.41                     | 0.56              |
| 22:AV:38:A:N1     | 24:AX:16:A:C6      | 2.74                     | 0.56              |
| 25:BA:893:C:H6    | 25:BA:893:C:O5'    | 1.89                     | 0.56              |
| 25:BA:956:G:C4'   | 37:BQ:83:MET:HE1   | 2.35                     | 0.56              |
| 25:BA:1819:A:H1'  | 25:BA:1821:A:C5    | 2.41                     | 0.56              |
| 25:BA:2443:C:H2'  | 25:BA:2444:G:H8    | 1.71                     | 0.56              |
| 34:BN:66:LYS:O    | 34:BN:70:LYS:HB3   | 2.05                     | 0.56              |
| 41:BU:58:ARG:O    | 41:BU:62:ILE:HD13  | 2.05                     | 0.56              |
| 42:BV:38:LEU:C    | 42:BV:39:LEU:HD13  | 2.30                     | 0.56              |
| 45:BY:7:VAL:HB    | 45:BY:8:LYS:HZ2    | 1.70                     | 0.56              |
| 1:CA:263:A:OP2    | 20:CT:79:ARG:NH1   | 2.38                     | 0.56              |
| 1:CA:607:A:C2     | 16:CP:31:LYS:HG3   | 2.40                     | 0.56              |
| 3:CC:54:ARG:NH1   | 3:CC:56:ASP:OD1    | 2.38                     | 0.56              |
| 5:CE:144:THR:O    | 5:CE:148:VAL:HG23  | 2.05                     | 0.56              |
| 10:CJ:50:ILE:HG12 | 14:CN:41:ARG:HD3   | 1.88                     | 0.56              |
| 13:CM:82:MET:O    | 13:CM:84:ILE:N     | 2.37                     | 0.56              |
| 13:CM:126:LYS:O   | 13:CM:126:LYS:CG   | 2.53                     | 0.56              |
| 19:CS:10:PHE:CZ   | 19:CS:70:LYS:HE2   | 2.40                     | 0.56              |
| 25:DA:458:G:O3'   | 25:DA:459:U:H6     | 1.88                     | 0.56              |
| 25:DA:1110:G:H2'  | 25:DA:1111:A:H8    | 1.69                     | 0.56              |
| 25:DA:1615:C:OP2  | 25:DA:1617:C:N4    | 2.37                     | 0.56              |
| 25:DA:1756:G:H4'  | 25:DA:1758:G:O4'   | 2.06                     | 0.56              |
| 25:DA:1952:A:C5   | 35:DO:22:ILE:HD12  | 2.41                     | 0.56              |
| 25:DA:2134:A:H62  | 25:DA:2157:G:H1'   | 1.69                     | 0.56              |
| 28:DD:44:ASN:CB   | 28:DD:48:ARG:O     | 2.53                     | 0.56              |
| 35:DO:4:PRO:O     | 35:DO:5:GLN:HB2    | 2.06                     | 0.56              |
| 42:DV:55:ALA:HB2  | 42:DV:101:GLY:OXT  | 2.05                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 43:DW:76:VAL:HG22 | 43:DW:102:HIS:O   | 2.06                     | 0.56              |
| 45:DY:73:ARG:NH2  | 45:DY:82:PRO:HD3  | 2.20                     | 0.56              |
| 46:DZ:99:TYR:CD2  | 46:DZ:99:TYR:N    | 2.71                     | 0.56              |
| 50:D3:29:ARG:HB2  | 50:D3:33:GLN:HE22 | 1.70                     | 0.56              |
| 1:AA:652:U:C4     | 1:AA:752:G:N3     | 2.73                     | 0.56              |
| 1:AA:1050:G:H2'   | 1:AA:1050:G:N3    | 2.19                     | 0.56              |
| 1:AA:1370:G:H5''  | 9:AI:12:GLU:HG3   | 1.88                     | 0.56              |
| 2:AB:71:VAL:HG22  | 2:AB:93:VAL:CG2   | 2.35                     | 0.56              |
| 3:AC:16:ARG:HH11  | 3:AC:16:ARG:CB    | 2.19                     | 0.56              |
| 8:AH:73:ASP:OD2   | 8:AH:75:ARG:HD3   | 2.06                     | 0.56              |
| 10:AJ:22:LYS:NZ   | 10:AJ:23:ILE:HG23 | 2.20                     | 0.56              |
| 12:AL:41:ARG:HD2  | 12:AL:43:VAL:HG12 | 1.88                     | 0.56              |
| 16:AP:21:VAL:O    | 16:AP:33:ILE:HG12 | 2.04                     | 0.56              |
| 21:AU:18:TYR:CD1  | 21:AU:24:ARG:CZ   | 2.89                     | 0.56              |
| 23:AW:38:A:H3'    | 23:AW:39:U:H5'    | 1.88                     | 0.56              |
| 25:BA:6:A:O2'     | 34:BN:130:HIS:HB3 | 2.05                     | 0.56              |
| 25:BA:528:A:C2    | 25:BA:2042:A:H2'  | 2.40                     | 0.56              |
| 25:BA:2127:G:C5   | 25:BA:2162:G:N2   | 2.73                     | 0.56              |
| 25:BA:2458:G:C4   | 25:BA:2490:G:N1   | 2.73                     | 0.56              |
| 29:BE:110:GLY:HA3 | 29:BE:162:ALA:HB2 | 1.88                     | 0.56              |
| 30:BF:51:THR:CG2  | 30:BF:92:PRO:N    | 2.67                     | 0.56              |
| 32:BH:71:LEU:O    | 32:BH:74:ASN:HB2  | 2.06                     | 0.56              |
| 32:BH:72:ILE:O    | 32:BH:76:VAL:HG23 | 2.05                     | 0.56              |
| 35:BO:24:VAL:HA   | 35:BO:39:ILE:HG22 | 1.87                     | 0.56              |
| 36:BP:52:GLU:OE1  | 36:BP:55:ARG:NH2  | 2.32                     | 0.56              |
| 36:BP:65:ARG:NH1  | 55:B8:15:LYS:HB2  | 2.18                     | 0.56              |
| 36:BP:111:ARG:HG3 | 36:BP:128:HIS:ND1 | 2.20                     | 0.56              |
| 39:BS:13:ARG:HG3  | 39:BS:13:ARG:NH1  | 2.20                     | 0.56              |
| 42:BV:46:VAL:O    | 42:BV:47:VAL:HG13 | 2.06                     | 0.56              |
| 45:BY:2:ARG:C     | 45:BY:4:LYS:H     | 2.13                     | 0.56              |
| 47:B0:51:VAL:HG21 | 47:B0:79:VAL:O    | 2.06                     | 0.56              |
| 1:CA:411:A:C5     | 1:CA:413:G:H1'    | 2.41                     | 0.56              |
| 1:CA:873:A:H8     | 1:CA:873:A:O5'    | 1.89                     | 0.56              |
| 2:CB:109:SER:C    | 2:CB:111:ARG:H    | 2.13                     | 0.56              |
| 5:CE:100:VAL:C    | 5:CE:101:ILE:HD13 | 2.31                     | 0.56              |
| 9:CI:2:GLU:HG2    | 9:CI:2:GLU:O      | 2.04                     | 0.56              |
| 10:CJ:47:PHE:CZ   | 14:CN:37:PHE:CE2  | 2.94                     | 0.56              |
| 12:CL:18:VAL:HG23 | 12:CL:19:ARG:N    | 2.21                     | 0.56              |
| 22:CV:30:G:C2'    | 22:CV:31:G:O5'    | 2.54                     | 0.56              |
| 22:CV:65:G:H2'    | 22:CV:66:C:O4'    | 2.06                     | 0.56              |
| 23:CW:21:A:N6     | 23:CW:46:G:C4     | 2.74                     | 0.56              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:DA:13:A:H61     | 25:DA:525:U:H3'    | 1.69                     | 0.56              |
| 25:DA:529:A:H5'    | 25:DA:530:G:OP1    | 2.05                     | 0.56              |
| 25:DA:1212:G:H1'   | 25:DA:1237:A:H62   | 1.70                     | 0.56              |
| 25:DA:1992:G:H5'   | 25:DA:1994:C:H41   | 1.70                     | 0.56              |
| 25:DA:2090:G:H21   | 48:D1:45:ASN:ND2   | 1.99                     | 0.56              |
| 29:DE:111:ARG:HE   | 29:DE:160:TYR:HE1  | 1.51                     | 0.56              |
| 31:DG:96:ARG:HH11  | 31:DG:96:ARG:HG3   | 1.70                     | 0.56              |
| 35:DO:110:GLY:HA2  | 35:DO:112:MET:HE3  | 1.86                     | 0.56              |
| 36:DP:107:LYS:C    | 36:DP:109:GLY:H    | 2.12                     | 0.56              |
| 38:DR:86:ARG:HB3   | 38:DR:118:GLU:OE2  | 2.06                     | 0.56              |
| 44:DX:25:LYS:HD2   | 44:DX:82:GLN:OE1   | 2.05                     | 0.56              |
| 1:AA:1126:U:H6     | 1:AA:1126:U:OP1    | 1.87                     | 0.56              |
| 1:AA:1128:C:H4'    | 9:AI:16:ARG:HH12   | 1.70                     | 0.56              |
| 1:AA:1157:A:C4'    | 1:AA:1158:C:O5'    | 2.52                     | 0.56              |
| 3:AC:139:GLN:O     | 3:AC:143:GLU:HB2   | 2.05                     | 0.56              |
| 4:AD:8:VAL:O       | 4:AD:11:LEU:HD23   | 2.04                     | 0.56              |
| 5:AE:11:ILE:HD12   | 5:AE:31:LEU:HD12   | 1.88                     | 0.56              |
| 21:AU:25:LYS:HB2   | 21:AU:25:LYS:HZ2   | 1.71                     | 0.56              |
| 22:AV:63:C:H2'     | 22:AV:64:G:H8      | 1.70                     | 0.56              |
| 23:AY:29:G:H2'     | 23:AY:29:G:N3      | 2.21                     | 0.56              |
| 25:BA:1268:A:H2'   | 25:BA:1269:A:O4'   | 2.06                     | 0.56              |
| 25:BA:1451:C:H4'   | 25:BA:1452:A:O5'   | 2.06                     | 0.56              |
| 25:BA:1820:U:H5''  | 25:BA:1821:A:OP2   | 2.06                     | 0.56              |
| 25:BA:2751:G:H4'   | 25:BA:2752:C:OP1   | 2.05                     | 0.56              |
| 26:BB:34:U:H5''    | 26:BB:35:U:OP1     | 2.05                     | 0.56              |
| 28:BD:155:LEU:HD23 | 28:BD:177:LEU:HD22 | 1.86                     | 0.56              |
| 28:BD:226:MET:O    | 28:BD:234:GLY:CA   | 2.54                     | 0.56              |
| 29:BE:179:GLU:O    | 29:BE:180:ASN:HB2  | 2.06                     | 0.56              |
| 36:BP:46:LYS:HG2   | 36:BP:51:PHE:CE2   | 2.41                     | 0.56              |
| 38:BR:103:ARG:CB   | 38:BR:109:ALA:C    | 2.78                     | 0.56              |
| 39:BS:42:ASP:C     | 39:BS:44:LYS:H     | 2.13                     | 0.56              |
| 40:BT:13:ARG:HA    | 40:BT:13:ARG:CZ    | 2.36                     | 0.56              |
| 40:BT:117:ASP:OD2  | 40:BT:120:ARG:NE   | 2.38                     | 0.56              |
| 43:BW:8:ARG:HH11   | 43:BW:8:ARG:HB3    | 1.71                     | 0.56              |
| 43:BW:82:LEU:HB3   | 43:BW:84:ARG:NH1   | 2.19                     | 0.56              |
| 45:BY:55:TYR:HD1   | 45:BY:56:PRO:HG2   | 1.69                     | 0.56              |
| 46:BZ:63:ASP:C     | 46:BZ:65:GLN:H     | 2.13                     | 0.56              |
| 48:B1:89:GLU:HA    | 48:B1:92:LYS:HB3   | 1.88                     | 0.56              |
| 1:CA:365:U:O2'     | 1:CA:366:C:C5      | 2.58                     | 0.56              |
| 1:CA:817:C:H4'     | 1:CA:818:G:O5'     | 2.03                     | 0.56              |
| 3:CC:31:HIS:ND1    | 3:CC:31:HIS:N      | 2.53                     | 0.56              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 10:CJ:22:LYS:C    | 10:CJ:22:LYS:HD2   | 2.31                     | 0.56              |
| 15:CO:82:ILE:HG22 | 15:CO:83:GLU:N     | 2.21                     | 0.56              |
| 19:CS:33:THR:OG1  | 19:CS:34:TRP:N     | 2.39                     | 0.56              |
| 25:DA:483:A:H4'   | 45:DY:49:VAL:CG1   | 2.35                     | 0.56              |
| 25:DA:2126:A:H4'  | 25:DA:2127:G:O5'   | 2.05                     | 0.56              |
| 25:DA:2267:A:H5'' | 25:DA:2268:A:H5'   | 1.87                     | 0.56              |
| 25:DA:2282:G:O2'  | 25:DA:2283:C:OP2   | 2.19                     | 0.56              |
| 30:DF:168:ARG:HG3 | 30:DF:175:THR:HG21 | 1.87                     | 0.56              |
| 31:DG:146:TYR:C   | 31:DG:148:MET:H    | 2.13                     | 0.56              |
| 34:DN:126:PRO:O   | 34:DN:127:ASP:HB2  | 2.05                     | 0.56              |
| 36:DP:127:ALA:O   | 36:DP:147:LEU:HA   | 2.06                     | 0.56              |
| 43:DW:68:ARG:HH22 | 43:DW:112:GLY:HA2  | 1.71                     | 0.56              |
| 45:DY:43:ASN:HB3  | 45:DY:64:GLU:HA    | 1.88                     | 0.56              |
| 46:DZ:17:ALA:O    | 46:DZ:20:ARG:HB2   | 2.05                     | 0.56              |
| 46:DZ:61:LEU:HD12 | 46:DZ:65:GLN:NE2   | 2.21                     | 0.56              |
| 50:D3:8:LEU:HD12  | 50:D3:31:LEU:HA    | 1.88                     | 0.56              |
| 1:AA:243:A:C4'    | 1:AA:244:U:O5'     | 2.43                     | 0.56              |
| 2:AB:124:SER:OG   | 2:AB:125:PRO:HD2   | 2.05                     | 0.56              |
| 2:AB:221:LEU:O    | 2:AB:224:GLN:N     | 2.37                     | 0.56              |
| 5:AE:81:GLU:HG2   | 5:AE:90:VAL:HG12   | 1.88                     | 0.56              |
| 5:AE:150:ARG:CZ   | 5:AE:150:ARG:HB2   | 2.35                     | 0.56              |
| 9:AI:5:TYR:HE2    | 9:AI:16:ARG:HB3    | 1.71                     | 0.56              |
| 10:AJ:48:THR:CA   | 10:AJ:62:HIS:HB3   | 2.35                     | 0.56              |
| 20:AT:36:LEU:HD23 | 20:AT:36:LEU:N     | 2.21                     | 0.56              |
| 23:AW:14:A:C6     | 23:AW:15:G:H1'     | 2.40                     | 0.56              |
| 23:AW:37:A:H2'    | 23:AW:38:A:O4'     | 2.06                     | 0.56              |
| 25:BA:74:A:OP2    | 25:BA:74:A:C2      | 2.59                     | 0.56              |
| 25:BA:182:A:N3    | 25:BA:433:C:O2'    | 2.32                     | 0.56              |
| 25:BA:215:G:H4'   | 25:BA:216:A:O5'    | 2.04                     | 0.56              |
| 25:BA:1523:U:H2'  | 25:BA:1524:G:C8    | 2.40                     | 0.56              |
| 25:BA:1680:U:O2'  | 25:BA:1763:G:N7    | 2.31                     | 0.56              |
| 28:BD:26:LYS:CE   | 28:BD:82:ILE:H     | 2.19                     | 0.56              |
| 30:BF:22:ALA:C    | 30:BF:26:ALA:HB2   | 2.31                     | 0.56              |
| 30:BF:194:MET:HE3 | 30:BF:199:TRP:HD1  | 1.70                     | 0.56              |
| 38:BR:55:ALA:HA   | 38:BR:80:PHE:CE1   | 2.41                     | 0.56              |
| 39:BS:85:VAL:C    | 39:BS:106:ARG:HG3  | 2.31                     | 0.56              |
| 41:BU:7:GLY:O     | 41:BU:8:VAL:HG23   | 2.06                     | 0.56              |
| 43:BW:33:ARG:O    | 43:BW:37:ARG:HB2   | 2.05                     | 0.56              |
| 1:CA:49:U:O4      | 1:CA:364:A:N7      | 2.39                     | 0.56              |
| 2:CB:140:HIS:O    | 2:CB:143:GLU:HB2   | 2.05                     | 0.56              |
| 2:CB:200:ILE:HG22 | 2:CB:202:PRO:HD3   | 1.87                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:CE:98:THR:CG2   | 5:CE:99:GLY:O     | 2.51                     | 0.56              |
| 5:CE:126:ARG:CG   | 5:CE:126:ARG:NH1  | 2.68                     | 0.56              |
| 15:CO:82:ILE:CG2  | 15:CO:83:GLU:N    | 2.69                     | 0.56              |
| 25:DA:1818:U:H2'  | 28:DD:157:ARG:HG3 | 1.86                     | 0.56              |
| 28:DD:25:THR:O    | 28:DD:26:LYS:HG2  | 2.05                     | 0.56              |
| 30:DF:31:HIS:CB   | 36:DP:9:ASN:HD21  | 2.16                     | 0.56              |
| 36:DP:46:LYS:HG2  | 36:DP:51:PHE:CE2  | 2.41                     | 0.56              |
| 36:DP:85:LEU:H    | 36:DP:85:LEU:CD2  | 2.19                     | 0.56              |
| 37:DQ:137:TYR:CZ  | 46:DZ:81:ARG:NH2  | 2.65                     | 0.56              |
| 40:DT:16:ARG:HH12 | 40:DT:19:LEU:HG   | 1.71                     | 0.56              |
| 43:DW:64:MET:O    | 43:DW:65:LEU:CB   | 2.54                     | 0.56              |
| 44:DX:24:GLY:O    | 44:DX:82:GLN:HA   | 2.06                     | 0.56              |
| 46:DZ:61:LEU:HB3  | 46:DZ:62:PRO:HD2  | 1.88                     | 0.56              |
| 1:AA:738:C:C5'    | 6:AF:69:GLU:HB2   | 2.22                     | 0.56              |
| 1:AA:1251:A:O2'   | 1:AA:1252:A:O4'   | 2.23                     | 0.56              |
| 2:AB:134:GLU:HA   | 2:AB:137:ARG:HB3  | 1.88                     | 0.56              |
| 3:AC:79:ARG:CZ    | 11:CK:100:ALA:HB2 | 2.36                     | 0.56              |
| 7:AG:41:ARG:O     | 7:AG:42:ILE:C     | 2.48                     | 0.56              |
| 14:AN:23:ARG:O    | 14:AN:24:CYS:C    | 2.47                     | 0.56              |
| 18:AR:58:LEU:H    | 18:AR:58:LEU:HD12 | 1.69                     | 0.56              |
| 22:AV:17:C:H3'    | 22:AV:18:U:H5'    | 1.87                     | 0.56              |
| 25:BA:448:U:C2'   | 30:BF:84:VAL:HG13 | 2.36                     | 0.56              |
| 25:BA:481:G:OP2   | 45:BY:47:LYS:HG3  | 2.06                     | 0.56              |
| 30:BF:64:ILE:C    | 30:BF:65:TRP:HD1  | 2.12                     | 0.56              |
| 30:BF:78:ILE:HD13 | 30:BF:78:ILE:H    | 1.69                     | 0.56              |
| 31:BG:165:THR:OG1 | 31:BG:168:GLU:HB2 | 2.05                     | 0.56              |
| 36:BP:52:GLU:OE1  | 36:BP:55:ARG:HD2  | 2.05                     | 0.56              |
| 42:BV:49:THR:HB   | 42:BV:50:PRO:CD   | 2.34                     | 0.56              |
| 49:B2:44:LEU:O    | 49:B2:45:SER:HB2  | 2.05                     | 0.56              |
| 1:CA:1112:C:H1'   | 3:CC:179:ARG:HD3  | 1.87                     | 0.56              |
| 2:CB:28:PHE:CD1   | 2:CB:190:THR:HA   | 2.41                     | 0.56              |
| 15:CO:66:LEU:H    | 15:CO:66:LEU:HD12 | 1.71                     | 0.56              |
| 19:CS:5:LEU:C     | 19:CS:6:LYS:HE3   | 2.31                     | 0.56              |
| 21:CU:6:ARG:NE    | 21:CU:15:ARG:HH12 | 2.04                     | 0.56              |
| 25:DA:389:G:H22   | 36:DP:72:PRO:HD3  | 1.71                     | 0.56              |
| 25:DA:2286:A:H61  | 53:D6:24:GLU:CB   | 2.16                     | 0.56              |
| 25:DA:2702:U:OP1  | 25:DA:2702:U:H6   | 1.89                     | 0.56              |
| 26:DB:13:A:O2'    | 26:DB:14:U:C5'    | 2.54                     | 0.56              |
| 27:DC:41:VAL:HG12 | 27:DC:213:TYR:HA  | 1.88                     | 0.56              |
| 27:DC:51:PRO:HB2  | 27:DC:203:GLY:O   | 2.05                     | 0.56              |
| 30:DF:175:THR:O   | 30:DF:176:LEU:HB2 | 2.05                     | 0.56              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 31:DG:67:LYS:HE2   | 51:D4:6:HIS:NE2   | 2.19                     | 0.56              |
| 32:DH:17:VAL:HG12  | 32:DH:17:VAL:O    | 2.05                     | 0.56              |
| 33:DI:125:GLU:OE1  | 33:DI:141:LYS:HA  | 2.05                     | 0.56              |
| 40:DT:88:ILE:CG2   | 40:DT:89:VAL:HG23 | 2.29                     | 0.56              |
| 42:DV:38:LEU:O     | 42:DV:51:VAL:HA   | 2.05                     | 0.56              |
| 46:DZ:170:THR:HG22 | 46:DZ:171:ILE:H   | 1.70                     | 0.56              |
| 47:D0:48:GLY:HA3   | 47:D0:80:HIS:ND1  | 2.21                     | 0.56              |
| 48:D1:45:ASN:HD21  | 48:D1:47:GLN:HE21 | 1.50                     | 0.56              |
| 1:AA:261:U:OP2     | 20:AT:79:ARG:NH2  | 2.39                     | 0.56              |
| 1:AA:982:U:O5'     | 1:AA:982:U:C6     | 2.49                     | 0.56              |
| 1:AA:1015:A:N3     | 1:AA:1218:C:O2'   | 2.36                     | 0.56              |
| 1:AA:1380:U:H5''   | 1:AA:1381:U:OP1   | 2.06                     | 0.56              |
| 3:AC:32:LEU:HD22   | 3:AC:59:ARG:NH1   | 2.21                     | 0.56              |
| 6:AF:27:GLN:O      | 6:AF:28:ARG:C     | 2.48                     | 0.56              |
| 6:AF:45:LEU:O      | 6:AF:46:ARG:CG    | 2.53                     | 0.56              |
| 7:AG:26:PHE:HB2    | 7:AG:62:PHE:HZ    | 1.70                     | 0.56              |
| 10:AJ:13:HIS:HE1   | 10:AJ:14:LYS:HE3  | 1.70                     | 0.56              |
| 10:AJ:67:THR:O     | 10:AJ:67:THR:HG23 | 2.06                     | 0.56              |
| 12:AL:6:THR:N      | 12:AL:9:GLN:HE21  | 2.03                     | 0.56              |
| 13:AM:25:ILE:N     | 13:AM:25:ILE:CD1  | 2.68                     | 0.56              |
| 13:AM:89:GLY:C     | 13:AM:90:LEU:O    | 2.47                     | 0.56              |
| 22:AV:40:C:H2'     | 22:AV:41:C:H6     | 1.69                     | 0.56              |
| 24:AX:13:A:H3'     | 24:AX:14:A:H5''   | 1.86                     | 0.56              |
| 25:BA:221:A:C5     | 25:BA:266:G:C5    | 2.94                     | 0.56              |
| 25:BA:489:G:N7     | 43:BW:49:LYS:NZ   | 2.52                     | 0.56              |
| 25:BA:670:A:C8     | 25:BA:670:A:OP2   | 2.59                     | 0.56              |
| 25:BA:1171:G:H3'   | 25:BA:1173:G:H4'  | 1.88                     | 0.56              |
| 25:BA:2168:G:H22   | 25:BA:2171:A:P    | 2.28                     | 0.56              |
| 28:BD:45:ASN:O     | 28:BD:46:GLN:HG3  | 2.05                     | 0.56              |
| 32:BH:61:HIS:HA    | 32:BH:64:LEU:HD12 | 1.87                     | 0.56              |
| 33:BI:38:LEU:H     | 33:BI:38:LEU:CD1  | 2.01                     | 0.56              |
| 34:BN:3:THR:HG22   | 34:BN:5:VAL:CG1   | 2.35                     | 0.56              |
| 36:BP:85:LEU:H     | 36:BP:85:LEU:CD2  | 2.19                     | 0.56              |
| 42:BV:39:LEU:C     | 42:BV:40:LEU:HD23 | 2.31                     | 0.56              |
| 43:BW:4:LYS:CE     | 43:BW:6:ILE:HD12  | 2.33                     | 0.56              |
| 50:B3:48:GLU:O     | 50:B3:51:ALA:HB2  | 2.06                     | 0.56              |
| 1:CA:828:A:H62     | 1:CA:858:G:H21    | 1.54                     | 0.56              |
| 1:CA:1144:G:C2     | 1:CA:1145:C:O2    | 2.59                     | 0.56              |
| 2:CB:28:PHE:O      | 2:CB:28:PHE:CG    | 2.58                     | 0.56              |
| 2:CB:98:LEU:HD23   | 2:CB:98:LEU:N     | 2.21                     | 0.56              |
| 2:CB:155:LEU:HG    | 2:CB:159:PRO:HG3  | 1.88                     | 0.56              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 16:CP:19:ILE:HB   | 16:CP:37:GLY:CA    | 2.36                     | 0.56              |
| 18:CR:59:SER:N    | 18:CR:62:GLU:HB2   | 2.21                     | 0.56              |
| 23:CW:57:G:H2'    | 23:CW:58:A:C5'     | 2.35                     | 0.56              |
| 23:CY:28:G:C4     | 23:CY:29:G:N7      | 2.74                     | 0.56              |
| 25:DA:34:C:N4     | 25:DA:454:A:O2'    | 2.38                     | 0.56              |
| 25:DA:890:A:N6    | 25:DA:892:G:O6     | 2.39                     | 0.56              |
| 25:DA:1342:A:C5   | 25:DA:1397:U:C6    | 2.94                     | 0.56              |
| 25:DA:1902:C:C5'  | 28:DD:246:PRO:HD3  | 2.36                     | 0.56              |
| 25:DA:2171:A:C4'  | 25:DA:2172:U:OP1   | 2.43                     | 0.56              |
| 25:DA:2667:C:H1'  | 32:DH:109:PHE:HD2  | 1.71                     | 0.56              |
| 26:DB:66:A:N6     | 26:DB:108:U:C6     | 2.74                     | 0.56              |
| 27:DC:77:ILE:HD11 | 27:DC:100:ILE:HD11 | 1.88                     | 0.56              |
| 32:DH:153:LYS:HG3 | 32:DH:161:GLY:HA3  | 1.88                     | 0.56              |
| 33:DI:77:LEU:CD1  | 33:DI:78:THR:N     | 2.69                     | 0.56              |
| 37:DQ:51:ARG:O    | 37:DQ:55:VAL:HG12  | 2.05                     | 0.56              |
| 40:DT:42:ILE:HD12 | 40:DT:42:ILE:N     | 2.14                     | 0.56              |
| 41:DU:101:ARG:C   | 41:DU:102:GLU:CG   | 2.79                     | 0.56              |
| 44:DX:60:ARG:HH22 | 54:D7:47:ARG:NE    | 2.03                     | 0.56              |
| 1:AA:279:A:H1'    | 1:AA:281:G:C6      | 2.41                     | 0.55              |
| 1:AA:397:A:N7     | 1:AA:547:A:O2'     | 2.36                     | 0.55              |
| 1:AA:1300:G:O2'   | 1:AA:1301:U:P      | 2.63                     | 0.55              |
| 4:AD:108:LEU:O    | 4:AD:109:GLY:C     | 2.49                     | 0.55              |
| 8:AH:40:ALA:C     | 8:AH:42:GLU:N      | 2.65                     | 0.55              |
| 9:AI:40:LEU:C     | 9:AI:42:ARG:H      | 2.14                     | 0.55              |
| 10:AJ:24:VAL:HG22 | 10:AJ:72:VAL:HG11  | 1.87                     | 0.55              |
| 11:AK:20:TYR:O    | 11:AK:30:VAL:HG12  | 2.06                     | 0.55              |
| 20:AT:49:ALA:C    | 20:AT:100:ILE:HD11 | 2.31                     | 0.55              |
| 24:AX:22:A:H2'    | 24:AX:22:A:N3      | 2.20                     | 0.55              |
| 25:BA:866:A:C6    | 25:BA:914:C:C6     | 2.94                     | 0.55              |
| 25:BA:1336:A:H2'  | 25:BA:1337:G:H8    | 1.70                     | 0.55              |
| 25:BA:1719:G:C2'  | 25:BA:1720:U:H5'   | 2.36                     | 0.55              |
| 25:BA:1902:C:O2'  | 28:BD:244:ARG:CG   | 2.54                     | 0.55              |
| 27:BC:21:THR:HG21 | 27:BC:191:ALA:CB   | 2.36                     | 0.55              |
| 28:BD:81:ALA:HA   | 28:BD:113:VAL:HG13 | 1.88                     | 0.55              |
| 30:BF:1:MET:SD    | 30:BF:26:ALA:HA    | 2.46                     | 0.55              |
| 33:BI:114:LEU:O   | 33:BI:115:ALA:HB3  | 2.06                     | 0.55              |
| 35:BO:80:ASP:H    | 40:BT:70:VAL:CG1   | 2.19                     | 0.55              |
| 36:BP:107:LYS:C   | 36:BP:109:GLY:N    | 2.63                     | 0.55              |
| 36:BP:128:HIS:O   | 36:BP:147:LEU:HB3  | 2.06                     | 0.55              |
| 38:BR:37:THR:HG23 | 38:BR:40:LYS:HB2   | 1.86                     | 0.55              |
| 51:B4:56:GLU:O    | 51:B4:57:ILE:HD13  | 2.06                     | 0.55              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 51:B4:57:ILE:HG22  | 51:B4:57:ILE:O    | 2.05                     | 0.55              |
| 1:CA:871:U:H4'     | 1:CA:872:A:OP1    | 2.05                     | 0.55              |
| 2:CB:31:TYR:HD1    | 2:CB:202:PRO:HB3  | 1.69                     | 0.55              |
| 3:CC:148:GLY:HA3   | 3:CC:172:ARG:O    | 2.06                     | 0.55              |
| 3:CC:173:VAL:HG12  | 3:CC:175:LEU:HG   | 1.88                     | 0.55              |
| 4:CD:146:ILE:HD12  | 4:CD:146:ILE:N    | 2.21                     | 0.55              |
| 4:CD:176:LEU:CD1   | 4:CD:177:ASP:H    | 2.12                     | 0.55              |
| 9:CI:17:VAL:HG21   | 9:CI:81:ILE:HD13  | 1.88                     | 0.55              |
| 12:CL:27:LEU:HD22  | 12:CL:27:LEU:N    | 2.21                     | 0.55              |
| 12:CL:46:LYS:O     | 12:CL:47:LYS:C    | 2.48                     | 0.55              |
| 12:CL:58:VAL:O     | 12:CL:65:GLU:HA   | 2.06                     | 0.55              |
| 15:CO:62:GLN:O     | 15:CO:63:ARG:C    | 2.49                     | 0.55              |
| 17:CQ:52:LYS:O     | 17:CQ:55:ASP:CG   | 2.49                     | 0.55              |
| 22:CV:2:G:H2'      | 22:CV:3:C:H6      | 1.71                     | 0.55              |
| 22:CV:30:G:O6      | 22:CV:43:G:C6     | 2.59                     | 0.55              |
| 22:CV:30:G:H2'     | 22:CV:31:G:O5'    | 2.06                     | 0.55              |
| 29:DE:176:ILE:HG23 | 29:DE:178:GLU:HB3 | 1.87                     | 0.55              |
| 33:DI:61:ARG:HH21  | 33:DI:64:GLU:CD   | 2.13                     | 0.55              |
| 36:DP:85:LEU:CA    | 36:DP:88:LEU:HB3  | 2.32                     | 0.55              |
| 46:DZ:19:ARG:HH12  | 46:DZ:84:GLU:C    | 2.14                     | 0.55              |
| 47:D0:53:MET:CB    | 47:D0:59:LEU:HD23 | 2.29                     | 0.55              |
| 50:D3:6:VAL:HG12   | 50:D3:56:VAL:HG13 | 1.88                     | 0.55              |
| 50:D3:23:LEU:HD12  | 50:D3:23:LEU:N    | 2.20                     | 0.55              |
| 53:D6:13:CYS:HB2   | 53:D6:22:ALA:HB3  | 1.88                     | 0.55              |
| 55:D8:6:THR:HB     | 55:D8:63:PRO:HG3  | 1.87                     | 0.55              |
| 1:AA:9:G:H5''      | 5:AE:122:GLU:OE1  | 2.06                     | 0.55              |
| 1:AA:939:G:H5''    | 7:AG:102:ARG:NH1  | 2.21                     | 0.55              |
| 1:AA:1101:A:H4'    | 1:AA:1102:A:O5'   | 2.06                     | 0.55              |
| 1:AA:1201:A:C4'    | 1:AA:1202:G:O5'   | 2.36                     | 0.55              |
| 1:AA:1251:A:O2'    | 1:AA:1369:C:O2'   | 2.21                     | 0.55              |
| 2:AB:78:GLN:HG2    | 2:AB:94:ASN:HD22  | 1.71                     | 0.55              |
| 3:AC:110:ASN:O     | 3:AC:141:VAL:HG22 | 2.06                     | 0.55              |
| 6:AF:91:VAL:CG1    | 18:AR:72:ARG:HH11 | 2.14                     | 0.55              |
| 8:AH:21:LYS:N      | 8:AH:65:TYR:OH    | 2.39                     | 0.55              |
| 10:AJ:22:LYS:HE3   | 10:AJ:23:ILE:HG12 | 1.88                     | 0.55              |
| 17:AQ:33:GLY:O     | 17:AQ:34:LYS:O    | 2.24                     | 0.55              |
| 25:BA:32:C:C2'     | 25:BA:33:U:H5'    | 2.35                     | 0.55              |
| 25:BA:196:A:H5''   | 36:BP:46:LYS:HE3  | 1.89                     | 0.55              |
| 25:BA:322:A:C5'    | 25:BA:323:G:OP2   | 2.53                     | 0.55              |
| 25:BA:631:A:OP1    | 36:BP:64:LYS:HE2  | 2.07                     | 0.55              |
| 25:BA:956:G:OP2    | 37:BQ:14:ARG:NH2  | 2.33                     | 0.55              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:BA:2136:C:H41   | 25:BA:2156:G:H21   | 1.53                     | 0.55              |
| 25:BA:2712:U:C2'   | 25:BA:2713:A:H5''  | 2.36                     | 0.55              |
| 27:BC:68:LEU:HB3   | 27:BC:70:LYS:HE2   | 1.88                     | 0.55              |
| 28:BD:8:PRO:HB3    | 28:BD:14:ARG:HB2   | 1.86                     | 0.55              |
| 28:BD:13:ARG:CA    | 28:BD:16:MET:HE3   | 2.35                     | 0.55              |
| 28:BD:165:ILE:HG22 | 28:BD:167:GLY:H    | 1.72                     | 0.55              |
| 31:BG:113:ARG:O    | 31:BG:114:ILE:C    | 2.50                     | 0.55              |
| 32:BH:149:ARG:HD3  | 32:BH:164:TYR:CD1  | 2.41                     | 0.55              |
| 35:BO:119:PRO:O    | 35:BO:120:GLU:HB2  | 2.06                     | 0.55              |
| 40:BT:77:PRO:O     | 40:BT:78:LEU:CB    | 2.53                     | 0.55              |
| 45:BY:20:TYR:CE1   | 45:BY:42:VAL:HA    | 2.41                     | 0.55              |
| 1:CA:566:G:OP1     | 1:CA:566:G:C8      | 2.45                     | 0.55              |
| 1:CA:1051:C:C4     | 1:CA:1052:U:O4     | 2.59                     | 0.55              |
| 1:CA:1064:G:OP1    | 1:CA:1386:G:H4'    | 2.06                     | 0.55              |
| 1:CA:1225:A:H2'    | 1:CA:1225:A:N3     | 2.20                     | 0.55              |
| 1:CA:1391:U:H2'    | 1:CA:1392:G:C8     | 2.40                     | 0.55              |
| 2:CB:220:ASP:O     | 2:CB:223:ILE:HG12  | 2.06                     | 0.55              |
| 3:CC:7:PRO:O       | 3:CC:11:ARG:HG2    | 2.06                     | 0.55              |
| 4:CD:106:TYR:CE1   | 4:CD:113:SER:HA    | 2.41                     | 0.55              |
| 9:CI:29:ASN:OD1    | 9:CI:64:THR:HA     | 2.07                     | 0.55              |
| 19:CS:16:LEU:HD11  | 19:CS:41:VAL:HG21  | 1.87                     | 0.55              |
| 19:CS:45:VAL:C     | 19:CS:62:ILE:HG21  | 2.31                     | 0.55              |
| 20:CT:71:THR:HG22  | 20:CT:72:LEU:N     | 2.20                     | 0.55              |
| 25:DA:1428:C:N4    | 25:DA:1570:A:OP2   | 2.30                     | 0.55              |
| 28:DD:43:ARG:HH11  | 28:DD:44:ASN:CG    | 2.13                     | 0.55              |
| 29:DE:65:GLY:HA2   | 29:DE:70:ALA:CB    | 2.37                     | 0.55              |
| 30:DF:127:GLU:HA   | 30:DF:127:GLU:OE1  | 2.05                     | 0.55              |
| 32:DH:118:PRO:HG2  | 32:DH:121:ILE:HD12 | 1.88                     | 0.55              |
| 33:DI:76:THR:HG22  | 33:DI:77:LEU:HD12  | 1.87                     | 0.55              |
| 36:DP:128:HIS:O    | 36:DP:147:LEU:HB3  | 2.06                     | 0.55              |
| 38:DR:107:ASP:C    | 38:DR:107:ASP:OD2  | 2.46                     | 0.55              |
| 40:DT:3:ARG:HB3    | 40:DT:6:LEU:HB2    | 1.87                     | 0.55              |
| 41:DU:104:GLN:CD   | 41:DU:104:GLN:N    | 2.62                     | 0.55              |
| 43:DW:92:ARG:HG2   | 43:DW:92:ARG:NH1   | 2.20                     | 0.55              |
| 43:DW:111:HIS:CD2  | 43:DW:112:GLY:H    | 2.24                     | 0.55              |
| 46:DZ:118:GLN:HG2  | 46:DZ:119:GLU:N    | 2.17                     | 0.55              |
| 1:AA:401:C:H2'     | 1:AA:402:G:H8      | 1.71                     | 0.55              |
| 1:AA:914:A:C4      | 1:AA:915:A:C8      | 2.94                     | 0.55              |
| 1:AA:1130:A:O2'    | 9:AI:3:GLN:NE2     | 2.40                     | 0.55              |
| 11:AK:34:ASP:O     | 11:AK:37:GLY:N     | 2.39                     | 0.55              |
| 12:AL:83:VAL:HG22  | 12:AL:100:ILE:HG23 | 1.86                     | 0.55              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:AW:39:U:C2'     | 23:AW:40:C:H5'     | 2.36                     | 0.55              |
| 24:AX:13:A:N3      | 24:AX:13:A:C3'     | 2.64                     | 0.55              |
| 25:BA:481:G:P      | 45:BY:47:LYS:HE3   | 2.47                     | 0.55              |
| 25:BA:1131:G:O2'   | 34:BN:82:LEU:HD13  | 2.06                     | 0.55              |
| 25:BA:1288:U:OP1   | 25:BA:1289:C:N4    | 2.38                     | 0.55              |
| 25:BA:1407:C:H42   | 25:BA:1595:G:H1    | 1.53                     | 0.55              |
| 25:BA:2000:G:O2'   | 25:BA:2689:U:C5    | 2.54                     | 0.55              |
| 28:BD:92:ILE:HD13  | 28:BD:92:ILE:H     | 1.71                     | 0.55              |
| 31:BG:46:ALA:C     | 31:BG:51:ARG:HG3   | 2.32                     | 0.55              |
| 34:BN:123:TYR:HE1  | 34:BN:130:HIS:NE2  | 1.96                     | 0.55              |
| 35:BO:111:PHE:O    | 35:BO:115:VAL:HG23 | 2.06                     | 0.55              |
| 36:BP:105:LEU:O    | 36:BP:106:LEU:HB2  | 2.05                     | 0.55              |
| 37:BQ:29:PHE:HB3   | 37:BQ:65:PHE:CE1   | 2.41                     | 0.55              |
| 37:BQ:59:ARG:O     | 37:BQ:60:ARG:HB2   | 2.06                     | 0.55              |
| 38:BR:5:LYS:O      | 38:BR:6:SER:CB     | 2.53                     | 0.55              |
| 39:BS:67:ARG:HH12  | 39:BS:98:VAL:HG13  | 1.71                     | 0.55              |
| 40:BT:89:VAL:CG1   | 40:BT:91:ARG:HE    | 2.19                     | 0.55              |
| 41:BU:79:PHE:CD2   | 41:BU:79:PHE:C     | 2.81                     | 0.55              |
| 43:BW:5:ALA:O      | 43:BW:6:ILE:CG1    | 2.54                     | 0.55              |
| 52:B5:40:LYS:HB2   | 52:B5:41:PRO:HD2   | 1.88                     | 0.55              |
| 2:CB:124:SER:OG    | 2:CB:125:PRO:HD2   | 2.05                     | 0.55              |
| 2:CB:136:VAL:HA    | 2:CB:139:LYS:HB2   | 1.88                     | 0.55              |
| 13:CM:65:LYS:HB2   | 13:CM:69:GLU:CB    | 2.36                     | 0.55              |
| 17:CQ:66:SER:O     | 17:CQ:70:ARG:NH1   | 2.39                     | 0.55              |
| 25:DA:27:G:H1'     | 25:DA:513:A:H62    | 1.71                     | 0.55              |
| 25:DA:1162:G:O3'   | 42:DV:24:LYS:NZ    | 2.38                     | 0.55              |
| 28:DD:68:LYS:HB2   | 28:DD:70:TRP:CZ2   | 2.40                     | 0.55              |
| 28:DD:177:LEU:HD11 | 28:DD:183:ARG:HB2  | 1.88                     | 0.55              |
| 28:DD:224:ALA:O    | 28:DD:225:ALA:HB2  | 2.06                     | 0.55              |
| 32:DH:136:ILE:HD12 | 32:DH:136:ILE:N    | 2.21                     | 0.55              |
| 35:DO:20:MET:HG2   | 35:DO:21:CYS:N     | 2.22                     | 0.55              |
| 39:DS:3:ARG:HG2    | 39:DS:4:LEU:H      | 1.70                     | 0.55              |
| 40:DT:36:GLU:HG2   | 40:DT:36:GLU:O     | 2.05                     | 0.55              |
| 42:DV:16:PRO:HA    | 42:DV:96:ILE:HG22  | 1.89                     | 0.55              |
| 42:DV:66:ARG:HH11  | 42:DV:66:ARG:CB    | 2.19                     | 0.55              |
| 43:DW:6:ILE:HG13   | 43:DW:104:THR:HG23 | 1.88                     | 0.55              |
| 45:DY:33:LYS:HG3   | 45:DY:34:LYS:H     | 1.71                     | 0.55              |
| 45:DY:81:LYS:HB3   | 45:DY:97:ARG:CD    | 2.36                     | 0.55              |
| 47:D0:41:ARG:HD2   | 47:D0:41:ARG:N     | 2.19                     | 0.55              |
| 53:D6:20:ASN:HD22  | 53:D6:21:TYR:H     | 1.52                     | 0.55              |
| 1:AA:1205:U:H5''   | 3:AC:190:ARG:NH2   | 2.21                     | 0.55              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 12:AL:27:LEU:HD11  | 12:AL:64:TYR:CE1   | 2.41                     | 0.55              |
| 22:AV:16:C:O2'     | 22:AV:17:C:H5'     | 2.07                     | 0.55              |
| 25:BA:642:G:H21    | 25:BA:646:A:H2     | 1.53                     | 0.55              |
| 25:BA:873:G:H1     | 25:BA:904:C:H42    | 1.55                     | 0.55              |
| 25:BA:1204:A:O2'   | 25:BA:1205:U:O5'   | 2.23                     | 0.55              |
| 25:BA:1340:U:O2    | 25:BA:1602:U:H5''  | 2.05                     | 0.55              |
| 25:BA:2468:G:O2'   | 25:BA:2469:A:H8    | 1.88                     | 0.55              |
| 33:BI:5:LEU:CD1    | 33:BI:19:VAL:HG12  | 2.31                     | 0.55              |
| 37:BQ:10:ARG:HH11  | 37:BQ:10:ARG:HG3   | 1.67                     | 0.55              |
| 37:BQ:54:MET:HB3   | 37:BQ:64:ILE:HD11  | 1.88                     | 0.55              |
| 38:BR:2:ARG:CZ     | 38:BR:5:LYS:HE2    | 2.37                     | 0.55              |
| 41:BU:28:ARG:HA    | 41:BU:34:LYS:HB3   | 1.89                     | 0.55              |
| 43:BW:48:ALA:O     | 43:BW:49:LYS:C     | 2.48                     | 0.55              |
| 50:B3:50:VAL:O     | 50:B3:53:LEU:HD12  | 2.05                     | 0.55              |
| 1:CA:484:G:H5'     | 1:CA:486:U:O4'     | 2.05                     | 0.55              |
| 3:CC:76:VAL:HG23   | 3:CC:77:ILE:HG13   | 1.88                     | 0.55              |
| 4:CD:101:LEU:HD11  | 4:CD:105:VAL:HG23  | 1.89                     | 0.55              |
| 9:CI:55:ALA:HB2    | 9:CI:58:HIS:ND1    | 2.22                     | 0.55              |
| 12:CL:27:LEU:HD23  | 12:CL:62:SER:OG    | 2.06                     | 0.55              |
| 13:CM:108:ARG:HH11 | 13:CM:108:ARG:HA   | 1.69                     | 0.55              |
| 16:CP:18:ARG:O     | 16:CP:20:VAL:HG12  | 2.06                     | 0.55              |
| 25:DA:13:A:H2      | 25:DA:14:A:N6      | 2.03                     | 0.55              |
| 25:DA:1779:U:H5    | 25:DA:1784:A:N7    | 2.05                     | 0.55              |
| 25:DA:1818:U:C2'   | 28:DD:157:ARG:HG3  | 2.36                     | 0.55              |
| 33:DI:86:THR:HG22  | 33:DI:86:THR:O     | 2.07                     | 0.55              |
| 34:DN:47:ALA:HB2   | 34:DN:112:LEU:HD11 | 1.87                     | 0.55              |
| 34:DN:102:ALA:O    | 34:DN:106:MET:HE3  | 2.06                     | 0.55              |
| 36:DP:47:ASP:HB3   | 36:DP:48:PRO:HA    | 1.86                     | 0.55              |
| 39:DS:20:ARG:C     | 39:DS:22:GLY:H     | 2.15                     | 0.55              |
| 40:DT:11:GLU:CD    | 40:DT:11:GLU:N     | 2.64                     | 0.55              |
| 40:DT:64:ARG:HD2   | 40:DT:73:GLU:CG    | 2.37                     | 0.55              |
| 1:AA:60:A:C4'      | 1:AA:61:G:O5'      | 2.30                     | 0.55              |
| 1:AA:1299:A:C5     | 1:AA:1301:U:C2     | 2.95                     | 0.55              |
| 2:AB:78:GLN:O      | 2:AB:94:ASN:ND2    | 2.32                     | 0.55              |
| 4:AD:206:PHE:O     | 4:AD:207:TYR:HD2   | 1.90                     | 0.55              |
| 5:AE:93:PRO:HG2    | 8:AH:105:ARG:HE    | 1.69                     | 0.55              |
| 7:AG:62:PHE:HA     | 7:AG:124:LEU:CD2   | 2.36                     | 0.55              |
| 9:AI:4:TYR:N       | 9:AI:4:TYR:CD1     | 2.73                     | 0.55              |
| 10:AJ:38:ILE:CD1   | 10:AJ:71:LEU:HD23  | 2.22                     | 0.55              |
| 15:AO:10:LYS:O     | 15:AO:14:GLU:HB3   | 2.06                     | 0.55              |
| 22:AV:20:G:C2      | 22:AV:58:A:N3      | 2.74                     | 0.55              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 25:BA:1665:A:H1'   | 35:BO:1:MET:HE3   | 1.89                     | 0.55              |
| 28:BD:25:THR:O     | 28:BD:27:THR:N    | 2.33                     | 0.55              |
| 30:BF:93:LYS:HB3   | 30:BF:94:PRO:HD2  | 1.89                     | 0.55              |
| 34:BN:133:GLN:HG2  | 34:BN:135:PRO:HD3 | 1.89                     | 0.55              |
| 45:BY:2:ARG:N      | 45:BY:4:LYS:HG2   | 2.22                     | 0.55              |
| 45:BY:42:VAL:HB    | 45:BY:65:ALA:CB   | 2.29                     | 0.55              |
| 46:BZ:135:GLU:O    | 46:BZ:136:PHE:HB3 | 2.06                     | 0.55              |
| 53:B6:17:LYS:HB3   | 53:B6:18:ARG:NH1  | 2.22                     | 0.55              |
| 55:B8:63:PRO:HB2   | 55:B8:64:TYR:HD1  | 1.71                     | 0.55              |
| 1:CA:8:A:O2'       | 5:CE:103:GLY:HA2  | 2.07                     | 0.55              |
| 2:CB:80:ILE:HD13   | 2:CB:212:GLN:HA   | 1.89                     | 0.55              |
| 7:CG:150:ALA:O     | 11:CK:57:THR:HG21 | 2.06                     | 0.55              |
| 13:CM:40:ASN:HD21  | 13:CM:42:ALA:HB3  | 1.72                     | 0.55              |
| 15:CO:23:GLY:O     | 15:CO:27:VAL:HB   | 2.07                     | 0.55              |
| 22:CV:40:C:H2'     | 22:CV:41:C:C6     | 2.41                     | 0.55              |
| 23:CW:39:U:OP1     | 23:CW:39:U:H4'    | 2.05                     | 0.55              |
| 25:DA:1465:G:O4'   | 25:DA:1528:A:H8   | 1.89                     | 0.55              |
| 25:DA:1558:A:HO2'  | 25:DA:1559:G:P    | 2.29                     | 0.55              |
| 25:DA:1693:U:OP2   | 25:DA:1694:C:C4   | 2.59                     | 0.55              |
| 25:DA:2522:U:O2'   | 25:DA:2647:U:OP1  | 2.22                     | 0.55              |
| 33:DI:76:THR:HG22  | 33:DI:77:LEU:H    | 1.71                     | 0.55              |
| 34:DN:43:THR:O     | 34:DN:46:VAL:HG12 | 2.05                     | 0.55              |
| 34:DN:128:HIS:O    | 34:DN:130:HIS:N   | 2.39                     | 0.55              |
| 36:DP:98:GLU:HG3   | 36:DP:99:LEU:N    | 2.22                     | 0.55              |
| 36:DP:112:LEU:HD22 | 36:DP:113:LYS:H   | 1.71                     | 0.55              |
| 40:DT:36:GLU:CG    | 40:DT:38:ASN:HD21 | 2.18                     | 0.55              |
| 42:DV:1:MET:CG     | 42:DV:1:MET:CE    | 2.83                     | 0.55              |
| 45:DY:19:LYS:O     | 45:DY:20:TYR:CG   | 2.60                     | 0.55              |
| 55:D8:61:LEU:N     | 55:D8:63:PRO:HD2  | 2.22                     | 0.55              |
| 1:AA:656:C:H4'     | 15:AO:62:GLN:NE2  | 2.22                     | 0.55              |
| 12:AL:7:ILE:O      | 12:AL:9:GLN:N     | 2.40                     | 0.55              |
| 19:AS:43:GLU:C     | 19:AS:45:VAL:H    | 2.14                     | 0.55              |
| 23:AW:51:U:H2'     | 23:AW:52:G:C8     | 2.42                     | 0.55              |
| 25:BA:2437:U:O2'   | 25:BA:2438:U:H5'  | 2.07                     | 0.55              |
| 25:BA:2712:U:OP1   | 25:BA:2714:G:H4'  | 2.06                     | 0.55              |
| 27:BC:82:LYS:O     | 27:BC:86:ALA:HB3  | 2.06                     | 0.55              |
| 30:BF:139:PHE:HB2  | 30:BF:166:ALA:HB1 | 1.89                     | 0.55              |
| 32:BH:156:ALA:C    | 32:BH:158:HIS:N   | 2.58                     | 0.55              |
| 34:BN:31:ALA:O     | 34:BN:34:LEU:HB2  | 2.07                     | 0.55              |
| 36:BP:6:LEU:O      | 36:BP:7:ARG:HG2   | 2.06                     | 0.55              |
| 36:BP:124:LYS:HA   | 36:BP:143:GLY:O   | 2.06                     | 0.55              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 41:BU:61:TRP:CD2   | 41:BU:94:ASN:HA   | 2.40                     | 0.55              |
| 43:BW:100:THR:O    | 43:BW:100:THR:CG2 | 2.49                     | 0.55              |
| 45:BY:14:LEU:HG    | 45:BY:15:VAL:N    | 2.22                     | 0.55              |
| 45:BY:17:SER:HB2   | 45:BY:71:LYS:CE   | 2.37                     | 0.55              |
| 1:CA:280:C:C2      | 17:CQ:38:ARG:HG3  | 2.42                     | 0.55              |
| 1:CA:528:C:H5'     | 1:CA:535:A:N6     | 2.21                     | 0.55              |
| 1:CA:748:C:O4'     | 1:CA:749:C:H5     | 1.89                     | 0.55              |
| 3:CC:52:LEU:HD23   | 3:CC:52:LEU:H     | 1.71                     | 0.55              |
| 12:CL:26:ALA:C     | 12:CL:27:LEU:HD22 | 2.31                     | 0.55              |
| 13:CM:5:ALA:O      | 13:CM:7:VAL:N     | 2.39                     | 0.55              |
| 16:CP:19:ILE:HG22  | 16:CP:36:ILE:CG1  | 2.34                     | 0.55              |
| 16:CP:58:TYR:O     | 16:CP:61:SER:N    | 2.40                     | 0.55              |
| 18:CR:37:VAL:HG23  | 18:CR:38:GLU:N    | 2.22                     | 0.55              |
| 19:CS:9:VAL:O      | 19:CS:11:VAL:N    | 2.40                     | 0.55              |
| 25:DA:527:C:H4'    | 25:DA:528:A:O5'   | 2.07                     | 0.55              |
| 25:DA:729:G:C5     | 28:DD:208:LYS:HB2 | 2.41                     | 0.55              |
| 25:DA:1798:U:H5''  | 28:DD:260:ARG:HB3 | 1.87                     | 0.55              |
| 25:DA:1858:G:O2'   | 25:DA:1884:A:N6   | 2.39                     | 0.55              |
| 29:DE:119:ARG:HD2  | 29:DE:120:TRP:NE1 | 2.22                     | 0.55              |
| 30:DF:46:ARG:O     | 30:DF:47:GLY:C    | 2.49                     | 0.55              |
| 30:DF:114:VAL:HG21 | 30:DF:202:PHE:CZ  | 2.41                     | 0.55              |
| 33:DI:10:GLU:O     | 33:DI:11:ASN:HB3  | 2.06                     | 0.55              |
| 36:DP:88:LEU:HD11  | 36:DP:95:VAL:CG2  | 2.36                     | 0.55              |
| 39:DS:5:THR:C      | 39:DS:7:TYR:N     | 2.64                     | 0.55              |
| 40:DT:13:ARG:NE    | 40:DT:13:ARG:CA   | 2.66                     | 0.55              |
| 41:DU:90:VAL:HA    | 42:DV:11:GLN:HE22 | 1.71                     | 0.55              |
| 42:DV:81:TYR:C     | 42:DV:82:ARG:CG   | 2.80                     | 0.55              |
| 45:DY:77:PRO:O     | 45:DY:78:ALA:HB2  | 2.05                     | 0.55              |
| 45:DY:90:LEU:N     | 45:DY:90:LEU:HD22 | 2.22                     | 0.55              |
| 50:D3:52:HIS:ND1   | 50:D3:53:LEU:HG   | 2.21                     | 0.55              |
| 53:D6:36:LEU:O     | 53:D6:37:ARG:HG3  | 2.07                     | 0.55              |
| 56:D9:19:ARG:O     | 56:D9:24:TYR:HE1  | 1.89                     | 0.55              |
| 1:AA:281:G:H8      | 1:AA:281:G:OP2    | 1.89                     | 0.55              |
| 1:AA:297:G:N2      | 1:AA:300:A:OP2    | 2.35                     | 0.55              |
| 1:AA:974:A:OP1     | 14:AN:31:ARG:HD3  | 2.06                     | 0.55              |
| 1:AA:1201:A:H4'    | 1:AA:1202:G:C5'   | 2.35                     | 0.55              |
| 5:AE:88:LYS:HB3    | 5:AE:123:LEU:HB2  | 1.88                     | 0.55              |
| 6:AF:8:ILE:CD1     | 6:AF:26:ILE:HD13  | 2.33                     | 0.55              |
| 8:AH:13:ILE:O      | 8:AH:17:THR:HG23  | 2.07                     | 0.55              |
| 12:AL:6:THR:CG2    | 12:AL:9:GLN:HG3   | 2.29                     | 0.55              |
| 23:AW:38:A:C2'     | 23:AW:39:U:H5''   | 2.37                     | 0.55              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:BA:644:A:H4'   | 25:BA:645:C:C5     | 2.42                     | 0.55              |
| 28:BD:65:ILE:HD13 | 28:BD:65:ILE:O     | 2.07                     | 0.55              |
| 29:BE:77:ILE:CG2  | 29:BE:78:LEU:HG    | 2.34                     | 0.55              |
| 31:BG:125:PHE:HB2 | 31:BG:166:ASP:OD2  | 2.06                     | 0.55              |
| 38:BR:53:HIS:HB2  | 38:BR:94:TYR:HE1   | 1.71                     | 0.55              |
| 39:BS:42:ASP:O    | 39:BS:43:GLU:HB2   | 2.07                     | 0.55              |
| 40:BT:26:ASP:HB2  | 40:BT:48:ILE:HG13  | 1.88                     | 0.55              |
| 40:BT:90:GLN:NE2  | 40:BT:124:ASP:OD2  | 2.39                     | 0.55              |
| 42:BV:47:VAL:O    | 42:BV:48:GLY:C     | 2.50                     | 0.55              |
| 44:BX:11:PRO:O    | 44:BX:12:VAL:C     | 2.50                     | 0.55              |
| 44:BX:12:VAL:HG12 | 44:BX:27:THR:HG23  | 1.87                     | 0.55              |
| 46:BZ:24:LEU:HB3  | 46:BZ:41:LEU:HG    | 1.89                     | 0.55              |
| 55:B8:50:LEU:HA   | 55:B8:53:PRO:HG3   | 1.87                     | 0.55              |
| 7:CG:111:ARG:HG2  | 7:CG:113:GLU:OE2   | 2.07                     | 0.55              |
| 7:CG:113:GLU:O    | 7:CG:119:ARG:HD3   | 2.06                     | 0.55              |
| 16:CP:53:VAL:HG13 | 16:CP:79:VAL:HG22  | 1.87                     | 0.55              |
| 23:CW:21:A:H62    | 23:CW:46:G:H1'     | 1.72                     | 0.55              |
| 25:DA:99:U:H4'    | 25:DA:102:G:H1'    | 1.89                     | 0.55              |
| 25:DA:604:G:C5    | 25:DA:605:C:C4     | 2.95                     | 0.55              |
| 25:DA:1943:U:H4'  | 25:DA:1944:U:O5'   | 2.05                     | 0.55              |
| 25:DA:2481:G:O2'  | 25:DA:2482:G:O5'   | 2.24                     | 0.55              |
| 25:DA:2884:U:H1'  | 52:D5:52:TYR:OH    | 2.06                     | 0.55              |
| 33:DI:71:ILE:HD13 | 33:DI:71:ILE:O     | 2.07                     | 0.55              |
| 35:DO:77:ILE:HD11 | 40:DT:72:VAL:CG1   | 2.37                     | 0.55              |
| 36:DP:124:LYS:HA  | 36:DP:143:GLY:O    | 2.06                     | 0.55              |
| 37:DQ:1:MET:HE2   | 37:DQ:1:MET:C      | 2.32                     | 0.55              |
| 39:DS:46:VAL:HG12 | 39:DS:47:THR:N     | 2.22                     | 0.55              |
| 40:DT:96:ARG:HH11 | 40:DT:96:ARG:HG2   | 1.71                     | 0.55              |
| 45:DY:42:VAL:HG12 | 45:DY:65:ALA:HB3   | 1.88                     | 0.55              |
| 45:DY:94:LYS:HD2  | 45:DY:101:LYS:HZ3  | 1.71                     | 0.55              |
| 46:DZ:33:LEU:HD12 | 46:DZ:34:ASN:H     | 1.71                     | 0.55              |
| 46:DZ:134:PRO:HB3 | 46:DZ:137:ILE:HD11 | 1.88                     | 0.55              |
| 46:DZ:150:LEU:CD2 | 46:DZ:171:ILE:HD12 | 2.37                     | 0.55              |
| 47:D0:9:SER:OG    | 47:D0:10:THR:N     | 2.40                     | 0.55              |
| 1:AA:927:G:OP2    | 1:AA:1503:A:N7     | 2.39                     | 0.55              |
| 1:AA:949:A:N3     | 1:AA:971:G:O6      | 2.40                     | 0.55              |
| 1:AA:950:U:H2'    | 1:AA:951:G:H8      | 1.71                     | 0.55              |
| 6:AF:69:GLU:CD    | 6:AF:69:GLU:N      | 2.65                     | 0.55              |
| 7:AG:15:ASP:CB    | 7:AG:24:THR:HG22   | 2.36                     | 0.55              |
| 8:AH:112:LEU:CD2  | 8:AH:133:LEU:HA    | 2.37                     | 0.55              |
| 9:AI:17:VAL:HA    | 9:AI:63:ILE:HG12   | 1.89                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 12:AL:84:LEU:HD22 | 12:AL:85:ILE:H    | 1.72                     | 0.55              |
| 15:AO:82:ILE:HD13 | 15:AO:82:ILE:C    | 2.31                     | 0.55              |
| 19:AS:29:ARG:NH1  | 19:AS:30:LEU:HB2  | 2.21                     | 0.55              |
| 22:AV:52:C:H2'    | 22:AV:53:G:O5'    | 2.07                     | 0.55              |
| 25:BA:195:A:OP1   | 36:BP:46:LYS:HE2  | 2.06                     | 0.55              |
| 25:BA:332:A:C4'   | 25:BA:333:G:OP1   | 2.50                     | 0.55              |
| 25:BA:1126:A:H4'  | 25:BA:1127:A:O5'  | 2.06                     | 0.55              |
| 25:BA:2318:G:H2'  | 25:BA:2319:G:OP1  | 2.07                     | 0.55              |
| 28:BD:31:LYS:NZ   | 28:BD:102:LYS:HZ1 | 2.04                     | 0.55              |
| 29:BE:47:VAL:HG12 | 29:BE:49:LEU:HD12 | 1.88                     | 0.55              |
| 34:BN:22:THR:HB   | 34:BN:25:ARG:HB2  | 1.89                     | 0.55              |
| 36:BP:59:LEU:CG   | 55:B8:13:ARG:NH2  | 2.70                     | 0.55              |
| 36:BP:71:VAL:CG2  | 36:BP:72:PRO:HD3  | 2.36                     | 0.55              |
| 39:BS:67:ARG:HG2  | 39:BS:67:ARG:NH1  | 2.22                     | 0.55              |
| 43:BW:5:ALA:O     | 43:BW:6:ILE:HB    | 2.07                     | 0.55              |
| 46:BZ:10:ARG:NH2  | 46:BZ:26:GLY:H    | 2.04                     | 0.55              |
| 1:CA:542:G:OP1    | 4:CD:10:ARG:NH2   | 2.39                     | 0.55              |
| 1:CA:748:C:O4'    | 1:CA:749:C:C5     | 2.59                     | 0.55              |
| 3:CC:101:LEU:HD23 | 3:CC:102:ASN:N    | 2.22                     | 0.55              |
| 4:CD:29:PRO:C     | 4:CD:30:LYS:HG2   | 2.32                     | 0.55              |
| 5:CE:142:LEU:O    | 5:CE:143:ARG:HG2  | 2.07                     | 0.55              |
| 10:CJ:61:GLU:OE2  | 14:CN:45:ARG:NH1  | 2.40                     | 0.55              |
| 12:CL:21:LYS:N    | 12:CL:21:LYS:CD   | 2.70                     | 0.55              |
| 14:CN:39:LEU:HD11 | 14:CN:47:LEU:HD12 | 1.89                     | 0.55              |
| 16:CP:23:ASP:HB3  | 16:CP:26:ARG:HG3  | 1.88                     | 0.55              |
| 23:CW:6:G:N2      | 23:CW:68:C:N3     | 2.54                     | 0.55              |
| 23:CW:34:G:C6     | 24:CX:14:A:C6     | 2.95                     | 0.55              |
| 25:DA:414:C:O2    | 25:DA:1864:U:O2'  | 2.24                     | 0.55              |
| 25:DA:2336:A:H61  | 47:D0:43:THR:CG2  | 2.19                     | 0.55              |
| 27:DC:77:ILE:O    | 27:DC:77:ILE:HG23 | 2.06                     | 0.55              |
| 28:DD:267:SER:C   | 28:DD:269:PHE:H   | 2.15                     | 0.55              |
| 34:DN:57:ALA:O    | 34:DN:58:ASP:O    | 2.25                     | 0.55              |
| 36:DP:48:PRO:O    | 36:DP:51:PHE:N    | 2.39                     | 0.55              |
| 42:DV:3:ALA:O     | 42:DV:4:ILE:HD13  | 2.06                     | 0.55              |
| 44:DX:60:ARG:NH2  | 54:D7:47:ARG:NH2  | 2.53                     | 0.55              |
| 46:DZ:19:ARG:NH1  | 46:DZ:84:GLU:HA   | 2.22                     | 0.55              |
| 52:D5:57:VAL:C    | 52:D5:58:LEU:CD2  | 2.69                     | 0.55              |
| 1:AA:523:A:H61    | 12:AL:92:ASP:HB2  | 1.71                     | 0.55              |
| 1:AA:792:A:C4     | 1:AA:794:A:C5     | 2.95                     | 0.55              |
| 1:AA:1265:G:C6    | 1:AA:1266:G:C6    | 2.94                     | 0.55              |
| 3:AC:153:VAL:HG22 | 3:AC:198:VAL:CG1  | 2.37                     | 0.55              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 3:AC:184:TYR:HE1  | 3:AC:199:LYS:HB3   | 1.71                     | 0.55              |
| 7:AG:15:ASP:HB3   | 7:AG:24:THR:HG23   | 1.88                     | 0.55              |
| 9:AI:3:GLN:CD     | 9:AI:20:ARG:HH12   | 2.14                     | 0.55              |
| 12:AL:17:LYS:NZ   | 12:AL:18:VAL:HG22  | 2.21                     | 0.55              |
| 16:AP:11:SER:HB2  | 16:AP:14:ASN:HB3   | 1.88                     | 0.55              |
| 25:BA:627:A:H62   | 36:BP:116:GLY:HA2  | 1.72                     | 0.55              |
| 25:BA:1012:U:O4   | 34:BN:28:THR:HG21  | 2.06                     | 0.55              |
| 25:BA:1311:G:O6   | 54:B7:9:ARG:NH2    | 2.39                     | 0.55              |
| 25:BA:2282:G:H4'  | 25:BA:2283:C:O5'   | 2.06                     | 0.55              |
| 37:BQ:114:ALA:C   | 37:BQ:116:GLU:H    | 2.14                     | 0.55              |
| 47:B0:23:VAL:HG13 | 47:B0:38:VAL:HG22  | 1.88                     | 0.55              |
| 47:B0:53:MET:HA   | 47:B0:58:THR:O     | 2.07                     | 0.55              |
| 55:B8:30:ARG:HA   | 55:B8:30:ARG:NE    | 2.21                     | 0.55              |
| 1:CA:197:A:H4'    | 1:CA:198:G:O5'     | 2.06                     | 0.55              |
| 1:CA:461:A:N6     | 1:CA:471:G:C6      | 2.75                     | 0.55              |
| 2:CB:233:SER:OG   | 2:CB:234:PRO:HD2   | 2.07                     | 0.55              |
| 4:CD:25:ARG:HH12  | 4:CD:30:LYS:HB2    | 1.72                     | 0.55              |
| 4:CD:138:TYR:CD2  | 4:CD:139:ARG:N     | 2.75                     | 0.55              |
| 4:CD:155:LEU:O    | 4:CD:156:GLU:C     | 2.50                     | 0.55              |
| 6:CF:72:VAL:CG1   | 6:CF:73:ASN:N      | 2.69                     | 0.55              |
| 7:CG:22:LEU:HG    | 7:CG:62:PHE:HE2    | 1.71                     | 0.55              |
| 13:CM:92:HIS:HA   | 13:CM:110:ARG:NH2  | 2.22                     | 0.55              |
| 16:CP:49:LEU:HD12 | 16:CP:49:LEU:C     | 2.32                     | 0.55              |
| 17:CQ:67:LYS:CA   | 17:CQ:70:ARG:NH1   | 2.69                     | 0.55              |
| 25:DA:8:A:H2'     | 25:DA:9:U:C6       | 2.42                     | 0.55              |
| 25:DA:918:A:N3    | 26:DB:80:U:O2'     | 2.37                     | 0.55              |
| 25:DA:1338:G:N7   | 44:DX:62:LYS:NZ    | 2.53                     | 0.55              |
| 31:DG:77:ILE:CG2  | 31:DG:80:PHE:H     | 2.20                     | 0.55              |
| 31:DG:126:ASP:OD1 | 31:DG:130:ASN:HB2  | 2.06                     | 0.55              |
| 32:DH:20:ALA:CB   | 32:DH:21:PRO:HD2   | 2.34                     | 0.55              |
| 34:DN:26:LEU:CG   | 34:DN:30:ILE:HD11  | 2.36                     | 0.55              |
| 36:DP:52:GLU:OE1  | 36:DP:55:ARG:NH2   | 2.36                     | 0.55              |
| 36:DP:71:VAL:CG2  | 36:DP:72:PRO:HD3   | 2.36                     | 0.55              |
| 39:DS:27:SER:HA   | 39:DS:88:ASP:CB    | 2.37                     | 0.55              |
| 39:DS:88:ASP:CG   | 39:DS:90:GLY:H     | 2.14                     | 0.55              |
| 40:DT:102:ILE:HB  | 40:DT:110:ILE:HD11 | 1.88                     | 0.55              |
| 41:DU:12:ARG:HA   | 41:DU:15:LYS:HD2   | 1.88                     | 0.55              |
| 42:DV:76:LYS:HB3  | 42:DV:79:VAL:HG11  | 1.88                     | 0.55              |
| 43:DW:48:ALA:O    | 43:DW:49:LYS:C     | 2.50                     | 0.55              |
| 46:DZ:166:SER:H   | 46:DZ:167:PRO:HA   | 1.71                     | 0.55              |
| 55:D8:60:LEU:O    | 55:D8:63:PRO:O     | 2.25                     | 0.55              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:AA:1057:G:H5''   | 3:AC:154:SER:HB2  | 1.89                     | 0.55              |
| 2:AB:166:ASP:OD1   | 2:AB:169:LYS:HB2  | 2.07                     | 0.55              |
| 5:AE:64:ARG:HA     | 5:AE:64:ARG:HE    | 1.72                     | 0.55              |
| 6:AF:49:ALA:HB1    | 18:AR:80:PRO:HB3  | 1.89                     | 0.55              |
| 10:AJ:49:VAL:HG21  | 14:AN:41:ARG:O    | 2.07                     | 0.55              |
| 13:AM:16:ASP:N     | 13:AM:16:ASP:OD2  | 2.40                     | 0.55              |
| 22:AV:35:C:H42     | 24:AX:18:G:H1     | 1.55                     | 0.55              |
| 22:AV:54:G:O2'     | 22:AV:55:U:P      | 2.64                     | 0.55              |
| 25:BA:271(L):U:H4' | 25:BA:271(M):G:C5 | 2.42                     | 0.55              |
| 25:BA:448:U:O3'    | 30:BF:84:VAL:HG12 | 2.07                     | 0.55              |
| 25:BA:1490:A:H5'   | 25:BA:1491:G:OP2  | 2.06                     | 0.55              |
| 25:BA:1965:C:C4    | 25:BA:1966:A:C6   | 2.95                     | 0.55              |
| 25:BA:2078:C:C4    | 25:BA:2079:U:O4   | 2.59                     | 0.55              |
| 25:BA:2832:U:H1'   | 25:BA:2834:G:C4   | 2.42                     | 0.55              |
| 26:BB:83:G:H5''    | 50:B3:52:HIS:CD2  | 2.42                     | 0.55              |
| 29:BE:40:GLU:CD    | 29:BE:40:GLU:N    | 2.64                     | 0.55              |
| 32:BH:47:GLU:HG2   | 32:BH:48:GLY:H    | 1.71                     | 0.55              |
| 32:BH:151:ILE:O    | 32:BH:152:ARG:HG2 | 2.07                     | 0.55              |
| 35:BO:80:ASP:HB2   | 40:BT:70:VAL:HG13 | 1.89                     | 0.55              |
| 37:BQ:29:PHE:HD2   | 37:BQ:65:PHE:CE1  | 2.25                     | 0.55              |
| 40:BT:32:TYR:CG    | 40:BT:81:PRO:HB2  | 2.42                     | 0.55              |
| 42:BV:65:GLY:CA    | 42:BV:91:TYR:HE1  | 2.19                     | 0.55              |
| 43:BW:62:HIS:O     | 43:BW:63:ASP:C    | 2.50                     | 0.55              |
| 44:BX:24:GLY:O     | 44:BX:82:GLN:HA   | 2.07                     | 0.55              |
| 45:BY:8:LYS:CE     | 45:BY:72:VAL:O    | 2.55                     | 0.55              |
| 48:B1:67:ILE:N     | 48:B1:68:PRO:HD2  | 2.22                     | 0.55              |
| 51:B4:40:ILE:HA    | 51:B4:57:ILE:HB   | 1.88                     | 0.55              |
| 1:CA:522:C:H41     | 12:CL:53:ARG:HH22 | 1.55                     | 0.55              |
| 8:CH:97:VAL:O      | 8:CH:100:ILE:HG13 | 2.07                     | 0.55              |
| 11:CK:67:ASP:OD2   | 11:CK:71:LYS:HE3  | 2.07                     | 0.55              |
| 13:CM:124:PRO:O    | 22:CV:31:G:N7     | 2.40                     | 0.55              |
| 25:DA:896:A:H2     | 46:DZ:113:ALA:HB3 | 1.69                     | 0.55              |
| 25:DA:1451:C:O2'   | 25:DA:1457:A:N6   | 2.40                     | 0.55              |
| 28:DD:211:ARG:HA   | 28:DD:214:TRP:CD2 | 2.42                     | 0.55              |
| 29:DE:39:PRO:HA    | 29:DE:43:GLY:HA2  | 1.87                     | 0.55              |
| 33:DI:52:ARG:NH1   | 33:DI:52:ARG:HB3  | 2.21                     | 0.55              |
| 33:DI:53:ALA:O     | 33:DI:57:ARG:HG3  | 2.07                     | 0.55              |
| 44:DX:28:PHE:CE2   | 44:DX:92:LEU:HD11 | 2.42                     | 0.55              |
| 46:DZ:48:PHE:O     | 46:DZ:50:GLN:N    | 2.40                     | 0.55              |
| 1:AA:1029:C:H1'    | 1:AA:1033:G:H1    | 1.71                     | 0.54              |
| 2:AB:233:SER:OG    | 2:AB:234:PRO:HD2  | 2.07                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:AC:182:ILE:HG12  | 3:AC:203:PHE:HD1   | 1.71                     | 0.54              |
| 14:AN:15:LYS:HE3   | 14:AN:16:PHE:CE2   | 2.42                     | 0.54              |
| 17:AQ:83:ASP:O     | 17:AQ:86:GLU:HB2   | 2.07                     | 0.54              |
| 25:BA:242:G:N7     | 55:B8:5:LYS:HG2    | 2.22                     | 0.54              |
| 25:BA:311:A:C8     | 25:BA:311:A:OP1    | 2.60                     | 0.54              |
| 25:BA:414:C:O2     | 25:BA:1864:U:O2'   | 2.23                     | 0.54              |
| 25:BA:448:U:C2'    | 30:BF:84:VAL:CG1   | 2.84                     | 0.54              |
| 25:BA:668:G:C5     | 25:BA:670:A:C8     | 2.94                     | 0.54              |
| 25:BA:800:A:H4'    | 25:BA:801:G:O5'    | 2.07                     | 0.54              |
| 25:BA:2698:U:H2'   | 25:BA:2699:C:C6    | 2.42                     | 0.54              |
| 28:BD:30:GLU:CD    | 28:BD:63:ARG:NH2   | 2.65                     | 0.54              |
| 31:BG:128:ARG:O    | 31:BG:130:ASN:N    | 2.36                     | 0.54              |
| 31:BG:138:GLN:O    | 31:BG:138:GLN:HG2  | 2.07                     | 0.54              |
| 36:BP:56:SER:O     | 36:BP:57:THR:CG2   | 2.54                     | 0.54              |
| 36:BP:147:LEU:HD23 | 36:BP:148:LEU:O    | 2.05                     | 0.54              |
| 37:BQ:65:PHE:HB2   | 37:BQ:105:GLU:HG2  | 1.89                     | 0.54              |
| 39:BS:24:LEU:CB    | 39:BS:85:VAL:HG12  | 2.25                     | 0.54              |
| 42:BV:65:GLY:O     | 42:BV:90:PRO:HA    | 2.07                     | 0.54              |
| 50:B3:26:LEU:HD21  | 50:B3:46:ASN:CB    | 2.36                     | 0.54              |
| 1:CA:243:A:H4'     | 1:CA:244:U:O5'     | 2.07                     | 0.54              |
| 1:CA:274:A:C4'     | 1:CA:275:G:O5'     | 2.53                     | 0.54              |
| 2:CB:60:ASP:O      | 2:CB:64:ARG:HG2    | 2.07                     | 0.54              |
| 2:CB:68:ILE:HG22   | 2:CB:70:PHE:CE1    | 2.42                     | 0.54              |
| 2:CB:238:LEU:HD23  | 2:CB:238:LEU:H     | 1.72                     | 0.54              |
| 3:CC:22:TRP:HB3    | 3:CC:59:ARG:HB2    | 1.87                     | 0.54              |
| 3:CC:86:VAL:O      | 3:CC:90:GLU:HG2    | 2.06                     | 0.54              |
| 3:CC:97:LYS:O      | 3:CC:99:VAL:HG13   | 2.06                     | 0.54              |
| 6:CF:9:VAL:C       | 6:CF:10:LEU:HD12   | 2.32                     | 0.54              |
| 11:CK:82:VAL:CG1   | 11:CK:108:ILE:HG12 | 2.37                     | 0.54              |
| 25:DA:82:G:C5      | 25:DA:83:G:C6      | 2.94                     | 0.54              |
| 25:DA:298:G:H1'    | 25:DA:340:A:H61    | 1.71                     | 0.54              |
| 25:DA:767:U:H2'    | 25:DA:768:G:C8     | 2.42                     | 0.54              |
| 25:DA:1497:U:O2    | 25:DA:1497:U:C2'   | 2.54                     | 0.54              |
| 25:DA:1799:G:O2'   | 25:DA:1800:C:P     | 2.65                     | 0.54              |
| 25:DA:2406:U:N3    | 36:DP:72:PRO:HG2   | 2.22                     | 0.54              |
| 32:DH:154:PRO:HG3  | 32:DH:163:TYR:CD1  | 2.42                     | 0.54              |
| 36:DP:114:ILE:O    | 36:DP:114:ILE:HG13 | 2.07                     | 0.54              |
| 38:DR:106:GLY:O    | 38:DR:107:ASP:HB3  | 2.08                     | 0.54              |
| 40:DT:48:ILE:H     | 40:DT:48:ILE:HD12  | 1.72                     | 0.54              |
| 41:DU:66:ASN:O     | 41:DU:70:ARG:HB2   | 2.07                     | 0.54              |
| 44:DX:47:PHE:N     | 44:DX:47:PHE:HD1   | 2.05                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 46:DZ:134:PRO:CB   | 46:DZ:137:ILE:HD11 | 2.37                     | 0.54              |
| 53:D6:15:GLU:O     | 53:D6:15:GLU:HG2   | 2.07                     | 0.54              |
| 53:D6:19:ARG:CG    | 53:D6:20:ASN:N     | 2.69                     | 0.54              |
| 54:D7:41:ARG:HD3   | 54:D7:45:ALA:CB    | 2.37                     | 0.54              |
| 55:D8:4:MET:SD     | 55:D8:61:LEU:CD2   | 2.94                     | 0.54              |
| 55:D8:61:LEU:C     | 55:D8:63:PRO:HD2   | 2.32                     | 0.54              |
| 1:AA:17:U:H2'      | 1:AA:18:C:C6       | 2.43                     | 0.54              |
| 1:AA:1049:U:C1'    | 1:AA:1201:A:C5     | 2.72                     | 0.54              |
| 2:AB:42:ILE:HD13   | 2:AB:203:GLY:CA    | 2.36                     | 0.54              |
| 6:AF:33:TYR:HB2    | 6:AF:75:LEU:HD12   | 1.89                     | 0.54              |
| 9:AI:28:VAL:CG2    | 9:AI:63:ILE:HB     | 2.35                     | 0.54              |
| 9:AI:99:LEU:HD12   | 9:AI:101:PHE:CE1   | 2.42                     | 0.54              |
| 19:AS:15:LEU:C     | 19:AS:19:VAL:HG23  | 2.31                     | 0.54              |
| 20:AT:45:GLN:C     | 20:AT:47:GLY:H     | 2.15                     | 0.54              |
| 23:AW:34:G:N7      | 24:AX:14:A:C6      | 2.76                     | 0.54              |
| 25:BA:84:A:O2'     | 25:BA:85:G:O4'     | 2.25                     | 0.54              |
| 25:BA:1657:C:H5''  | 29:BE:133:LYS:O    | 2.08                     | 0.54              |
| 25:BA:1964:G:O2'   | 25:BA:1965:C:OP1   | 2.23                     | 0.54              |
| 25:BA:2449:U:C5'   | 25:BA:2450:A:OP1   | 2.55                     | 0.54              |
| 29:BE:53:PRO:HB2   | 29:BE:54:GLN:HG2   | 1.89                     | 0.54              |
| 29:BE:201:THR:HG23 | 29:BE:202:LYS:N    | 2.22                     | 0.54              |
| 31:BG:106:LEU:HA   | 31:BG:110:ALA:CB   | 2.37                     | 0.54              |
| 32:BH:85:LYS:CD    | 32:BH:133:VAL:HB   | 2.36                     | 0.54              |
| 34:BN:123:TYR:HH   | 34:BN:130:HIS:HE2  | 1.52                     | 0.54              |
| 36:BP:56:SER:O     | 36:BP:57:THR:HG22  | 2.07                     | 0.54              |
| 37:BQ:35:VAL:HB    | 37:BQ:102:VAL:HG22 | 1.88                     | 0.54              |
| 42:BV:22:VAL:O     | 42:BV:23:GLU:CB    | 2.56                     | 0.54              |
| 46:BZ:5:LEU:CD2    | 46:BZ:43:GLU:HB3   | 2.13                     | 0.54              |
| 1:CA:1504:G:H4'    | 1:CA:1505:G:OP2    | 2.08                     | 0.54              |
| 2:CB:19:HIS:CG     | 2:CB:20:GLU:H      | 2.24                     | 0.54              |
| 2:CB:239:VAL:O     | 2:CB:241:GLU:N     | 2.40                     | 0.54              |
| 3:CC:29:TYR:O      | 3:CC:30:ARG:C      | 2.50                     | 0.54              |
| 7:CG:60:LYS:HA     | 7:CG:60:LYS:HZ3    | 1.71                     | 0.54              |
| 13:CM:2:ALA:O      | 13:CM:10:PRO:HD2   | 2.06                     | 0.54              |
| 13:CM:82:MET:HE2   | 13:CM:93:ARG:CA    | 2.36                     | 0.54              |
| 18:CR:86:VAL:HG12  | 18:CR:87:ARG:CD    | 2.34                     | 0.54              |
| 19:CS:43:GLU:C     | 19:CS:45:VAL:HG13  | 2.32                     | 0.54              |
| 23:CY:27:G:C2      | 23:CY:43:C:N4      | 2.75                     | 0.54              |
| 25:DA:434:U:HO2'   | 25:DA:435:C:H5     | 1.55                     | 0.54              |
| 25:DA:1231:G:H2'   | 25:DA:1232:G:H8    | 1.72                     | 0.54              |
| 25:DA:2122:U:H2'   | 25:DA:2123:G:C8    | 2.43                     | 0.54              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 25:DA:2208:A:H1'   | 25:DA:2219:G:C4     | 2.42                     | 0.54              |
| 30:DF:129:PHE:CD2  | 30:DF:163:VAL:HG21  | 2.42                     | 0.54              |
| 42:DV:49:THR:CB    | 42:DV:50:PRO:CD     | 2.86                     | 0.54              |
| 46:DZ:11:GLU:OE2   | 46:DZ:13:GLU:HG2    | 2.06                     | 0.54              |
| 46:DZ:52:SER:C     | 46:DZ:53:ILE:HG12   | 2.33                     | 0.54              |
| 46:DZ:102:LEU:HD22 | 46:DZ:139:VAL:HG22  | 1.88                     | 0.54              |
| 48:D1:3:LYS:HG2    | 48:D1:4:VAL:HG12    | 1.88                     | 0.54              |
| 50:D3:8:LEU:HD11   | 50:D3:31:LEU:HD23   | 1.89                     | 0.54              |
| 55:D8:16:ILE:HD12  | 55:D8:57:ARG:HG2    | 1.89                     | 0.54              |
| 4:AD:12:CYS:HB2    | 4:AD:19:LEU:H       | 1.72                     | 0.54              |
| 4:AD:192:GLU:O     | 4:AD:193:ASP:C      | 2.50                     | 0.54              |
| 5:AE:57:LYS:O      | 5:AE:61:TYR:HD2     | 1.87                     | 0.54              |
| 9:AI:17:VAL:CG1    | 9:AI:81:ILE:HD13    | 2.36                     | 0.54              |
| 17:AQ:73:VAL:HG12  | 17:AQ:74:LEU:N      | 2.23                     | 0.54              |
| 19:AS:36:ARG:HH12  | 19:AS:75:ALA:HB3    | 1.72                     | 0.54              |
| 20:AT:25:ARG:HH11  | 20:AT:25:ARG:CG     | 2.19                     | 0.54              |
| 20:AT:98:PRO:C     | 20:AT:100:ILE:H     | 2.14                     | 0.54              |
| 25:BA:614(A):U:O5' | 25:BA:614(A):U:H6   | 1.90                     | 0.54              |
| 25:BA:1796:U:H2'   | 25:BA:1797:C:C6     | 2.42                     | 0.54              |
| 25:BA:2811:G:H5'   | 29:BE:60:ASN:HD22   | 1.73                     | 0.54              |
| 28:BD:96:HIS:ND1   | 28:BD:102:LYS:HD3   | 2.21                     | 0.54              |
| 30:BF:22:ALA:HB1   | 30:BF:26:ALA:CB     | 2.37                     | 0.54              |
| 31:BG:9:ARG:O      | 31:BG:12:TYR:N      | 2.41                     | 0.54              |
| 31:BG:20:ILE:O     | 31:BG:24:GLY:HA2    | 2.08                     | 0.54              |
| 31:BG:117:PHE:CE1  | 31:BG:119:GLY:N     | 2.76                     | 0.54              |
| 35:BO:64:ARG:NH1   | 35:BO:81:ASP:OD2    | 2.41                     | 0.54              |
| 36:BP:127:ALA:O    | 36:BP:147:LEU:HA    | 2.06                     | 0.54              |
| 42:BV:72:VAL:CG2   | 42:BV:85:LYS:HB3    | 2.23                     | 0.54              |
| 43:BW:57:ASN:O     | 43:BW:58:ALA:C      | 2.49                     | 0.54              |
| 1:CA:407:G:H5'     | 4:CD:3:ARG:HH12     | 1.72                     | 0.54              |
| 1:CA:913:A:O2'     | 1:CA:914:A:P        | 2.65                     | 0.54              |
| 4:CD:133:VAL:HG11  | 4:CD:138:TYR:CD1    | 2.42                     | 0.54              |
| 8:CH:91:ARG:CG     | 8:CH:91:ARG:NH1     | 2.60                     | 0.54              |
| 9:CI:53:VAL:HB     | 9:CI:92:TYR:CE2     | 2.42                     | 0.54              |
| 11:CK:124:LYS:HB3  | 11:CK:125:PHE:CE1   | 2.41                     | 0.54              |
| 12:CL:79:GLU:CD    | 12:CL:79:GLU:N      | 2.61                     | 0.54              |
| 23:CW:4:C:H6       | 23:CW:4:C:O5'       | 1.89                     | 0.54              |
| 25:DA:848:G:H2'    | 25:DA:849:A:C8      | 2.43                     | 0.54              |
| 25:DA:1019:U:H3    | 25:DA:1142(A):A:H62 | 1.56                     | 0.54              |
| 25:DA:1721:G:C6    | 25:DA:1739:U:OP2    | 2.60                     | 0.54              |
| 25:DA:1801:G:OP2   | 28:DD:154:LYS:HE2   | 2.08                     | 0.54              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:DA:2702:U:OP1  | 25:DA:2702:U:C6    | 2.61                     | 0.54              |
| 26:DB:14:U:C4'    | 26:DB:15:A:OP2     | 2.55                     | 0.54              |
| 33:DI:116:LEU:O   | 33:DI:116:LEU:HG   | 2.08                     | 0.54              |
| 41:DU:46:ALA:O    | 41:DU:50:ARG:HG3   | 2.08                     | 0.54              |
| 43:DW:65:LEU:HD22 | 43:DW:68:ARG:H     | 1.72                     | 0.54              |
| 1:AA:191:G:H1'    | 20:AT:105:SER:HB2  | 1.89                     | 0.54              |
| 1:AA:992:U:O2'    | 1:AA:993:G:P       | 2.66                     | 0.54              |
| 1:AA:1490:C:OP2   | 58:AA:7111:PAR:N64 | 2.40                     | 0.54              |
| 3:AC:22:TRP:CH2   | 3:AC:32:LEU:HB3    | 2.43                     | 0.54              |
| 4:AD:172:PRO:C    | 4:AD:187:ARG:HH12  | 2.14                     | 0.54              |
| 14:AN:26:ARG:NH2  | 14:AN:47:LEU:HD21  | 2.23                     | 0.54              |
| 18:AR:58:LEU:HD12 | 18:AR:58:LEU:N     | 2.22                     | 0.54              |
| 25:BA:479:A:O2'   | 25:BA:481:G:H5'    | 2.07                     | 0.54              |
| 25:BA:520:G:H2'   | 25:BA:521:G:H8     | 1.72                     | 0.54              |
| 25:BA:1912:A:C2   | 25:BA:1919:A:C6    | 2.95                     | 0.54              |
| 25:BA:2473:U:O2   | 25:BA:2473:U:C2'   | 2.55                     | 0.54              |
| 25:BA:2615:U:C2   | 52:B5:7:PRO:HA     | 2.42                     | 0.54              |
| 25:BA:2716:U:H2'  | 25:BA:2717:G:C8    | 2.42                     | 0.54              |
| 31:BG:2:PRO:HG2   | 51:B4:51:TYR:CZ    | 2.41                     | 0.54              |
| 34:BN:91:LEU:O    | 34:BN:95:PRO:HB3   | 2.08                     | 0.54              |
| 36:BP:88:LEU:HD11 | 36:BP:95:VAL:CG2   | 2.36                     | 0.54              |
| 40:BT:30:VAL:CG1  | 40:BT:31:SER:H     | 2.18                     | 0.54              |
| 43:BW:4:LYS:NZ    | 43:BW:6:ILE:CD1    | 2.71                     | 0.54              |
| 48:B1:48:LYS:NZ   | 48:B1:61:ARG:HG3   | 2.22                     | 0.54              |
| 55:B8:40:GLU:O    | 55:B8:44:LYS:HE3   | 2.07                     | 0.54              |
| 1:CA:854:G:H3'    | 1:CA:871:U:O4      | 2.08                     | 0.54              |
| 2:CB:84:GLU:HB3   | 2:CB:219:VAL:HG21  | 1.88                     | 0.54              |
| 8:CH:121:ASP:HB2  | 8:CH:125:ARG:NH2   | 2.22                     | 0.54              |
| 9:CI:81:ILE:O     | 9:CI:85:LEU:HG     | 2.07                     | 0.54              |
| 10:CJ:30:SER:OG   | 10:CJ:81:THR:HG22  | 2.08                     | 0.54              |
| 13:CM:44:ARG:C    | 13:CM:46:LYS:N     | 2.63                     | 0.54              |
| 15:CO:79:ARG:O    | 15:CO:83:GLU:HB2   | 2.06                     | 0.54              |
| 19:CS:45:VAL:HA   | 19:CS:62:ILE:CG2   | 2.37                     | 0.54              |
| 20:CT:53:LEU:CD2  | 20:CT:100:ILE:CB   | 2.85                     | 0.54              |
| 25:DA:604:G:OP2   | 36:DP:90:ARG:NH2   | 2.41                     | 0.54              |
| 25:DA:686:G:O6    | 54:D7:12:ARG:HG3   | 2.08                     | 0.54              |
| 29:DE:69:LYS:HD3  | 29:DE:89:ASP:HA    | 1.90                     | 0.54              |
| 33:DI:88:ILE:HB   | 33:DI:90:GLY:O     | 2.08                     | 0.54              |
| 35:DO:104:ARG:NH2 | 40:DT:43:GLN:HE22  | 2.06                     | 0.54              |
| 36:DP:59:LEU:O    | 36:DP:59:LEU:HG    | 2.07                     | 0.54              |
| 36:DP:62:LEU:HD23 | 36:DP:62:LEU:H     | 1.72                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 40:DT:32:TYR:CD2   | 40:DT:81:PRO:O     | 2.59                     | 0.54              |
| 41:DU:66:ASN:CB    | 41:DU:76:TYR:HB2   | 2.37                     | 0.54              |
| 42:DV:66:ARG:HH11  | 42:DV:66:ARG:HB3   | 1.72                     | 0.54              |
| 51:D4:38:LYS:O     | 51:D4:39:CYS:SG    | 2.64                     | 0.54              |
| 55:D8:23:VAL:HG12  | 55:D8:46:ARG:HH11  | 1.71                     | 0.54              |
| 1:AA:13:U:O2'      | 1:AA:915:A:OP2     | 2.24                     | 0.54              |
| 1:AA:470:C:H5''    | 1:AA:471:G:OP2     | 2.08                     | 0.54              |
| 1:AA:922:G:H4'     | 5:AE:20:GLN:HA     | 1.88                     | 0.54              |
| 1:AA:1048:G:N3     | 1:AA:1050:G:N7     | 2.56                     | 0.54              |
| 1:AA:1191:A:H5''   | 3:AC:4:LYS:HZ2     | 1.73                     | 0.54              |
| 2:AB:19:HIS:ND1    | 2:AB:20:GLU:HG2    | 2.23                     | 0.54              |
| 2:AB:155:LEU:HG    | 2:AB:159:PRO:HG3   | 1.88                     | 0.54              |
| 8:AH:10:LEU:HD23   | 8:AH:83:ILE:CG1    | 2.37                     | 0.54              |
| 8:AH:48:TYR:CD1    | 8:AH:49:GLU:N      | 2.76                     | 0.54              |
| 9:AI:8:GLY:C       | 9:AI:76:ALA:HB1    | 2.33                     | 0.54              |
| 19:AS:43:GLU:CA    | 19:AS:45:VAL:HG13  | 2.37                     | 0.54              |
| 22:AV:38:A:C2      | 24:AX:16:A:C6      | 2.96                     | 0.54              |
| 24:AX:11:U:O5'     | 24:AX:11:U:H6      | 1.91                     | 0.54              |
| 30:BF:164:ARG:HG2  | 30:BF:164:ARG:NH1  | 2.18                     | 0.54              |
| 32:BH:107:VAL:CG2  | 32:BH:107:VAL:O    | 2.55                     | 0.54              |
| 32:BH:158:HIS:O    | 32:BH:159:GLU:HB2  | 2.07                     | 0.54              |
| 33:BI:131:LYS:HG3  | 33:BI:132:PRO:HD2  | 1.90                     | 0.54              |
| 36:BP:98:GLU:HG3   | 36:BP:99:LEU:N     | 2.22                     | 0.54              |
| 36:BP:114:ILE:O    | 36:BP:114:ILE:HG13 | 2.07                     | 0.54              |
| 36:BP:146:VAL:HG22 | 36:BP:147:LEU:N    | 2.15                     | 0.54              |
| 37:BQ:27:VAL:HG12  | 37:BQ:29:PHE:H     | 1.72                     | 0.54              |
| 40:BT:81:PRO:C     | 40:BT:82:LEU:HD12  | 2.33                     | 0.54              |
| 44:BX:12:VAL:HG12  | 44:BX:17:ALA:HB1   | 1.88                     | 0.54              |
| 45:BY:27:VAL:HB    | 45:BY:29:GLU:OE1   | 2.07                     | 0.54              |
| 50:B3:10:LYS:NZ    | 50:B3:15:TYR:OH    | 2.28                     | 0.54              |
| 1:CA:189(K):U:H2'  | 1:CA:189(L):G:C8   | 2.43                     | 0.54              |
| 1:CA:686:U:O2'     | 1:CA:687:A:C5'     | 2.55                     | 0.54              |
| 1:CA:687:A:C2      | 1:CA:704:A:C6      | 2.95                     | 0.54              |
| 2:CB:204:ASN:HB3   | 2:CB:210:SER:OG    | 2.08                     | 0.54              |
| 6:CF:40:VAL:O      | 6:CF:41:GLU:HG3    | 2.08                     | 0.54              |
| 7:CG:22:LEU:O      | 7:CG:25:ALA:HB3    | 2.08                     | 0.54              |
| 13:CM:25:ILE:HD11  | 13:CM:66:LEU:CD2   | 2.38                     | 0.54              |
| 15:CO:18:PHE:CE1   | 15:CO:21:ASP:HB2   | 2.42                     | 0.54              |
| 23:CW:38:A:C2'     | 23:CW:39:U:H5''    | 2.38                     | 0.54              |
| 25:DA:811:U:H1'    | 25:DA:1251:C:O4'   | 2.08                     | 0.54              |
| 25:DA:2477:C:N3    | 56:D9:4:ARG:NH1    | 2.55                     | 0.54              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:DA:2615:U:H2'  | 25:DA:2616:C:C6    | 2.41                     | 0.54              |
| 28:DD:158:ALA:HB3 | 28:DD:161:THR:HG21 | 1.89                     | 0.54              |
| 28:DD:243:GLY:O   | 28:DD:244:ARG:HB3  | 2.07                     | 0.54              |
| 29:DE:75:VAL:O    | 29:DE:77:ILE:N     | 2.41                     | 0.54              |
| 29:DE:101:ARG:NH2 | 29:DE:171:GLU:CB   | 2.68                     | 0.54              |
| 33:DI:32:PRO:C    | 33:DI:34:GLY:N     | 2.65                     | 0.54              |
| 33:DI:132:PRO:O   | 33:DI:133:HIS:ND1  | 2.40                     | 0.54              |
| 34:DN:73:THR:CG2  | 34:DN:82:LEU:HD11  | 2.37                     | 0.54              |
| 37:DQ:26:TYR:CD1  | 37:DQ:26:TYR:O     | 2.61                     | 0.54              |
| 40:DT:121:ILE:O   | 40:DT:124:ASP:HB2  | 2.08                     | 0.54              |
| 41:DU:69:CYS:CB   | 41:DU:79:PHE:HD1   | 2.19                     | 0.54              |
| 46:DZ:3:TYR:N     | 46:DZ:3:TYR:CD1    | 2.75                     | 0.54              |
| 1:AA:119:A:O2'    | 1:AA:120:A:OP2     | 2.20                     | 0.54              |
| 1:AA:366:C:H6     | 1:AA:366:C:O5'     | 1.90                     | 0.54              |
| 7:AG:9:VAL:O      | 7:AG:10:ARG:C      | 2.51                     | 0.54              |
| 11:AK:64:ALA:O    | 11:AK:68:ALA:N     | 2.34                     | 0.54              |
| 13:AM:23:TYR:CE1  | 13:AM:70:LEU:HD22  | 2.42                     | 0.54              |
| 19:AS:33:THR:OG1  | 19:AS:34:TRP:N     | 2.39                     | 0.54              |
| 25:BA:242:G:H5''  | 55:B8:62:LEU:HD13  | 1.89                     | 0.54              |
| 25:BA:669:G:N3    | 25:BA:669:G:C2'    | 2.69                     | 0.54              |
| 25:BA:2318:G:HO2' | 25:BA:2319:G:P     | 2.29                     | 0.54              |
| 29:BE:70:ALA:O    | 29:BE:71:GLY:O     | 2.25                     | 0.54              |
| 29:BE:132:HIS:CD2 | 29:BE:135:HIS:NE2  | 2.75                     | 0.54              |
| 35:BO:86:ILE:HD12 | 35:BO:86:ILE:N     | 2.23                     | 0.54              |
| 36:BP:117:GLU:OE1 | 36:BP:117:GLU:N    | 2.37                     | 0.54              |
| 40:BT:28:VAL:HG12 | 40:BT:29:ARG:HH21  | 1.73                     | 0.54              |
| 42:BV:2:PHE:CD2   | 42:BV:3:ALA:N      | 2.76                     | 0.54              |
| 45:BY:8:LYS:H     | 45:BY:8:LYS:CD     | 2.05                     | 0.54              |
| 45:BY:37:VAL:HG23 | 45:BY:39:VAL:HG23  | 1.90                     | 0.54              |
| 46:BZ:67:LEU:HD22 | 46:BZ:90:VAL:HG11  | 1.88                     | 0.54              |
| 49:B2:67:LYS:HA   | 49:B2:70:GLN:NE2   | 2.22                     | 0.54              |
| 1:CA:490:G:H2'    | 1:CA:491:G:H8      | 1.73                     | 0.54              |
| 1:CA:1435:G:H2'   | 1:CA:1436:U:C6     | 2.43                     | 0.54              |
| 1:CA:1443:G:H22   | 1:CA:1460:A:H1'    | 1.73                     | 0.54              |
| 5:CE:60:TYR:HE1   | 5:CE:64:ARG:HD3    | 1.71                     | 0.54              |
| 10:CJ:50:ILE:N    | 10:CJ:50:ILE:HD13  | 2.22                     | 0.54              |
| 23:CW:36:A:N1     | 23:CW:37:A:C5      | 2.76                     | 0.54              |
| 25:DA:889:C:O2'   | 25:DA:890:A:P      | 2.66                     | 0.54              |
| 25:DA:1273:U:O2'  | 25:DA:1275:A:OP1   | 2.24                     | 0.54              |
| 25:DA:2820:A:OP1  | 38:DR:4:LEU:HA     | 2.06                     | 0.54              |
| 28:DD:252:TRP:O   | 28:DD:253:GLN:C    | 2.51                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:DG:13:GLU:O     | 31:DG:13:GLU:HG3   | 2.08                     | 0.54              |
| 31:DG:77:ILE:O     | 31:DG:81:LYS:O     | 2.25                     | 0.54              |
| 32:DH:35:VAL:CG1   | 32:DH:71:LEU:HG    | 2.36                     | 0.54              |
| 33:DI:61:ARG:HA    | 33:DI:61:ARG:CZ    | 2.37                     | 0.54              |
| 39:DS:18:ILE:O     | 39:DS:19:LYS:O     | 2.25                     | 0.54              |
| 41:DU:97:ASP:OD1   | 41:DU:98:LEU:N     | 2.41                     | 0.54              |
| 51:D4:1:MET:HB3    | 51:D4:6:HIS:CD2    | 2.43                     | 0.54              |
| 1:AA:457:C:H2'     | 1:AA:458:C:H6      | 1.72                     | 0.54              |
| 1:AA:950:U:H2'     | 1:AA:951:G:C8      | 2.43                     | 0.54              |
| 2:AB:11:LEU:CD1    | 2:AB:217:ARG:NH2   | 2.71                     | 0.54              |
| 3:AC:70:VAL:HG12   | 3:AC:72:LYS:H      | 1.73                     | 0.54              |
| 3:AC:73:PRO:HA     | 3:AC:76:VAL:HG13   | 1.89                     | 0.54              |
| 4:AD:8:VAL:HG11    | 4:AD:21:LEU:HB2    | 1.90                     | 0.54              |
| 7:AG:86:GLN:HB2    | 7:AG:148:ASN:ND2   | 2.23                     | 0.54              |
| 9:AI:118:LYS:NZ    | 9:AI:118:LYS:HB3   | 2.21                     | 0.54              |
| 10:AJ:33:GLN:O     | 10:AJ:75:ILE:HG12  | 2.07                     | 0.54              |
| 10:AJ:50:ILE:HD13  | 10:AJ:50:ILE:H     | 1.72                     | 0.54              |
| 20:AT:53:LEU:CD1   | 20:AT:102:GLY:HA3  | 2.24                     | 0.54              |
| 25:BA:1188:U:H4'   | 42:BV:79:VAL:CG2   | 2.37                     | 0.54              |
| 25:BA:1558:A:H4'   | 25:BA:1559:G:O5'   | 2.08                     | 0.54              |
| 25:BA:2746:U:O5'   | 25:BA:2746:U:H6    | 1.91                     | 0.54              |
| 26:BB:11:C:H5''    | 26:BB:12:C:OP2     | 2.07                     | 0.54              |
| 26:BB:66:A:N6      | 26:BB:108:U:C5     | 2.76                     | 0.54              |
| 27:BC:49:ILE:HG22  | 27:BC:50:ASP:N     | 2.23                     | 0.54              |
| 28:BD:36:PRO:O     | 28:BD:37:LEU:HD23  | 2.07                     | 0.54              |
| 28:BD:211:ARG:O    | 28:BD:214:TRP:HB2  | 2.08                     | 0.54              |
| 28:BD:224:ALA:O    | 28:BD:225:ALA:CB   | 2.55                     | 0.54              |
| 29:BE:61:ARG:HB3   | 29:BE:62:PRO:HD3   | 1.90                     | 0.54              |
| 30:BF:39:TRP:O     | 30:BF:43:LYS:HG2   | 2.08                     | 0.54              |
| 31:BG:37:VAL:HG11  | 31:BG:94:LEU:HD12  | 1.86                     | 0.54              |
| 31:BG:160:VAL:HG12 | 31:BG:161:THR:N    | 2.22                     | 0.54              |
| 32:BH:54:ARG:O     | 32:BH:54:ARG:HG3   | 2.08                     | 0.54              |
| 35:BO:119:PRO:O    | 35:BO:120:GLU:CB   | 2.56                     | 0.54              |
| 39:BS:101:LEU:HD13 | 39:BS:101:LEU:H    | 1.72                     | 0.54              |
| 41:BU:59:ARG:O     | 41:BU:60:LEU:C     | 2.50                     | 0.54              |
| 42:BV:66:ARG:HH11  | 42:BV:66:ARG:HG2   | 1.73                     | 0.54              |
| 49:B2:13:ALA:O     | 49:B2:16:LEU:HB2   | 2.07                     | 0.54              |
| 1:CA:470:C:C5'     | 1:CA:471:G:OP2     | 2.55                     | 0.54              |
| 3:CC:46:GLU:O      | 3:CC:47:LEU:HB2    | 2.07                     | 0.54              |
| 10:CJ:83:GLU:HB3   | 10:CJ:84:GLN:NE2   | 2.22                     | 0.54              |
| 11:CK:99:GLN:HG2   | 11:CK:105:VAL:HG11 | 1.89                     | 0.54              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 12:CL:119:LYS:HB2 | 12:CL:120:TYR:CD1  | 2.43                     | 0.54              |
| 15:CO:61:GLY:O    | 15:CO:64:ARG:HB3   | 2.08                     | 0.54              |
| 17:CQ:67:LYS:C    | 17:CQ:69:LYS:H     | 2.15                     | 0.54              |
| 23:CW:32:U:H2'    | 23:CW:33:U:H5'     | 1.88                     | 0.54              |
| 25:DA:859:G:N2    | 25:DA:917:A:OP2    | 2.37                     | 0.54              |
| 25:DA:1965:C:O5'  | 25:DA:1965:C:H6    | 1.91                     | 0.54              |
| 25:DA:2680:C:H5'  | 29:DE:189:PRO:HA   | 1.89                     | 0.54              |
| 32:DH:124:GLU:HB2 | 32:DH:132:ARG:CD   | 2.35                     | 0.54              |
| 34:DN:26:LEU:HG   | 34:DN:30:ILE:HD11  | 1.88                     | 0.54              |
| 34:DN:51:PHE:CE2  | 34:DN:119:ARG:HD2  | 2.43                     | 0.54              |
| 34:DN:67:LEU:HB3  | 34:DN:88:GLU:HG2   | 1.88                     | 0.54              |
| 41:DU:79:PHE:C    | 41:DU:79:PHE:CD2   | 2.86                     | 0.54              |
| 43:DW:68:ARG:HD2  | 43:DW:110:LYS:HB3  | 1.90                     | 0.54              |
| 45:DY:49:VAL:HG12 | 45:DY:50:ARG:N     | 2.22                     | 0.54              |
| 45:DY:57:GLN:HE21 | 45:DY:58:GLY:N     | 2.06                     | 0.54              |
| 46:DZ:19:ARG:NH2  | 46:DZ:84:GLU:O     | 2.40                     | 0.54              |
| 4:AD:43:HIS:O     | 4:AD:44:GLY:C      | 2.50                     | 0.54              |
| 7:AG:118:VAL:HG23 | 7:AG:119:ARG:N     | 2.21                     | 0.54              |
| 20:AT:81:LYS:O    | 20:AT:85:MET:HB2   | 2.07                     | 0.54              |
| 20:AT:91:LEU:C    | 20:AT:93:GLU:H     | 2.16                     | 0.54              |
| 25:BA:529:A:H5''  | 25:BA:530:G:OP1    | 2.08                     | 0.54              |
| 25:BA:562:U:O4    | 25:BA:2033:A:N1    | 2.39                     | 0.54              |
| 25:BA:614:U:O2    | 25:BA:614:U:C5'    | 2.52                     | 0.54              |
| 25:BA:1365:A:H5'' | 48:B1:41:ARG:HH12  | 1.72                     | 0.54              |
| 25:BA:2602:A:H62  | 47:B0:2:ALA:HB3    | 1.72                     | 0.54              |
| 27:BC:55:ASP:CG   | 27:BC:56:GLN:N     | 2.65                     | 0.54              |
| 27:BC:77:ILE:HG21 | 27:BC:123:VAL:N    | 2.23                     | 0.54              |
| 30:BF:167:ALA:HB1 | 30:BF:173:VAL:HG11 | 1.90                     | 0.54              |
| 31:BG:47:LYS:HZ2  | 31:BG:82:LEU:HD12  | 1.73                     | 0.54              |
| 31:BG:72:ARG:NH1  | 31:BG:86:MET:HB2   | 2.15                     | 0.54              |
| 32:BH:64:LEU:HA   | 32:BH:67:LEU:HB3   | 1.90                     | 0.54              |
| 33:BI:83:ALA:O    | 33:BI:89:TYR:HE1   | 1.90                     | 0.54              |
| 43:BW:13:SER:HB3  | 43:BW:16:LYS:HG3   | 1.90                     | 0.54              |
| 45:BY:28:LYS:HB3  | 45:BY:37:VAL:CG2   | 2.37                     | 0.54              |
| 48:B1:18:ILE:HG12 | 48:B1:37:ILE:HG23  | 1.88                     | 0.54              |
| 55:B8:31:HIS:ND1  | 55:B8:32:LEU:CB    | 2.71                     | 0.54              |
| 1:CA:532:A:H2'    | 1:CA:533:A:OP1     | 2.08                     | 0.54              |
| 1:CA:533:A:C4'    | 1:CA:534:U:OP1     | 2.50                     | 0.54              |
| 1:CA:1457:G:H2'   | 1:CA:1458:G:C8     | 2.42                     | 0.54              |
| 4:CD:96:LEU:HD23  | 4:CD:139:ARG:CZ    | 2.38                     | 0.54              |
| 5:CE:127:ASN:OD1  | 5:CE:127:ASN:C     | 2.50                     | 0.54              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 9:CI:55:ALA:CB     | 9:CI:58:HIS:ND1   | 2.70                     | 0.54              |
| 25:DA:762:U:H4'    | 25:DA:763:G:O5'   | 2.08                     | 0.54              |
| 25:DA:1815:A:H4'   | 25:DA:1816:G:O5'  | 2.07                     | 0.54              |
| 25:DA:2291:U:O2'   | 25:DA:2374:C:O2   | 2.25                     | 0.54              |
| 25:DA:2543:G:H2'   | 25:DA:2544:G:C8   | 2.43                     | 0.54              |
| 25:DA:2848:G:N2    | 25:DA:2867:G:C4   | 2.76                     | 0.54              |
| 28:DD:25:THR:HG22  | 28:DD:26:LYS:N    | 2.20                     | 0.54              |
| 29:DE:53:PRO:O     | 29:DE:54:GLN:O    | 2.25                     | 0.54              |
| 32:DH:30:LYS:HE3   | 32:DH:81:GLU:CA   | 2.37                     | 0.54              |
| 36:DP:6:LEU:O      | 36:DP:7:ARG:HG2   | 2.07                     | 0.54              |
| 37:DQ:39:PRO:HA    | 37:DQ:97:VAL:O    | 2.07                     | 0.54              |
| 37:DQ:110:THR:OG1  | 37:DQ:112:GLU:HG2 | 2.08                     | 0.54              |
| 38:DR:92:GLY:O     | 38:DR:93:GLY:C    | 2.51                     | 0.54              |
| 40:DT:32:TYR:CD2   | 40:DT:32:TYR:N    | 2.68                     | 0.54              |
| 41:DU:92:ARG:NH1   | 42:DV:11:GLN:CB   | 2.56                     | 0.54              |
| 43:DW:1:MET:HA     | 43:DW:1:MET:HE3   | 1.89                     | 0.54              |
| 47:D0:73:GLY:C     | 47:D0:75:LEU:N    | 2.66                     | 0.54              |
| 1:AA:974:A:C1'     | 14:AN:31:ARG:HE   | 2.21                     | 0.54              |
| 1:AA:1047:G:C2'    | 1:AA:1048:G:H5'   | 2.38                     | 0.54              |
| 1:AA:1108:G:H5'    | 3:AC:176:HIS:ND1  | 2.20                     | 0.54              |
| 8:AH:8:ASP:O       | 8:AH:11:THR:N     | 2.36                     | 0.54              |
| 9:AI:42:ARG:O      | 9:AI:43:ALA:C     | 2.50                     | 0.54              |
| 13:AM:3:ARG:CD     | 31:BG:113:ARG:NH2 | 2.71                     | 0.54              |
| 25:BA:604:G:OP2    | 36:BP:90:ARG:NH2  | 2.41                     | 0.54              |
| 25:BA:811:U:O4     | 36:BP:21:ARG:NH2  | 2.40                     | 0.54              |
| 25:BA:1340:U:C4'   | 25:BA:1341:U:OP2  | 2.55                     | 0.54              |
| 25:BA:2701:C:H3'   | 25:BA:2702:U:C5'  | 2.27                     | 0.54              |
| 25:BA:2787:C:H1'   | 29:BE:61:ARG:CG   | 2.38                     | 0.54              |
| 29:BE:119:ARG:O    | 29:BE:120:TRP:CD2 | 2.61                     | 0.54              |
| 31:BG:132:ASN:ND2  | 31:BG:132:ASN:N   | 2.55                     | 0.54              |
| 33:BI:40:THR:O     | 33:BI:41:GLU:C    | 2.51                     | 0.54              |
| 33:BI:44:LEU:O     | 33:BI:47:LEU:HB3  | 2.08                     | 0.54              |
| 34:BN:18:ALA:O     | 34:BN:21:LYS:N    | 2.33                     | 0.54              |
| 35:BO:11:ALA:O     | 35:BO:98:VAL:HG23 | 2.08                     | 0.54              |
| 36:BP:58:THR:O     | 36:BP:58:THR:HG22 | 2.07                     | 0.54              |
| 36:BP:105:LEU:HD12 | 36:BP:105:LEU:N   | 2.23                     | 0.54              |
| 40:BT:45:PHE:CE1   | 40:BT:74:ARG:HG3  | 2.43                     | 0.54              |
| 46:BZ:119:GLU:HB2  | 46:BZ:122:ARG:HG2 | 1.90                     | 0.54              |
| 48:B1:8:SER:HB2    | 48:B1:66:HIS:CD2  | 2.43                     | 0.54              |
| 1:CA:128:G:N2      | 1:CA:130:A:H62    | 2.06                     | 0.54              |
| 1:CA:827:U:H3      | 1:CA:872:A:H61    | 1.55                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:1067:A:H1'    | 1:CA:1068:G:O4'    | 2.07                     | 0.54              |
| 2:CB:87:ARG:NE     | 2:CB:233:SER:HB2   | 2.22                     | 0.54              |
| 4:CD:19:LEU:CD2    | 4:CD:21:LEU:HD11   | 2.38                     | 0.54              |
| 14:CN:36:PHE:C     | 14:CN:36:PHE:CD1   | 2.86                     | 0.54              |
| 16:CP:8:ARG:HH11   | 16:CP:8:ARG:HG3    | 1.71                     | 0.54              |
| 16:CP:8:ARG:HB3    | 16:CP:28:ARG:NH1   | 2.23                     | 0.54              |
| 21:CU:3:LYS:HG2    | 21:CU:14:TRP:CD1   | 2.43                     | 0.54              |
| 22:CV:55:U:O2'     | 22:CV:56:U:H5'     | 2.08                     | 0.54              |
| 25:DA:77:C:O3'     | 49:D2:14:ARG:NH2   | 2.40                     | 0.54              |
| 25:DA:154:G:O6     | 25:DA:172:C:N4     | 2.37                     | 0.54              |
| 25:DA:587:C:O2     | 36:DP:33:ARG:NH1   | 2.41                     | 0.54              |
| 25:DA:614(A):U:C4' | 25:DA:614(B):G:OP1 | 2.52                     | 0.54              |
| 25:DA:871:U:OP1    | 37:DQ:5:ARG:HG3    | 2.08                     | 0.54              |
| 25:DA:1697:G:C3'   | 25:DA:1698:A:C5'   | 2.78                     | 0.54              |
| 25:DA:2729:G:H1'   | 29:DE:187:ALA:CB   | 2.38                     | 0.54              |
| 28:DD:30:GLU:HG3   | 28:DD:63:ARG:CZ    | 2.38                     | 0.54              |
| 29:DE:128:SER:OG   | 29:DE:129:HIS:N    | 2.38                     | 0.54              |
| 31:DG:68:PRO:CG    | 31:DG:90:LEU:HD12  | 2.37                     | 0.54              |
| 32:DH:103:LEU:HD21 | 32:DH:115:VAL:HB   | 1.89                     | 0.54              |
| 32:DH:130:ARG:O    | 32:DH:130:ARG:HD2  | 2.08                     | 0.54              |
| 33:DI:125:GLU:OE2  | 33:DI:141:LYS:HG2  | 2.08                     | 0.54              |
| 34:DN:15:LEU:HB3   | 34:DN:136:GLU:HA   | 1.89                     | 0.54              |
| 41:DU:106:PHE:O    | 41:DU:110:VAL:HG23 | 2.08                     | 0.54              |
| 42:DV:25:LEU:CD1   | 42:DV:94:LEU:HD21  | 2.38                     | 0.54              |
| 44:DX:12:VAL:HG11  | 44:DX:27:THR:HG1   | 1.73                     | 0.54              |
| 45:DY:75:ILE:CG1   | 45:DY:80:GLY:H     | 2.21                     | 0.54              |
| 47:D0:41:ARG:HD3   | 47:D0:44:ARG:HD2   | 1.90                     | 0.54              |
| 53:D6:15:GLU:CG    | 53:D6:47:THR:OG1   | 2.56                     | 0.54              |
| 53:D6:25:LYS:HD3   | 55:D8:34:TRP:HZ2   | 1.73                     | 0.54              |
| 1:AA:535:A:O2'     | 1:AA:536:C:OP1     | 2.22                     | 0.54              |
| 2:AB:119:GLU:O     | 2:AB:122:PHE:HB3   | 2.08                     | 0.54              |
| 3:AC:58:GLU:O      | 3:AC:59:ARG:HG3    | 2.08                     | 0.54              |
| 5:AE:100:VAL:HG13  | 5:AE:118:ILE:HG22  | 1.89                     | 0.54              |
| 8:AH:19:VAL:HG21   | 8:AH:21:LYS:HE3    | 1.91                     | 0.54              |
| 9:AI:37:PHE:HB3    | 9:AI:43:ALA:HB2    | 1.89                     | 0.54              |
| 12:AL:84:LEU:HD22  | 12:AL:85:ILE:N     | 2.22                     | 0.54              |
| 13:AM:28:ALA:O     | 13:AM:30:ALA:N     | 2.41                     | 0.54              |
| 13:AM:90:LEU:O     | 13:AM:91:ARG:CB    | 2.54                     | 0.54              |
| 19:AS:41:VAL:O     | 19:AS:44:MET:HB2   | 2.08                     | 0.54              |
| 22:AV:37:U:H2'     | 22:AV:38:A:O4'     | 2.08                     | 0.54              |
| 25:BA:685:A:O2'    | 25:BA:689:A:N6     | 2.41                     | 0.54              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 25:BA:1301:A:C4'   | 25:BA:1302:A:OP1  | 2.49                     | 0.54              |
| 25:BA:2320:A:C5    | 25:BA:2333:A:N6   | 2.74                     | 0.54              |
| 28:BD:210:GLY:O    | 28:BD:211:ARG:C   | 2.51                     | 0.54              |
| 35:BO:7:TYR:CE1    | 35:BO:20:MET:HB2  | 2.43                     | 0.54              |
| 40:BT:29:ARG:HD3   | 40:BT:84:GLN:O    | 2.08                     | 0.54              |
| 46:BZ:39:VAL:CG2   | 46:BZ:44:PHE:HB2  | 2.38                     | 0.54              |
| 1:CA:1030(A):G:H1' | 1:CA:1031:G:H22   | 1.73                     | 0.54              |
| 6:CF:77:ARG:O      | 6:CF:79:LEU:N     | 2.41                     | 0.54              |
| 7:CG:110:GLN:O     | 7:CG:111:ARG:HB2  | 2.07                     | 0.54              |
| 18:CR:74:ARG:NH2   | 18:CR:81:PHE:HA   | 2.22                     | 0.54              |
| 20:CT:53:LEU:HB3   | 20:CT:102:GLY:HA3 | 1.90                     | 0.54              |
| 22:CV:28:U:O2'     | 22:CV:29:C:H5'    | 2.08                     | 0.54              |
| 22:CV:55:U:C2'     | 22:CV:56:U:H5'    | 2.37                     | 0.54              |
| 25:DA:1820:U:C4'   | 25:DA:1821:A:OP2  | 2.46                     | 0.54              |
| 28:DD:22:SER:O     | 28:DD:23:GLU:C    | 2.51                     | 0.54              |
| 29:DE:14:ILE:HG12  | 29:DE:21:VAL:HG23 | 1.89                     | 0.54              |
| 29:DE:173:VAL:HG12 | 29:DE:174:ASP:H   | 1.73                     | 0.54              |
| 30:DF:7:TYR:N      | 30:DF:7:TYR:CD1   | 2.76                     | 0.54              |
| 31:DG:110:ALA:C    | 31:DG:112:PRO:HD2 | 2.32                     | 0.54              |
| 33:DI:37:VAL:HG13  | 33:DI:38:LEU:HD12 | 1.89                     | 0.54              |
| 38:DR:52:ILE:O     | 38:DR:55:ALA:HB3  | 2.08                     | 0.54              |
| 42:DV:8:GLY:O      | 42:DV:10:LYS:CE   | 2.55                     | 0.54              |
| 45:DY:81:LYS:HB3   | 45:DY:97:ARG:HD3  | 1.88                     | 0.54              |
| 47:D0:69:PHE:CD2   | 47:D0:79:VAL:HG22 | 2.43                     | 0.54              |
| 1:AA:76:C:H42      | 1:AA:93:G:H1      | 1.56                     | 0.53              |
| 1:AA:192:U:H4'     | 20:AT:103:GLY:HA2 | 1.89                     | 0.53              |
| 2:AB:82:ARG:O      | 2:AB:85:ALA:HB3   | 2.07                     | 0.53              |
| 2:AB:108:ILE:CG2   | 2:AB:152:PHE:CE1  | 2.91                     | 0.53              |
| 2:AB:180:LEU:C     | 2:AB:182:ILE:H    | 2.16                     | 0.53              |
| 4:AD:13:ARG:HH22   | 4:AD:36:ARG:HH11  | 1.55                     | 0.53              |
| 5:AE:20:GLN:O      | 5:AE:21:ALA:C     | 2.50                     | 0.53              |
| 5:AE:91:LEU:CD2    | 5:AE:138:ALA:HB1  | 2.38                     | 0.53              |
| 5:AE:101:ILE:CD1   | 5:AE:119:LEU:HD23 | 2.38                     | 0.53              |
| 6:AF:41:GLU:O      | 6:AF:43:LEU:N     | 2.40                     | 0.53              |
| 12:AL:41:ARG:HD2   | 12:AL:43:VAL:CG1  | 2.38                     | 0.53              |
| 14:AN:23:ARG:NH1   | 14:AN:30:ALA:HB2  | 2.22                     | 0.53              |
| 15:AO:87:ILE:CG2   | 15:AO:88:ARG:N    | 2.70                     | 0.53              |
| 22:AV:17:C:OP1     | 22:AV:62:C:H5'    | 2.08                     | 0.53              |
| 23:AW:38:A:H2'     | 23:AW:39:U:H5''   | 1.90                     | 0.53              |
| 23:AY:28:G:H2'     | 23:AY:29:G:C8     | 2.42                     | 0.53              |
| 25:BA:1819:A:H1'   | 25:BA:1821:A:N6   | 2.22                     | 0.53              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:BA:2472:G:H5'   | 25:BA:2473:U:H5''  | 1.90                     | 0.53              |
| 32:BH:146:ALA:O    | 32:BH:150:ALA:HB2  | 2.09                     | 0.53              |
| 35:BO:17:ARG:HA    | 35:BO:17:ARG:HH11  | 1.73                     | 0.53              |
| 36:BP:58:THR:O     | 36:BP:61:ARG:CZ    | 2.56                     | 0.53              |
| 36:BP:79:ARG:CD    | 36:BP:109:GLY:C    | 2.81                     | 0.53              |
| 37:BQ:1:MET:O      | 37:BQ:2:LEU:HB2    | 2.08                     | 0.53              |
| 41:BU:61:TRP:CZ3   | 41:BU:94:ASN:HB2   | 2.43                     | 0.53              |
| 41:BU:108:GLU:CD   | 42:BV:44:LYS:HD3   | 2.32                     | 0.53              |
| 45:BY:43:ASN:O     | 45:BY:44:ILE:O     | 2.26                     | 0.53              |
| 46:BZ:10:ARG:HD2   | 46:BZ:36:LYS:HD3   | 1.90                     | 0.53              |
| 46:BZ:14:LYS:O     | 46:BZ:15:PRO:C     | 2.50                     | 0.53              |
| 1:CA:509:A:O2'     | 1:CA:510:A:OP1     | 2.21                     | 0.53              |
| 3:CC:184:TYR:HA    | 3:CC:200:ALA:O     | 2.08                     | 0.53              |
| 9:CI:15:ALA:HB2    | 9:CI:65:VAL:CG2    | 2.23                     | 0.53              |
| 11:CK:32:ILE:CD1   | 11:CK:68:ALA:O     | 2.56                     | 0.53              |
| 18:CR:58:LEU:HD12  | 18:CR:58:LEU:N     | 2.23                     | 0.53              |
| 25:DA:13:A:C2      | 25:DA:14:A:N6      | 2.75                     | 0.53              |
| 25:DA:571:A:H1'    | 25:DA:573:G:C8     | 2.42                     | 0.53              |
| 25:DA:750:A:O2'    | 25:DA:752:A:OP1    | 2.26                     | 0.53              |
| 25:DA:1300:U:H1'   | 25:DA:1626:G:C2    | 2.43                     | 0.53              |
| 25:DA:1799:G:C8    | 25:DA:1819:A:N6    | 2.75                     | 0.53              |
| 25:DA:1819:A:H5''  | 25:DA:1820:U:H5'   | 1.89                     | 0.53              |
| 25:DA:2377:A:H2'   | 25:DA:2378:A:C8    | 2.42                     | 0.53              |
| 28:DD:155:LEU:HD12 | 28:DD:155:LEU:N    | 2.22                     | 0.53              |
| 32:DH:123:PHE:CE2  | 32:DH:133:VAL:HG22 | 2.43                     | 0.53              |
| 33:DI:14:ASP:O     | 33:DI:16:GLY:N     | 2.39                     | 0.53              |
| 35:DO:8:LEU:CD2    | 35:DO:8:LEU:N      | 2.71                     | 0.53              |
| 40:DT:8:LYS:HA     | 40:DT:11:GLU:OE1   | 2.07                     | 0.53              |
| 40:DT:26:ASP:OD2   | 40:DT:27:THR:N     | 2.40                     | 0.53              |
| 40:DT:28:VAL:HG12  | 40:DT:29:ARG:CZ    | 2.38                     | 0.53              |
| 41:DU:112:ARG:HG2  | 41:DU:112:ARG:NH1  | 2.20                     | 0.53              |
| 46:DZ:156:LYS:O    | 46:DZ:157:LEU:C    | 2.51                     | 0.53              |
| 55:D8:4:MET:O      | 55:D8:62:LEU:HD11  | 2.07                     | 0.53              |
| 1:AA:115:G:H1'     | 1:AA:116:A:N7      | 2.23                     | 0.53              |
| 1:AA:473:G:H2'     | 1:AA:474:G:H8      | 1.73                     | 0.53              |
| 1:AA:919:A:C2'     | 1:AA:920:U:H5'     | 2.39                     | 0.53              |
| 2:AB:52:GLU:O      | 2:AB:56:ARG:HG2    | 2.07                     | 0.53              |
| 2:AB:80:ILE:CG1    | 2:AB:215:LEU:HD12  | 2.37                     | 0.53              |
| 7:AG:145:ALA:C     | 7:AG:147:ALA:H     | 2.15                     | 0.53              |
| 10:AJ:44:VAL:CG1   | 10:AJ:45:ARG:N     | 2.70                     | 0.53              |
| 11:AK:19:ALA:HB3   | 11:AK:82:VAL:HG23  | 1.90                     | 0.53              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 12:AL:117:ARG:C    | 12:AL:119:LYS:O   | 2.51                     | 0.53              |
| 12:AL:117:ARG:HD2  | 12:AL:122:THR:HB  | 1.88                     | 0.53              |
| 18:AR:86:VAL:HG12  | 18:AR:87:ARG:HB3  | 1.89                     | 0.53              |
| 22:AV:38:A:H5''    | 22:AV:39:A:OP2    | 2.09                     | 0.53              |
| 25:BA:71:A:O2'     | 25:BA:72:U:OP2    | 2.21                     | 0.53              |
| 25:BA:332:A:O2'    | 25:BA:333:G:P     | 2.65                     | 0.53              |
| 25:BA:601:C:O2'    | 30:BF:104:LYS:NZ  | 2.41                     | 0.53              |
| 25:BA:1278:A:H5''  | 38:BR:36:THR:HG22 | 1.90                     | 0.53              |
| 25:BA:1497:U:H3    | 25:BA:1578:U:P    | 2.32                     | 0.53              |
| 25:BA:1601:G:N7    | 25:BA:1602:U:C4   | 2.76                     | 0.53              |
| 25:BA:1963:U:O2    | 25:BA:1963:U:C3'  | 2.56                     | 0.53              |
| 25:BA:2286:A:OP1   | 53:B6:30:THR:HB   | 2.08                     | 0.53              |
| 25:BA:2345:G:H2'   | 25:BA:2345:G:N3   | 2.23                     | 0.53              |
| 25:BA:2543:G:H2'   | 25:BA:2544:G:C8   | 2.44                     | 0.53              |
| 29:BE:132:HIS:HA   | 29:BE:135:HIS:NE2 | 2.23                     | 0.53              |
| 34:BN:70:LYS:C     | 34:BN:71:ILE:HD12 | 2.32                     | 0.53              |
| 36:BP:146:VAL:HG13 | 36:BP:147:LEU:N   | 2.23                     | 0.53              |
| 37:BQ:78:PRO:O     | 37:BQ:81:VAL:HG13 | 2.08                     | 0.53              |
| 38:BR:14:SER:HA    | 38:BR:17:ARG:CZ   | 2.38                     | 0.53              |
| 44:BX:90:GLU:O     | 44:BX:91:ALA:C    | 2.51                     | 0.53              |
| 48:B1:57:GLU:O     | 48:B1:58:ILE:HG23 | 2.07                     | 0.53              |
| 49:B2:43:GLN:O     | 49:B2:44:LEU:HD22 | 2.08                     | 0.53              |
| 1:CA:31:G:C6       | 1:CA:48:C:C1'     | 2.91                     | 0.53              |
| 1:CA:1510:U:H2'    | 1:CA:1511:G:C8    | 2.44                     | 0.53              |
| 4:CD:59:ARG:HA     | 4:CD:59:ARG:HE    | 1.72                     | 0.53              |
| 9:CI:3:GLN:O       | 9:CI:88:TYR:CE1   | 2.62                     | 0.53              |
| 20:CT:25:ARG:HH11  | 20:CT:25:ARG:HG3  | 1.72                     | 0.53              |
| 22:CV:30:G:C4      | 22:CV:31:G:C8     | 2.96                     | 0.53              |
| 22:CV:48:U:H5'     | 22:CV:49:C:H5'    | 1.91                     | 0.53              |
| 25:DA:1796:U:H2'   | 25:DA:1797:C:C6   | 2.43                     | 0.53              |
| 28:DD:77:ALA:HB2   | 28:DD:97:TYR:HA   | 1.90                     | 0.53              |
| 29:DE:3:GLY:HA3    | 29:DE:81:ILE:CG2  | 2.33                     | 0.53              |
| 30:DF:206:ILE:HD12 | 30:DF:206:ILE:C   | 2.33                     | 0.53              |
| 33:DI:35:LEU:O     | 33:DI:36:ALA:HB2  | 2.08                     | 0.53              |
| 50:D3:49:LYS:C     | 50:D3:51:ALA:H    | 2.17                     | 0.53              |
| 51:D4:16:CYS:SG    | 51:D4:36:CYS:HB3  | 2.48                     | 0.53              |
| 1:AA:641:U:O2'     | 1:AA:642:A:N7     | 2.39                     | 0.53              |
| 1:AA:1158:C:H42    | 1:AA:1181:G:H22   | 1.55                     | 0.53              |
| 1:AA:1316:G:O6     | 19:AS:5:LEU:HD23  | 2.09                     | 0.53              |
| 2:AB:179:LYS:HG2   | 2:AB:179:LYS:O    | 2.07                     | 0.53              |
| 2:AB:187:LEU:HD23  | 2:AB:201:ILE:O    | 2.07                     | 0.53              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:AG:15:ASP:CB     | 7:AG:24:THR:CG2    | 2.87                     | 0.53              |
| 9:AI:17:VAL:HG22   | 9:AI:63:ILE:HG12   | 1.91                     | 0.53              |
| 11:AK:82:VAL:HG12  | 11:AK:108:ILE:HG12 | 1.90                     | 0.53              |
| 13:AM:23:TYR:HB3   | 13:AM:67:GLU:CA    | 2.38                     | 0.53              |
| 20:AT:30:LYS:HD3   | 20:AT:30:LYS:O     | 2.08                     | 0.53              |
| 20:AT:49:ALA:C     | 20:AT:100:ILE:HD13 | 2.33                     | 0.53              |
| 23:AW:7:A:N6       | 23:AW:49:C:C4      | 2.76                     | 0.53              |
| 23:AW:38:A:N6      | 23:AW:39:U:C5      | 2.77                     | 0.53              |
| 25:BA:92:A:H2'     | 25:BA:93:G:H8      | 1.74                     | 0.53              |
| 25:BA:1812:A:H2'   | 25:BA:1813:G:H8    | 1.73                     | 0.53              |
| 25:BA:2283:C:H2'   | 25:BA:2284:C:O4'   | 2.08                     | 0.53              |
| 25:BA:2712:U:H5''  | 25:BA:2714:G:H5''  | 1.90                     | 0.53              |
| 25:BA:2866:U:H6    | 25:BA:2868:A:H1'   | 1.73                     | 0.53              |
| 26:BB:66:A:C6      | 26:BB:108:U:N3     | 2.76                     | 0.53              |
| 31:BG:114:ILE:O    | 31:BG:115:ARG:C    | 2.51                     | 0.53              |
| 31:BG:127:GLY:H    | 31:BG:166:ASP:CG   | 2.15                     | 0.53              |
| 33:BI:63:ALA:O     | 33:BI:67:ARG:HG2   | 2.08                     | 0.53              |
| 36:BP:3:LEU:O      | 36:BP:5:ASP:N      | 2.39                     | 0.53              |
| 36:BP:48:PRO:O     | 36:BP:51:PHE:N     | 2.39                     | 0.53              |
| 37:BQ:68:ILE:HG21  | 37:BQ:101:ARG:HD3  | 1.91                     | 0.53              |
| 40:BT:99:LEU:H     | 40:BT:99:LEU:HD12  | 1.72                     | 0.53              |
| 43:BW:6:ILE:HG12   | 43:BW:104:THR:CG2  | 2.38                     | 0.53              |
| 43:BW:78:GLU:OE2   | 43:BW:99:ARG:NH1   | 2.41                     | 0.53              |
| 54:B7:17:GLY:O     | 54:B7:21:ARG:HG2   | 2.07                     | 0.53              |
| 1:CA:511:C:O2'     | 1:CA:512:U:P       | 2.66                     | 0.53              |
| 1:CA:817:C:O2'     | 1:CA:818:G:H5''    | 2.08                     | 0.53              |
| 2:CB:59:GLU:HB2    | 2:CB:221:LEU:HD12  | 1.89                     | 0.53              |
| 2:CB:194:PRO:O     | 2:CB:195:ASP:C     | 2.50                     | 0.53              |
| 3:CC:141:VAL:HG11  | 3:CC:202:ILE:CG2   | 2.38                     | 0.53              |
| 5:CE:137:GLU:O     | 5:CE:141:GLN:HG3   | 2.08                     | 0.53              |
| 9:CI:15:ALA:HA     | 9:CI:65:VAL:HA     | 1.89                     | 0.53              |
| 11:CK:127:LYS:NZ   | 11:CK:127:LYS:HA   | 2.24                     | 0.53              |
| 12:CL:22:SER:C     | 12:CL:24:VAL:N     | 2.66                     | 0.53              |
| 13:CM:116:THR:C    | 13:CM:117:VAL:HG13 | 2.33                     | 0.53              |
| 13:CM:117:VAL:O    | 13:CM:118:ALA:O    | 2.25                     | 0.53              |
| 19:CS:44:MET:HA    | 19:CS:44:MET:CE    | 2.37                     | 0.53              |
| 25:DA:498:G:H21    | 45:DY:47:LYS:NZ    | 2.06                     | 0.53              |
| 25:DA:2668:G:H2'   | 25:DA:2669:G:H8    | 1.74                     | 0.53              |
| 29:DE:30:PRO:HD3   | 29:DE:180:ASN:ND2  | 2.23                     | 0.53              |
| 29:DE:59:VAL:O     | 29:DE:60:ASN:CB    | 2.55                     | 0.53              |
| 30:DF:125:LEU:HD21 | 30:DF:199:TRP:CE3  | 2.43                     | 0.53              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 32:DH:20:ALA:HB1   | 32:DH:21:PRO:CD   | 2.38                     | 0.53              |
| 33:DI:60:GLU:CG    | 33:DI:61:ARG:HH12 | 2.22                     | 0.53              |
| 36:DP:83:VAL:O     | 36:DP:83:VAL:HG13 | 2.09                     | 0.53              |
| 41:DU:31:SER:C     | 41:DU:33:ARG:H    | 2.16                     | 0.53              |
| 41:DU:92:ARG:NH1   | 41:DU:92:ARG:CG   | 2.68                     | 0.53              |
| 41:DU:105:VAL:O    | 41:DU:109:LEU:HG  | 2.09                     | 0.53              |
| 48:D1:41:ARG:HD3   | 48:D1:43:TYR:OH   | 2.08                     | 0.53              |
| 49:D2:34:GLU:O     | 49:D2:38:GLN:HG3  | 2.08                     | 0.53              |
| 50:D3:17:LYS:HD2   | 50:D3:20:LYS:HD2  | 1.89                     | 0.53              |
| 1:AA:265:G:H2'     | 1:AA:266:G:H5''   | 1.89                     | 0.53              |
| 7:AG:76:ARG:HD3    | 7:AG:89:MET:CG    | 2.38                     | 0.53              |
| 8:AH:119:LEU:HB3   | 8:AH:123:GLU:HB2  | 1.88                     | 0.53              |
| 17:AQ:11:VAL:HG22  | 17:AQ:20:THR:O    | 2.09                     | 0.53              |
| 19:AS:9:VAL:O      | 19:AS:10:PHE:CG   | 2.62                     | 0.53              |
| 19:AS:51:VAL:O     | 19:AS:57:HIS:HA   | 2.08                     | 0.53              |
| 23:AW:9:A:C5'      | 23:AW:46:G:H21    | 2.21                     | 0.53              |
| 25:BA:83:G:O2'     | 25:BA:102:G:N2    | 2.41                     | 0.53              |
| 25:BA:791:C:H4'    | 25:BA:792:G:OP1   | 2.06                     | 0.53              |
| 25:BA:1859:A:N6    | 25:BA:1883:G:O2'  | 2.41                     | 0.53              |
| 28:BD:76:PRO:HA    | 28:BD:118:VAL:HB  | 1.90                     | 0.53              |
| 28:BD:131:LEU:N    | 28:BD:131:LEU:CD1 | 2.71                     | 0.53              |
| 29:BE:28:ALA:HB3   | 29:BE:93:VAL:CG2  | 2.38                     | 0.53              |
| 32:BH:125:VAL:HG12 | 32:BH:125:VAL:O   | 2.07                     | 0.53              |
| 33:BI:117:GLU:HG3  | 33:BI:118:LYS:N   | 2.22                     | 0.53              |
| 35:BO:80:ASP:OD1   | 40:BT:71:GLY:O    | 2.26                     | 0.53              |
| 36:BP:71:VAL:HG22  | 36:BP:72:PRO:HD3  | 1.88                     | 0.53              |
| 36:BP:110:TYR:O    | 36:BP:111:ARG:C   | 2.52                     | 0.53              |
| 37:BQ:46:GLN:O     | 37:BQ:47:ILE:C    | 2.51                     | 0.53              |
| 38:BR:2:ARG:NH2    | 38:BR:5:LYS:HZ3   | 2.04                     | 0.53              |
| 45:BY:98:VAL:O     | 45:BY:99:CYS:SG   | 2.66                     | 0.53              |
| 49:B2:48:HIS:CD2   | 49:B2:49:LYS:N    | 2.76                     | 0.53              |
| 54:B7:30:VAL:HG12  | 54:B7:34:ARG:HG3  | 1.90                     | 0.53              |
| 1:CA:390:C:H2'     | 1:CA:391:G:C8     | 2.43                     | 0.53              |
| 1:CA:869:G:O2'     | 1:CA:872:A:N7     | 2.35                     | 0.53              |
| 1:CA:878:G:H5'     | 8:CH:89:PRO:HG2   | 1.89                     | 0.53              |
| 2:CB:42:ILE:HD13   | 2:CB:203:GLY:HA2  | 1.89                     | 0.53              |
| 2:CB:228:GLY:O     | 2:CB:230:VAL:HG13 | 2.08                     | 0.53              |
| 3:CC:94:LEU:HD12   | 3:CC:95:THR:OG1   | 2.08                     | 0.53              |
| 8:CH:39:LEU:O      | 8:CH:44:PHE:HB2   | 2.08                     | 0.53              |
| 9:CI:11:LYS:O      | 9:CI:13:ALA:N     | 2.41                     | 0.53              |
| 17:CQ:48:GLU:OE1   | 17:CQ:50:LYS:HD3  | 2.08                     | 0.53              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 18:CR:76:LEU:HD23  | 18:CR:76:LEU:H    | 1.70                     | 0.53              |
| 20:CT:53:LEU:HB3   | 20:CT:102:GLY:CA  | 2.38                     | 0.53              |
| 23:CW:36:A:H2'     | 23:CW:37:A:C4'    | 2.38                     | 0.53              |
| 25:DA:69:C:O2      | 25:DA:73:A:O2'    | 2.20                     | 0.53              |
| 25:DA:142:A:H8     | 25:DA:1595:G:H21  | 1.54                     | 0.53              |
| 25:DA:598:G:O4'    | 36:DP:11:GLY:C    | 2.51                     | 0.53              |
| 25:DA:930:U:H1'    | 25:DA:931:G:C6    | 2.43                     | 0.53              |
| 25:DA:1609:A:H1'   | 25:DA:1616:A:O4'  | 2.08                     | 0.53              |
| 25:DA:1769:G:O2'   | 25:DA:1958:C:OP1  | 2.24                     | 0.53              |
| 25:DA:1779:U:OP2   | 25:DA:1784:A:N6   | 2.33                     | 0.53              |
| 25:DA:1820:U:C2    | 28:DD:202:LYS:HB3 | 2.44                     | 0.53              |
| 25:DA:2468:G:O2'   | 25:DA:2469:A:H8   | 1.92                     | 0.53              |
| 25:DA:2750:A:C4'   | 25:DA:2751:G:OP2  | 2.49                     | 0.53              |
| 28:DD:32:SER:O     | 28:DD:36:PRO:HD2  | 2.08                     | 0.53              |
| 31:DG:107:LEU:HD11 | 31:DG:178:PHE:CD1 | 2.43                     | 0.53              |
| 31:DG:113:ARG:HD3  | 31:DG:140:ILE:O   | 2.07                     | 0.53              |
| 36:DP:146:VAL:HG13 | 36:DP:147:LEU:N   | 2.23                     | 0.53              |
| 37:DQ:47:ILE:HG22  | 37:DQ:48:GLU:N    | 2.23                     | 0.53              |
| 40:DT:14:TYR:N     | 40:DT:14:TYR:CD1  | 2.76                     | 0.53              |
| 42:DV:55:ALA:CB    | 42:DV:101:GLY:HA2 | 2.37                     | 0.53              |
| 46:DZ:5:LEU:HB3    | 46:DZ:59:LEU:HD22 | 1.90                     | 0.53              |
| 46:DZ:128:VAL:HG23 | 46:DZ:160:GLY:O   | 2.08                     | 0.53              |
| 53:D6:19:ARG:CD    | 53:D6:19:ARG:H    | 2.21                     | 0.53              |
| 1:AA:156:G:H1      | 1:AA:165:C:H42    | 1.55                     | 0.53              |
| 1:AA:410:G:H21     | 1:AA:432:A:H62    | 1.56                     | 0.53              |
| 1:AA:687:A:O2'     | 1:AA:688:G:OP2    | 2.27                     | 0.53              |
| 1:AA:1302:U:H5''   | 1:AA:1303:C:OP2   | 2.08                     | 0.53              |
| 2:AB:56:ARG:HH11   | 2:AB:56:ARG:HA    | 1.73                     | 0.53              |
| 2:AB:140:HIS:HA    | 2:AB:143:GLU:HG3  | 1.91                     | 0.53              |
| 4:AD:3:ARG:HG2     | 4:AD:118:ARG:HD3  | 1.90                     | 0.53              |
| 17:AQ:45:HIS:CB    | 17:AQ:65:ILE:HD13 | 2.39                     | 0.53              |
| 20:AT:84:LEU:C     | 20:AT:84:LEU:CD1  | 2.79                     | 0.53              |
| 25:BA:242:G:O2'    | 55:B8:6:THR:HG23  | 2.09                     | 0.53              |
| 25:BA:2068:U:H3    | 25:BA:2430:A:H2   | 1.53                     | 0.53              |
| 29:BE:51:PHE:CZ    | 29:BE:52:LEU:HD13 | 2.42                     | 0.53              |
| 32:BH:156:ALA:N    | 32:BH:158:HIS:H   | 2.05                     | 0.53              |
| 34:BN:17:ASP:OD1   | 34:BN:56:ASN:HB3  | 2.09                     | 0.53              |
| 35:BO:119:PRO:HB2  | 40:BT:68:TYR:CE1  | 2.44                     | 0.53              |
| 36:BP:33:ARG:NE    | 36:BP:40:SER:O    | 2.42                     | 0.53              |
| 36:BP:112:LEU:H    | 36:BP:128:HIS:CD2 | 2.26                     | 0.53              |
| 36:BP:138:LEU:CD1  | 36:BP:144:GLU:HG2 | 2.39                     | 0.53              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 37:BQ:116:GLU:O   | 37:BQ:120:ILE:HG12 | 2.08                     | 0.53              |
| 38:BR:13:HIS:ND1  | 38:BR:13:HIS:N     | 2.57                     | 0.53              |
| 39:BS:89:ARG:O    | 39:BS:90:GLY:C     | 2.51                     | 0.53              |
| 40:BT:89:VAL:HB   | 40:BT:91:ARG:NE    | 2.24                     | 0.53              |
| 41:BU:17:ILE:HB   | 41:BU:32:PHE:HE1   | 1.74                     | 0.53              |
| 43:BW:111:HIS:CG  | 43:BW:112:GLY:H    | 2.25                     | 0.53              |
| 49:B2:69:ARG:HG2  | 49:B2:69:ARG:NH1   | 2.20                     | 0.53              |
| 55:B8:50:LEU:CD1  | 55:B8:51:ALA:H     | 2.08                     | 0.53              |
| 1:CA:346:G:OP2    | 40:DT:35:LYS:CD    | 2.57                     | 0.53              |
| 1:CA:1404:C:H2'   | 1:CA:1405:G:C8     | 2.44                     | 0.53              |
| 2:CB:187:LEU:HA   | 2:CB:201:ILE:HB    | 1.90                     | 0.53              |
| 3:CC:6:HIS:NE2    | 3:CC:184:TYR:CE2   | 2.77                     | 0.53              |
| 12:CL:126:LYS:HG3 | 12:CL:127:GLU:H    | 1.73                     | 0.53              |
| 14:CN:23:ARG:HD2  | 14:CN:28:GLY:O     | 2.09                     | 0.53              |
| 14:CN:29:ARG:HG2  | 14:CN:40:CYS:SG    | 2.48                     | 0.53              |
| 22:CV:62:C:C2'    | 22:CV:63:C:H5'     | 2.38                     | 0.53              |
| 25:DA:84:A:C5'    | 45:DY:8:LYS:CG     | 2.84                     | 0.53              |
| 25:DA:1819:A:O4'  | 25:DA:1821:A:C6    | 2.62                     | 0.53              |
| 25:DA:2198:A:O2'  | 25:DA:2199:A:O5'   | 2.27                     | 0.53              |
| 25:DA:2245:U:H5'  | 25:DA:2246:G:H5'   | 1.90                     | 0.53              |
| 29:DE:4:ILE:CG1   | 29:DE:28:ALA:HB1   | 2.37                     | 0.53              |
| 32:DH:98:LEU:HA   | 32:DH:103:LEU:HA   | 1.89                     | 0.53              |
| 32:DH:153:LYS:HE2 | 32:DH:153:LYS:HA   | 1.91                     | 0.53              |
| 34:DN:34:LEU:HD21 | 34:DN:120:LEU:HB2  | 1.91                     | 0.53              |
| 36:DP:110:TYR:O   | 36:DP:111:ARG:C    | 2.52                     | 0.53              |
| 39:DS:85:VAL:HG23 | 39:DS:112:PHE:HZ   | 1.73                     | 0.53              |
| 41:DU:90:VAL:CG1  | 41:DU:91:ASP:H     | 2.12                     | 0.53              |
| 42:DV:47:VAL:HG13 | 42:DV:48:GLY:N     | 2.23                     | 0.53              |
| 45:DY:47:LYS:HA   | 45:DY:60:PHE:CD1   | 2.43                     | 0.53              |
| 46:DZ:104:PHE:O   | 46:DZ:106:GLY:N    | 2.41                     | 0.53              |
| 1:AA:1049:U:H1'   | 1:AA:1201:A:C4     | 2.38                     | 0.53              |
| 8:AH:8:ASP:O      | 8:AH:9:MET:C       | 2.52                     | 0.53              |
| 8:AH:86:ILE:HG21  | 8:AH:133:LEU:HD13  | 1.91                     | 0.53              |
| 10:AJ:34:VAL:HG22 | 10:AJ:74:ILE:HG22  | 1.91                     | 0.53              |
| 10:AJ:39:PRO:HA   | 10:AJ:70:ARG:HG3   | 1.90                     | 0.53              |
| 15:AO:33:THR:HG23 | 15:AO:63:ARG:HH12  | 1.73                     | 0.53              |
| 23:AW:36:A:H8     | 23:AW:36:A:O5'     | 1.92                     | 0.53              |
| 23:AW:53:G:N2     | 23:AW:62:C:C2      | 2.77                     | 0.53              |
| 25:BA:204:A:H1'   | 25:BA:206:U:C6     | 2.44                     | 0.53              |
| 25:BA:274:G:OP2   | 25:BA:274:G:N2     | 2.38                     | 0.53              |
| 25:BA:804:A:C2'   | 25:BA:806:C:C4     | 2.91                     | 0.53              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:BA:1286:A:C6    | 25:BA:1289:C:N3    | 2.76                     | 0.53              |
| 25:BA:2176:A:H2    | 27:BC:44:HIS:CE1   | 2.26                     | 0.53              |
| 25:BA:2847:U:O4    | 25:BA:2848:G:C2    | 2.61                     | 0.53              |
| 30:BF:22:ALA:C     | 30:BF:24:LEU:H     | 2.16                     | 0.53              |
| 32:BH:26:VAL:HG12  | 32:BH:79:VAL:HG21  | 1.89                     | 0.53              |
| 34:BN:120:LEU:C    | 34:BN:121:LYS:HD2  | 2.34                     | 0.53              |
| 36:BP:59:LEU:HG    | 55:B8:13:ARG:NH2   | 2.23                     | 0.53              |
| 36:BP:112:LEU:HD22 | 36:BP:113:LYS:H    | 1.72                     | 0.53              |
| 40:BT:28:VAL:CG2   | 40:BT:46:GLU:CA    | 2.86                     | 0.53              |
| 1:CA:579:G:H5'     | 1:CA:728:A:H1'     | 1.90                     | 0.53              |
| 1:CA:1363(A):A:H1' | 1:CA:1365:G:C5     | 2.44                     | 0.53              |
| 9:CI:114:TYR:CD2   | 9:CI:114:TYR:N     | 2.67                     | 0.53              |
| 12:CL:83:VAL:HG21  | 12:CL:100:ILE:HD13 | 1.90                     | 0.53              |
| 16:CP:28:ARG:NH1   | 16:CP:29:ASP:OD2   | 2.41                     | 0.53              |
| 20:CT:75:ASN:OD1   | 20:CT:75:ASN:N     | 2.41                     | 0.53              |
| 23:CW:19:G:H4'     | 23:CW:20:U:OP2     | 2.08                     | 0.53              |
| 24:CX:16:A:C4      | 24:CX:17:U:C6      | 2.97                     | 0.53              |
| 25:DA:780:G:H21    | 25:DA:783:A:H62    | 1.57                     | 0.53              |
| 25:DA:2370:G:O2'   | 53:D6:45:LYS:HD2   | 2.08                     | 0.53              |
| 28:DD:32:SER:O     | 28:DD:34:VAL:N     | 2.42                     | 0.53              |
| 29:DE:57:LYS:HB3   | 29:DE:57:LYS:NZ    | 2.22                     | 0.53              |
| 30:DF:34:TRP:CZ3   | 36:DP:8:PRO:HB3    | 2.44                     | 0.53              |
| 32:DH:98:LEU:HD12  | 32:DH:102:ALA:C    | 2.34                     | 0.53              |
| 33:DI:17:GLN:HE21  | 33:DI:19:VAL:HB    | 1.74                     | 0.53              |
| 36:DP:3:LEU:O      | 36:DP:5:ASP:N      | 2.39                     | 0.53              |
| 36:DP:34:GLY:O     | 36:DP:35:HIS:O     | 2.27                     | 0.53              |
| 36:DP:112:LEU:H    | 36:DP:128:HIS:CD2  | 2.26                     | 0.53              |
| 36:DP:148:LEU:N    | 36:DP:148:LEU:HD23 | 2.24                     | 0.53              |
| 38:DR:12:ARG:HG3   | 38:DR:12:ARG:NH1   | 2.22                     | 0.53              |
| 40:DT:64:ARG:HD2   | 40:DT:73:GLU:HG2   | 1.90                     | 0.53              |
| 43:DW:5:ALA:HB1    | 43:DW:50:VAL:HG23  | 1.91                     | 0.53              |
| 46:DZ:114:GLY:HA3  | 46:DZ:177:PRO:CG   | 2.37                     | 0.53              |
| 55:D8:6:THR:HG22   | 55:D8:63:PRO:HD3   | 1.91                     | 0.53              |
| 1:AA:1238:A:N6     | 1:AA:1301:U:H3     | 2.03                     | 0.53              |
| 5:AE:26:PHE:O      | 5:AE:27:ARG:CB     | 2.54                     | 0.53              |
| 10:AJ:24:VAL:HG21  | 10:AJ:37:PRO:HG3   | 1.91                     | 0.53              |
| 12:AL:24:VAL:HG22  | 12:AL:97:ARG:HB3   | 1.90                     | 0.53              |
| 12:AL:41:ARG:HH22  | 12:AL:57:LYS:HZ1   | 1.50                     | 0.53              |
| 18:AR:37:VAL:HG12  | 18:AR:79:LEU:CD2   | 2.39                     | 0.53              |
| 20:AT:20:LEU:O     | 20:AT:21:LYS:C     | 2.51                     | 0.53              |
| 20:AT:104:LEU:HD23 | 20:AT:105:SER:N    | 2.24                     | 0.53              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:AW:21:A:N6      | 23:AW:46:G:C4      | 2.77                     | 0.53              |
| 25:BA:1550:C:OP1   | 25:BA:1720:U:O2'   | 2.22                     | 0.53              |
| 25:BA:2320:A:N7    | 25:BA:2333:A:N1    | 2.55                     | 0.53              |
| 28:BD:35:LYS:HB3   | 28:BD:104:TYR:HE1  | 1.73                     | 0.53              |
| 28:BD:69:ARG:NH2   | 28:BD:192:THR:CB   | 2.72                     | 0.53              |
| 28:BD:143:HIS:CD2  | 28:BD:143:HIS:C    | 2.87                     | 0.53              |
| 28:BD:201:HIS:C    | 28:BD:203:ASN:N    | 2.67                     | 0.53              |
| 30:BF:3:GLU:CB     | 30:BF:24:LEU:HG    | 2.35                     | 0.53              |
| 30:BF:32:LEU:HD13  | 30:BF:112:MET:CE   | 2.39                     | 0.53              |
| 31:BG:63:ILE:HD12  | 31:BG:141:PHE:CD1  | 2.44                     | 0.53              |
| 32:BH:109:PHE:HE1  | 32:BH:152:ARG:NE   | 2.07                     | 0.53              |
| 33:BI:131:LYS:HE3  | 33:BI:132:PRO:HD3  | 1.90                     | 0.53              |
| 34:BN:62:VAL:CG1   | 34:BN:66:LYS:CB    | 2.86                     | 0.53              |
| 37:BQ:26:TYR:O     | 37:BQ:67:ARG:NH1   | 2.38                     | 0.53              |
| 37:BQ:29:PHE:CD2   | 37:BQ:65:PHE:CE1   | 2.96                     | 0.53              |
| 38:BR:32:GLY:HA2   | 38:BR:116:LEU:HD12 | 1.90                     | 0.53              |
| 44:BX:29:TRP:CE3   | 44:BX:78:LYS:HB3   | 2.44                     | 0.53              |
| 50:B3:26:LEU:HD23  | 50:B3:26:LEU:N     | 2.24                     | 0.53              |
| 1:CA:277:C:OP1     | 17:CQ:41:LYS:HE3   | 2.09                     | 0.53              |
| 1:CA:834:C:OP1     | 18:CR:60:ALA:HB2   | 2.08                     | 0.53              |
| 1:CA:837:G:H1      | 1:CA:849:C:H42     | 1.57                     | 0.53              |
| 2:CB:220:ASP:O     | 2:CB:221:LEU:C     | 2.50                     | 0.53              |
| 10:CJ:38:ILE:HG12  | 10:CJ:71:LEU:O     | 2.08                     | 0.53              |
| 13:CM:4:ILE:CG2    | 13:CM:5:ALA:H      | 2.19                     | 0.53              |
| 16:CP:43:LYS:HG2   | 16:CP:48:TRP:CG    | 2.43                     | 0.53              |
| 18:CR:86:VAL:O     | 18:CR:87:ARG:O     | 2.27                     | 0.53              |
| 25:DA:1341:U:O5'   | 25:DA:1341:U:H6    | 1.91                     | 0.53              |
| 29:DE:8:LYS:HD2    | 29:DE:188:VAL:HG13 | 1.90                     | 0.53              |
| 29:DE:47:VAL:HG23  | 29:DE:84:PHE:O     | 2.08                     | 0.53              |
| 29:DE:70:ALA:O     | 29:DE:71:GLY:C     | 2.51                     | 0.53              |
| 31:DG:142:PRO:HG2  | 31:DG:143:GLU:H    | 1.74                     | 0.53              |
| 32:DH:9:ILE:O      | 32:DH:9:ILE:HG13   | 2.09                     | 0.53              |
| 33:DI:19:VAL:HG22  | 33:DI:20:ASP:N     | 2.24                     | 0.53              |
| 36:DP:58:THR:O     | 36:DP:61:ARG:HG3   | 2.09                     | 0.53              |
| 36:DP:105:LEU:HD12 | 36:DP:105:LEU:N    | 2.23                     | 0.53              |
| 46:DZ:145:GLU:O    | 46:DZ:146:ILE:C    | 2.51                     | 0.53              |
| 48:D1:3:LYS:HG2    | 48:D1:4:VAL:N      | 2.24                     | 0.53              |
| 55:D8:63:PRO:HB2   | 55:D8:64:TYR:CD1   | 2.44                     | 0.53              |
| 1:AA:262:A:H5''    | 20:AT:76:ALA:HB2   | 1.89                     | 0.53              |
| 1:AA:1049:U:O2     | 1:AA:1201:A:N3     | 2.41                     | 0.53              |
| 3:AC:42:LEU:HD12   | 3:AC:45:LYS:NZ     | 2.24                     | 0.53              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 4:AD:189:PRO:CB    | 4:AD:194:LEU:HD21 | 2.30                     | 0.53              |
| 6:AF:1:MET:HE2     | 6:AF:1:MET:N      | 2.24                     | 0.53              |
| 8:AH:42:GLU:HG3    | 8:AH:109:ILE:HD11 | 1.91                     | 0.53              |
| 8:AH:86:ILE:HG13   | 8:AH:133:LEU:HD22 | 1.91                     | 0.53              |
| 11:AK:69:ALA:O     | 11:AK:72:ALA:N    | 2.41                     | 0.53              |
| 23:AW:31:A:H2'     | 23:AW:32:U:O4'    | 2.09                     | 0.53              |
| 25:BA:598:G:H1'    | 36:BP:12:ALA:HB2  | 1.90                     | 0.53              |
| 25:BA:643:A:N1     | 25:BA:2369:A:O2'  | 2.40                     | 0.53              |
| 25:BA:1131:G:O2'   | 25:BA:1132:A:O4'  | 2.26                     | 0.53              |
| 25:BA:1486:A:H61   | 25:BA:1504:C:H42  | 1.57                     | 0.53              |
| 25:BA:2176:A:C2    | 27:BC:44:HIS:CE1  | 2.97                     | 0.53              |
| 25:BA:2447:G:H1'   | 25:BA:2501:C:C4   | 2.43                     | 0.53              |
| 25:BA:2689:U:C4'   | 25:BA:2690:C:OP2  | 2.57                     | 0.53              |
| 25:BA:2873:A:N3    | 38:BR:6:SER:CB    | 2.68                     | 0.53              |
| 28:BD:6:PHE:CE1    | 28:BD:18:VAL:HG22 | 2.43                     | 0.53              |
| 29:BE:70:ALA:O     | 29:BE:71:GLY:C    | 2.52                     | 0.53              |
| 30:BF:9:ILE:HG22   | 30:BF:9:ILE:O     | 2.09                     | 0.53              |
| 30:BF:152:GLU:CD   | 30:BF:191:ARG:HD2 | 2.34                     | 0.53              |
| 36:BP:108:LYS:C    | 36:BP:110:TYR:H   | 2.17                     | 0.53              |
| 47:B0:34:GLY:O     | 47:B0:35:ASN:C    | 2.51                     | 0.53              |
| 1:CA:49:U:C4       | 1:CA:364:A:N7     | 2.77                     | 0.53              |
| 1:CA:323:U:O3'     | 20:CT:22:ARG:HD3  | 2.09                     | 0.53              |
| 1:CA:1266:G:N2     | 1:CA:1269:A:OP2   | 2.35                     | 0.53              |
| 2:CB:127:ILE:HG22  | 2:CB:127:ILE:O    | 2.09                     | 0.53              |
| 3:CC:47:LEU:HD11   | 3:CC:76:VAL:HG12  | 1.91                     | 0.53              |
| 5:CE:98:THR:HG22   | 5:CE:99:GLY:N     | 2.24                     | 0.53              |
| 12:CL:22:SER:O     | 12:CL:24:VAL:N    | 2.42                     | 0.53              |
| 18:CR:40:LEU:O     | 18:CR:43:PHE:N    | 2.37                     | 0.53              |
| 20:CT:8:ARG:O      | 20:CT:9:ASN:CG    | 2.52                     | 0.53              |
| 25:DA:13:A:N7      | 25:DA:525:U:C4    | 2.77                     | 0.53              |
| 25:DA:27:G:H22     | 25:DA:512:G:H2'   | 1.71                     | 0.53              |
| 25:DA:1607:C:N4    | 25:DA:1622:G:OP2  | 2.38                     | 0.53              |
| 25:DA:1681:G:H8    | 25:DA:1681:G:OP2  | 1.92                     | 0.53              |
| 25:DA:2147:G:H2'   | 25:DA:2148:G:O4'  | 2.09                     | 0.53              |
| 25:DA:2206:G:N2    | 25:DA:2207:G:H5'  | 2.23                     | 0.53              |
| 25:DA:2689:U:H4'   | 25:DA:2690:C:O5'  | 2.07                     | 0.53              |
| 25:DA:2832:U:H1'   | 25:DA:2834:G:C4   | 2.44                     | 0.53              |
| 29:DE:61:ARG:CB    | 29:DE:62:PRO:CD   | 2.86                     | 0.53              |
| 31:DG:161:THR:HG22 | 31:DG:162:THR:H   | 1.74                     | 0.53              |
| 32:DH:86:GLU:O     | 32:DH:87:LEU:CB   | 2.56                     | 0.53              |
| 33:DI:68:LEU:HA    | 33:DI:71:ILE:CG2  | 2.38                     | 0.53              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 37:DQ:59:ARG:O     | 37:DQ:60:ARG:CB    | 2.57                     | 0.53              |
| 37:DQ:70:PRO:HA    | 37:DQ:94:VAL:C     | 2.34                     | 0.53              |
| 40:DT:28:VAL:HG12  | 40:DT:29:ARG:NE    | 2.24                     | 0.53              |
| 40:DT:83:ILE:HG13  | 40:DT:84:GLN:H     | 1.74                     | 0.53              |
| 40:DT:129:ARG:HD2  | 40:DT:131:ALA:CB   | 2.38                     | 0.53              |
| 42:DV:31:ALA:O     | 42:DV:61:VAL:HG12  | 2.09                     | 0.53              |
| 45:DY:9:LYS:O      | 45:DY:27:VAL:HG22  | 2.09                     | 0.53              |
| 45:DY:42:VAL:HG11  | 45:DY:65:ALA:HB3   | 1.88                     | 0.53              |
| 49:D2:13:ALA:C     | 49:D2:15:LYS:N     | 2.64                     | 0.53              |
| 55:D8:7:HIS:CG     | 55:D8:59:LYS:HZ1   | 2.27                     | 0.53              |
| 1:AA:575:G:N2      | 1:AA:880:C:O2      | 2.42                     | 0.53              |
| 1:AA:980:C:H1'     | 14:AN:19:ARG:HA    | 1.90                     | 0.53              |
| 1:AA:1305:G:O2'    | 1:AA:1306:A:C8     | 2.62                     | 0.53              |
| 2:AB:213:LEU:O     | 2:AB:213:LEU:HD23  | 2.07                     | 0.53              |
| 3:AC:21:ARG:C      | 3:AC:22:TRP:HD1    | 2.16                     | 0.53              |
| 3:AC:140:ARG:HA    | 3:AC:143:GLU:OE1   | 2.07                     | 0.53              |
| 5:AE:53:LEU:O      | 5:AE:57:LYS:HB2    | 2.09                     | 0.53              |
| 13:AM:96:LEU:C     | 13:AM:110:ARG:HE   | 2.17                     | 0.53              |
| 19:AS:48:THR:CG2   | 19:AS:61:TYR:HD1   | 2.22                     | 0.53              |
| 20:AT:56:MET:SD    | 20:AT:85:MET:HE2   | 2.48                     | 0.53              |
| 23:AW:16:U:H5      | 23:AW:18:G:P       | 2.32                     | 0.53              |
| 25:BA:226:G:O2'    | 25:BA:227:A:H8     | 1.92                     | 0.53              |
| 25:BA:1394:U:C4    | 25:BA:1395:A:C6    | 2.97                     | 0.53              |
| 28:BD:73:VAL:O     | 28:BD:75:ILE:N     | 2.41                     | 0.53              |
| 28:BD:95:LEU:HD21  | 28:BD:105:ILE:HG21 | 1.90                     | 0.53              |
| 29:BE:75:VAL:O     | 29:BE:77:ILE:N     | 2.41                     | 0.53              |
| 30:BF:182:ASN:O    | 30:BF:184:TYR:N    | 2.42                     | 0.53              |
| 35:BO:24:VAL:CG2   | 35:BO:33:ALA:HB2   | 2.39                     | 0.53              |
| 35:BO:104:ARG:O    | 35:BO:105:GLU:C    | 2.52                     | 0.53              |
| 35:BO:104:ARG:HH22 | 40:BT:35:LYS:NZ    | 2.06                     | 0.53              |
| 1:CA:662:G:H2'     | 1:CA:663:A:C8      | 2.44                     | 0.53              |
| 1:CA:765:G:N1      | 1:CA:812:C:O2'     | 2.37                     | 0.53              |
| 1:CA:1048:G:OP1    | 14:CN:4:LYS:HB2    | 2.08                     | 0.53              |
| 1:CA:1095:U:H5'    | 1:CA:1109:C:O2     | 2.09                     | 0.53              |
| 1:CA:1502:A:H4'    | 1:CA:1503:A:OP1    | 2.09                     | 0.53              |
| 3:CC:19:GLU:O      | 3:CC:40:ARG:NH2    | 2.41                     | 0.53              |
| 13:CM:20:THR:C     | 13:CM:22:ILE:H     | 2.17                     | 0.53              |
| 16:CP:58:TYR:C     | 16:CP:58:TYR:CD1   | 2.86                     | 0.53              |
| 16:CP:58:TYR:C     | 16:CP:58:TYR:HD1   | 2.16                     | 0.53              |
| 17:CQ:63:ARG:HG2   | 17:CQ:64:PRO:HD2   | 1.91                     | 0.53              |
| 25:DA:17:G:H4'     | 41:DU:25:TRP:CH2   | 2.44                     | 0.53              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:DA:90:U:O2'     | 25:DA:92:A:H8      | 1.92                     | 0.53              |
| 25:DA:627:A:O2'    | 25:DA:636:G:N2     | 2.41                     | 0.53              |
| 25:DA:1819:A:H4'   | 25:DA:1820:U:C5'   | 2.34                     | 0.53              |
| 25:DA:2050:C:H2'   | 25:DA:2051:A:O4'   | 2.08                     | 0.53              |
| 25:DA:2880:C:HO2'  | 38:DR:90:ARG:HH11  | 1.56                     | 0.53              |
| 26:DB:88:C:H2'     | 26:DB:89:G:O4'     | 2.09                     | 0.53              |
| 28:DD:70:TRP:HZ3   | 28:DD:146:GLU:CD   | 2.16                     | 0.53              |
| 28:DD:144:ALA:HB3  | 28:DD:192:THR:HG23 | 1.89                     | 0.53              |
| 33:DI:77:LEU:HD11  | 33:DI:140:LEU:HA   | 1.89                     | 0.53              |
| 34:DN:107:LEU:HD12 | 34:DN:117:PHE:HB2  | 1.90                     | 0.53              |
| 36:DP:117:GLU:OE1  | 36:DP:117:GLU:N    | 2.37                     | 0.53              |
| 36:DP:138:LEU:CD1  | 36:DP:144:GLU:HG2  | 2.39                     | 0.53              |
| 37:DQ:45:GLN:CD    | 37:DQ:45:GLN:N     | 2.67                     | 0.53              |
| 37:DQ:120:ILE:O    | 37:DQ:123:HIS:HB2  | 2.08                     | 0.53              |
| 39:DS:71:ARG:CG    | 39:DS:104:GLY:HA2  | 2.32                     | 0.53              |
| 42:DV:64:HIS:CG    | 42:DV:92:THR:HG22  | 2.44                     | 0.53              |
| 46:DZ:28:MET:SD    | 46:DZ:37:VAL:HG11  | 2.49                     | 0.53              |
| 50:D3:52:HIS:CD2   | 50:D3:52:HIS:H     | 2.25                     | 0.53              |
| 53:D6:41:PRO:CD    | 53:D6:46:HIS:HA    | 2.39                     | 0.53              |
| 1:AA:438:G:O2'     | 1:AA:494:U:O4      | 2.22                     | 0.53              |
| 1:AA:1446:U:N3     | 1:AA:1452:C:O2     | 2.42                     | 0.53              |
| 2:AB:14:GLY:C      | 2:AB:15:VAL:HG22   | 2.34                     | 0.53              |
| 2:AB:69:LEU:HD23   | 2:AB:159:PRO:HG2   | 1.91                     | 0.53              |
| 5:AE:32:VAL:O      | 5:AE:43:LEU:HD12   | 2.09                     | 0.53              |
| 11:AK:27:ASN:HB2   | 11:AK:55:LYS:HE3   | 1.91                     | 0.53              |
| 11:AK:88:GLY:O     | 11:AK:89:ALA:C     | 2.52                     | 0.53              |
| 16:AP:12:LYS:O     | 16:AP:13:HIS:CB    | 2.57                     | 0.53              |
| 22:AV:52:C:C2'     | 22:AV:53:G:O5'     | 2.57                     | 0.53              |
| 25:BA:328:U:H4'    | 45:BY:68:HIS:CD2   | 2.43                     | 0.53              |
| 25:BA:625:G:O6     | 36:BP:107:LYS:HD3  | 2.08                     | 0.53              |
| 25:BA:708:C:H42    | 25:BA:723:G:H1     | 1.57                     | 0.53              |
| 25:BA:2691:C:N4    | 25:BA:2719:G:C2    | 2.76                     | 0.53              |
| 25:BA:2866:U:C6    | 25:BA:2868:A:H1'   | 2.43                     | 0.53              |
| 27:BC:59:ARG:HH22  | 27:BC:200:LYS:N    | 2.07                     | 0.53              |
| 27:BC:99:ILE:HG22  | 27:BC:99:ILE:O     | 2.09                     | 0.53              |
| 30:BF:158:THR:HG21 | 30:BF:163:VAL:HB   | 1.91                     | 0.53              |
| 32:BH:24:VAL:HG22  | 32:BH:35:VAL:O     | 2.08                     | 0.53              |
| 32:BH:85:LYS:O     | 32:BH:133:VAL:N    | 2.42                     | 0.53              |
| 33:BI:6:LEU:HG     | 33:BI:36:ALA:HA    | 1.90                     | 0.53              |
| 33:BI:138:ILE:HG12 | 33:BI:139:GLN:N    | 2.15                     | 0.53              |
| 34:BN:13:TRP:HB2   | 34:BN:133:GLN:OE1  | 2.08                     | 0.53              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 37:BQ:40:ALA:HB3   | 37:BQ:42:ILE:HD11  | 1.91                     | 0.53              |
| 41:BU:95:LEU:CD1   | 42:BV:4:ILE:HD13   | 2.30                     | 0.53              |
| 46:BZ:96:VAL:N     | 46:BZ:128:VAL:O    | 2.42                     | 0.53              |
| 46:BZ:104:PHE:HB3  | 46:BZ:141:VAL:CG1  | 2.38                     | 0.53              |
| 1:CA:511:C:H4'     | 1:CA:511:C:OP1     | 2.09                     | 0.53              |
| 1:CA:529:G:H4'     | 1:CA:533:A:C2      | 2.44                     | 0.53              |
| 1:CA:976:G:H5''    | 1:CA:1358:U:O2'    | 2.09                     | 0.53              |
| 1:CA:1151:A:H5'    | 10:CJ:41:PRO:HA    | 1.91                     | 0.53              |
| 1:CA:1505:G:H5'    | 1:CA:1506:U:H5''   | 1.90                     | 0.53              |
| 5:CE:50:GLU:HG3    | 5:CE:52:PRO:HD2    | 1.89                     | 0.53              |
| 7:CG:89:MET:HE1    | 7:CG:155:ARG:O     | 2.09                     | 0.53              |
| 11:CK:76:GLY:O     | 11:CK:77:MET:C     | 2.52                     | 0.53              |
| 12:CL:90:VAL:HG11  | 12:CL:93:LEU:CG    | 2.40                     | 0.53              |
| 25:DA:72:U:C5      | 49:D2:61:LEU:HB3   | 2.44                     | 0.53              |
| 25:DA:2319:G:O2'   | 25:DA:2320:A:O5'   | 2.26                     | 0.53              |
| 27:DC:49:ILE:H     | 27:DC:49:ILE:CD1   | 2.18                     | 0.53              |
| 28:DD:28:GLU:OE1   | 28:DD:29:PRO:HD3   | 2.09                     | 0.53              |
| 29:DE:57:LYS:C     | 29:DE:59:VAL:H     | 2.17                     | 0.53              |
| 30:DF:110:LEU:HD11 | 30:DF:181:LEU:HD12 | 1.91                     | 0.53              |
| 40:DT:33:LYS:HE2   | 40:DT:43:GLN:CG    | 2.39                     | 0.53              |
| 41:DU:79:PHE:C     | 41:DU:79:PHE:HD2   | 2.17                     | 0.53              |
| 41:DU:97:ASP:O     | 41:DU:100:VAL:N    | 2.26                     | 0.53              |
| 42:DV:65:GLY:HA3   | 42:DV:91:TYR:CE1   | 2.44                     | 0.53              |
| 45:DY:95:LYS:HA    | 45:DY:101:LYS:HB2  | 1.91                     | 0.53              |
| 46:DZ:23:LYS:C     | 46:DZ:25:PRO:HD3   | 2.33                     | 0.53              |
| 54:D7:18:PHE:O     | 54:D7:22:MET:HG2   | 2.09                     | 0.53              |
| 55:D8:38:GLY:O     | 55:D8:42:ARG:HB3   | 2.09                     | 0.53              |
| 1:AA:508:C:H1'     | 1:AA:509:A:N7      | 2.25                     | 0.52              |
| 1:AA:1432:G:OP1    | 40:BT:107:ASP:HB2  | 2.09                     | 0.52              |
| 1:AA:1502:A:H2     | 1:AA:1505:G:N2     | 2.02                     | 0.52              |
| 2:AB:41:ILE:HG22   | 2:AB:42:ILE:O      | 2.10                     | 0.52              |
| 4:AD:60:GLU:OE1    | 4:AD:199:ASN:N     | 2.31                     | 0.52              |
| 4:AD:62:GLN:OE1    | 4:AD:62:GLN:HA     | 2.08                     | 0.52              |
| 4:AD:148:VAL:HG12  | 4:AD:149:ALA:N     | 2.24                     | 0.52              |
| 5:AE:91:LEU:HD12   | 5:AE:120:THR:HG21  | 1.89                     | 0.52              |
| 5:AE:137:GLU:O     | 5:AE:141:GLN:HG3   | 2.09                     | 0.52              |
| 25:BA:641:C:O2'    | 25:BA:2350:C:OP1   | 2.20                     | 0.52              |
| 25:BA:1324:G:H1'   | 25:BA:1616:A:N6    | 2.24                     | 0.52              |
| 25:BA:1779:U:H5    | 25:BA:1784:A:N7    | 2.07                     | 0.52              |
| 25:BA:2056:G:H21   | 25:BA:2057:A:C1'   | 2.22                     | 0.52              |
| 25:BA:2111:C:H4'   | 25:BA:2112:G:OP1   | 2.09                     | 0.52              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 26:BB:44:G:H1'     | 26:BB:47:C:N4     | 2.24                     | 0.52              |
| 27:BC:65:PRO:HG2   | 27:BC:189:ILE:CA  | 2.39                     | 0.52              |
| 31:BG:72:ARG:HD3   | 31:BG:86:MET:HA   | 1.91                     | 0.52              |
| 31:BG:101:ILE:O    | 31:BG:104:GLU:HB3 | 2.07                     | 0.52              |
| 33:BI:117:GLU:CG   | 33:BI:118:LYS:H   | 2.20                     | 0.52              |
| 34:BN:15:LEU:CD1   | 34:BN:16:ILE:H    | 2.22                     | 0.52              |
| 37:BQ:109:VAL:HG22 | 37:BQ:113:GLN:OE1 | 2.09                     | 0.52              |
| 38:BR:79:LEU:HA    | 38:BR:83:ILE:HG13 | 1.91                     | 0.52              |
| 39:BS:34:HIS:CE1   | 39:BS:54:LEU:HD23 | 2.43                     | 0.52              |
| 40:BT:57:PHE:CD1   | 40:BT:58:ASN:N    | 2.77                     | 0.52              |
| 42:BV:49:THR:O     | 42:BV:50:PRO:C    | 2.52                     | 0.52              |
| 45:BY:95:LYS:HG2   | 45:BY:100:ALA:HA  | 1.91                     | 0.52              |
| 46:BZ:155:LEU:O    | 46:BZ:157:LEU:HG  | 2.09                     | 0.52              |
| 1:CA:129:U:O2'     | 1:CA:130:A:H2'    | 2.09                     | 0.52              |
| 1:CA:372:C:N4      | 1:CA:387:U:H2'    | 2.24                     | 0.52              |
| 1:CA:914:A:O2'     | 1:CA:915:A:H5'    | 2.08                     | 0.52              |
| 2:CB:77:ALA:O      | 2:CB:81:VAL:HG23  | 2.08                     | 0.52              |
| 2:CB:97:TRP:HZ2    | 2:CB:102:LEU:HD13 | 1.74                     | 0.52              |
| 16:CP:5:ARG:CB     | 16:CP:67:THR:OG1  | 2.53                     | 0.52              |
| 19:CS:36:ARG:NH1   | 19:CS:53:ASN:HA   | 2.24                     | 0.52              |
| 25:DA:142:A:H5''   | 25:DA:142(A):C:H5 | 1.74                     | 0.52              |
| 25:DA:727:A:OP1    | 25:DA:1431:U:O2'  | 2.26                     | 0.52              |
| 25:DA:2258:C:O5'   | 25:DA:2258:C:H6   | 1.92                     | 0.52              |
| 27:DC:93:TYR:O     | 27:DC:94:VAL:HG13 | 2.09                     | 0.52              |
| 29:DE:28:ALA:HB3   | 29:DE:93:VAL:HG22 | 1.91                     | 0.52              |
| 31:DG:88:ILE:C     | 31:DG:88:ILE:CD1  | 2.83                     | 0.52              |
| 32:DH:10:PRO:HD2   | 32:DH:50:VAL:O    | 2.08                     | 0.52              |
| 32:DH:147:ASN:N    | 32:DH:147:ASN:ND2 | 2.57                     | 0.52              |
| 33:DI:3:VAL:HB     | 33:DI:37:VAL:O    | 2.09                     | 0.52              |
| 34:DN:67:LEU:HD12  | 34:DN:67:LEU:H    | 1.72                     | 0.52              |
| 36:DP:79:ARG:NE    | 36:DP:109:GLY:HA3 | 2.25                     | 0.52              |
| 41:DU:21:ALA:HB1   | 41:DU:24:TYR:CD1  | 2.44                     | 0.52              |
| 41:DU:62:ILE:HD12  | 41:DU:76:TYR:OH   | 2.09                     | 0.52              |
| 41:DU:79:PHE:O     | 41:DU:79:PHE:HD2  | 1.91                     | 0.52              |
| 43:DW:27:LYS:HE3   | 43:DW:31:GLU:HG2  | 1.91                     | 0.52              |
| 2:AB:14:GLY:O      | 2:AB:15:VAL:CG1   | 2.48                     | 0.52              |
| 2:AB:91:PRO:HG3    | 2:AB:154:LEU:HD12 | 1.91                     | 0.52              |
| 4:AD:161:ASN:O     | 4:AD:165:MET:HG2  | 2.10                     | 0.52              |
| 6:AF:82:ARG:HB3    | 6:AF:85:VAL:HG23  | 1.89                     | 0.52              |
| 11:AK:41:THR:HG22  | 11:AK:42:TRP:N    | 2.22                     | 0.52              |
| 25:BA:74:A:H4'     | 25:BA:75:G:O5'    | 2.07                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:BA:1012:U:O4    | 34:BN:25:ARG:HD3   | 2.09                     | 0.52              |
| 25:BA:1453:U:O4    | 38:BR:73:VAL:HG13  | 2.08                     | 0.52              |
| 25:BA:2585:U:H5''  | 25:BA:2586:C:OP1   | 2.09                     | 0.52              |
| 25:BA:2780:G:C4'   | 25:BA:2781:A:OP2   | 2.57                     | 0.52              |
| 26:BB:3:C:H42      | 26:BB:118:G:H1     | 1.55                     | 0.52              |
| 27:BC:38:ASP:C     | 27:BC:40:THR:H     | 2.18                     | 0.52              |
| 28:BD:248:SER:HB2  | 28:BD:250:TRP:HE3  | 1.74                     | 0.52              |
| 29:BE:116:VAL:O    | 29:BE:117:MET:CB   | 2.53                     | 0.52              |
| 34:BN:11:PRO:HB3   | 34:BN:51:PHE:CE1   | 2.43                     | 0.52              |
| 36:BP:79:ARG:CD    | 36:BP:109:GLY:O    | 2.57                     | 0.52              |
| 38:BR:101:ALA:O    | 38:BR:102:GLU:HB2  | 2.08                     | 0.52              |
| 39:BS:106:ARG:HH12 | 39:BS:108:GLY:HA3  | 1.73                     | 0.52              |
| 41:BU:113:ALA:C    | 41:BU:115:ALA:H    | 2.16                     | 0.52              |
| 53:B6:13:CYS:O     | 53:B6:21:TYR:HA    | 2.08                     | 0.52              |
| 55:B8:23:VAL:CG1   | 55:B8:46:ARG:HB3   | 2.39                     | 0.52              |
| 55:B8:32:LEU:O     | 55:B8:33:ASN:CG    | 2.53                     | 0.52              |
| 1:CA:533:A:O2'     | 1:CA:534:U:P       | 2.67                     | 0.52              |
| 1:CA:818:G:O2'     | 1:CA:820:U:C4      | 2.62                     | 0.52              |
| 1:CA:1374:A:H4'    | 7:CG:31:MET:HE1    | 1.91                     | 0.52              |
| 1:CA:1405:G:OP2    | 58:CA:1741:PAR:O34 | 2.27                     | 0.52              |
| 2:CB:82:ARG:NH2    | 2:CB:92:TYR:OH     | 2.42                     | 0.52              |
| 3:CC:95:THR:O      | 3:CC:97:LYS:N      | 2.42                     | 0.52              |
| 3:CC:149:ALA:HA    | 3:CC:201:TYR:O     | 2.08                     | 0.52              |
| 4:CD:151:LYS:HG2   | 4:CD:151:LYS:O     | 2.09                     | 0.52              |
| 4:CD:172:PRO:CB    | 4:CD:187:ARG:HH22  | 2.22                     | 0.52              |
| 5:CE:90:VAL:HG21   | 5:CE:121:LYS:HB3   | 1.92                     | 0.52              |
| 11:CK:57:THR:HG22  | 11:CK:59:TYR:H     | 1.74                     | 0.52              |
| 13:CM:84:ILE:HD13  | 19:CS:65:ASN:CB    | 2.35                     | 0.52              |
| 14:CN:59:ALA:O     | 14:CN:60:SER:CB    | 2.57                     | 0.52              |
| 18:CR:75:ILE:C     | 18:CR:77:GLY:H     | 2.18                     | 0.52              |
| 19:CS:11:VAL:HG21  | 19:CS:16:LEU:HD11  | 1.91                     | 0.52              |
| 25:DA:2787:C:H1'   | 29:DE:61:ARG:HG3   | 1.91                     | 0.52              |
| 27:DC:78:ALA:HB2   | 27:DC:82:LYS:HB2   | 1.91                     | 0.52              |
| 29:DE:101:ARG:HH22 | 29:DE:171:GLU:HB2  | 1.71                     | 0.52              |
| 32:DH:153:LYS:CB   | 32:DH:154:PRO:CD   | 2.72                     | 0.52              |
| 35:DO:2:ILE:CD1    | 35:DO:6:THR:HG21   | 2.38                     | 0.52              |
| 36:DP:49:ARG:HD2   | 55:D8:59:LYS:HG2   | 1.91                     | 0.52              |
| 1:AA:8:A:H62       | 4:AD:208:SER:HB2   | 1.75                     | 0.52              |
| 1:AA:825:G:N2      | 1:AA:875:C:O2      | 2.40                     | 0.52              |
| 1:AA:970:C:N4      | 9:AI:128:ARG:O     | 2.42                     | 0.52              |
| 2:AB:102:LEU:HB2   | 2:AB:176:GLU:HG2   | 1.91                     | 0.52              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 3:AC:18:TRP:HD1   | 14:AN:54:PRO:HA    | 1.71                     | 0.52              |
| 3:AC:68:VAL:HG12  | 3:AC:70:VAL:HG23   | 1.91                     | 0.52              |
| 3:AC:111:LEU:CD2  | 3:AC:146:ALA:HB2   | 2.38                     | 0.52              |
| 4:AD:167:GLY:O    | 4:AD:168:ARG:C     | 2.52                     | 0.52              |
| 5:AE:84:PHE:O     | 5:AE:86:ALA:N      | 2.42                     | 0.52              |
| 9:AI:32:ASP:O     | 9:AI:35:GLU:HB3    | 2.10                     | 0.52              |
| 19:AS:47:HIS:O    | 19:AS:62:ILE:HG21  | 2.08                     | 0.52              |
| 22:AV:28:U:H3     | 22:AV:44:A:H61     | 1.57                     | 0.52              |
| 22:AV:55:U:H2'    | 22:AV:56:U:H5'     | 1.90                     | 0.52              |
| 23:AW:56:C:C4     | 23:AW:57:G:N7      | 2.77                     | 0.52              |
| 25:BA:221:A:C5    | 25:BA:266:G:N7     | 2.77                     | 0.52              |
| 25:BA:311:A:O4'   | 25:BA:332:A:N9     | 2.42                     | 0.52              |
| 25:BA:1792:G:H5'  | 28:BD:205:VAL:HG13 | 1.92                     | 0.52              |
| 25:BA:2820:A:H61  | 29:BE:192:ASN:HB2  | 1.74                     | 0.52              |
| 26:BB:40:U:O2'    | 26:BB:45:A:N6      | 2.42                     | 0.52              |
| 28:BD:45:ASN:OD1  | 28:BD:46:GLN:N     | 2.42                     | 0.52              |
| 36:BP:59:LEU:HG   | 36:BP:59:LEU:O     | 2.09                     | 0.52              |
| 39:BS:52:SER:O    | 39:BS:69:VAL:HG23  | 2.09                     | 0.52              |
| 39:BS:85:VAL:N    | 39:BS:106:ARG:HB2  | 2.23                     | 0.52              |
| 40:BT:29:ARG:CA   | 40:BT:29:ARG:HE    | 2.16                     | 0.52              |
| 41:BU:61:TRP:CH2  | 41:BU:94:ASN:CB    | 2.91                     | 0.52              |
| 45:BY:77:PRO:O    | 45:BY:78:ALA:CB    | 2.57                     | 0.52              |
| 48:B1:46:LEU:HD23 | 48:B1:46:LEU:H     | 1.74                     | 0.52              |
| 55:B8:59:LYS:C    | 55:B8:60:LEU:HD23  | 2.35                     | 0.52              |
| 1:CA:66:G:C5'     | 1:CA:173:U:O4      | 2.58                     | 0.52              |
| 2:CB:223:ILE:HA   | 2:CB:226:ARG:CD    | 2.39                     | 0.52              |
| 4:CD:134:ASP:O    | 4:CD:136:PRO:HD3   | 2.09                     | 0.52              |
| 5:CE:61:TYR:O     | 5:CE:62:ALA:C      | 2.52                     | 0.52              |
| 5:CE:105:VAL:O    | 5:CE:108:ALA:CB    | 2.57                     | 0.52              |
| 8:CH:28:ALA:CB    | 8:CH:57:PRO:HB2    | 2.39                     | 0.52              |
| 10:CJ:54:PHE:CE2  | 10:CJ:55:LYS:HD2   | 2.45                     | 0.52              |
| 12:CL:27:LEU:HG   | 12:CL:62:SER:CB    | 2.40                     | 0.52              |
| 12:CL:60:LEU:N    | 12:CL:60:LEU:HD22  | 2.25                     | 0.52              |
| 15:CO:32:LEU:O    | 15:CO:36:ILE:HG13  | 2.09                     | 0.52              |
| 21:CU:2:GLY:C     | 21:CU:4:GLY:H      | 2.17                     | 0.52              |
| 23:CW:69:G:H3'    | 23:CW:70:G:H5''    | 1.91                     | 0.52              |
| 25:DA:26:G:H1'    | 25:DA:515:A:H61    | 1.74                     | 0.52              |
| 25:DA:84:A:H61    | 25:DA:102:G:C2'    | 2.21                     | 0.52              |
| 25:DA:241:A:O3'   | 25:DA:242:G:H4'    | 2.08                     | 0.52              |
| 25:DA:9273:G:O2'  | 25:DA:9274:U:H5'   | 2.09                     | 0.52              |
| 25:DA:746:A:C6    | 25:DA:2611:U:H5''  | 2.44                     | 0.52              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 25:DA:830:G:H1'    | 25:DA:2448:A:N1   | 2.24                     | 0.52              |
| 25:DA:995:C:C6     | 41:DU:57:PHE:CD1  | 2.95                     | 0.52              |
| 25:DA:1693:U:OP2   | 25:DA:1694:C:H5   | 1.90                     | 0.52              |
| 25:DA:2111:C:H42   | 25:DA:2147:G:H22  | 1.56                     | 0.52              |
| 25:DA:2637:U:H5''  | 29:DE:82:ARG:HH21 | 1.74                     | 0.52              |
| 29:DE:110:GLY:HA2  | 29:DE:162:ALA:H   | 1.74                     | 0.52              |
| 30:DF:124:LEU:HD12 | 30:DF:125:LEU:N   | 2.24                     | 0.52              |
| 31:DG:146:TYR:C    | 31:DG:148:MET:N   | 2.64                     | 0.52              |
| 32:DH:18:GLU:O     | 32:DH:24:VAL:HA   | 2.10                     | 0.52              |
| 32:DH:87:LEU:HD13  | 32:DH:148:ILE:CG2 | 2.38                     | 0.52              |
| 32:DH:154:PRO:HD3  | 32:DH:161:GLY:C   | 2.34                     | 0.52              |
| 35:DO:8:LEU:HD22   | 35:DO:8:LEU:N     | 2.23                     | 0.52              |
| 36:DP:79:ARG:CD    | 36:DP:109:GLY:C   | 2.81                     | 0.52              |
| 39:DS:34:HIS:HB3   | 39:DS:53:SER:HB3  | 1.92                     | 0.52              |
| 46:DZ:44:PHE:HA    | 46:DZ:47:VAL:CG1  | 2.39                     | 0.52              |
| 50:D3:1:MET:HE2    | 50:D3:44:ARG:NH2  | 2.24                     | 0.52              |
| 1:AA:242:C:H3'     | 1:AA:242:C:C6     | 2.43                     | 0.52              |
| 2:AB:11:LEU:HD11   | 2:AB:217:ARG:HH21 | 1.74                     | 0.52              |
| 2:AB:118:LEU:CB    | 2:AB:142:LEU:HD13 | 2.40                     | 0.52              |
| 2:AB:219:VAL:O     | 2:AB:222:ILE:HB   | 2.09                     | 0.52              |
| 3:AC:58:GLU:HB2    | 3:AC:65:ALA:CB    | 2.34                     | 0.52              |
| 5:AE:76:ILE:HD11   | 5:AE:142:LEU:CD1  | 2.26                     | 0.52              |
| 11:AK:12:ARG:C     | 11:AK:13:GLN:HG3  | 2.34                     | 0.52              |
| 13:AM:3:ARG:NH1    | 31:BG:113:ARG:NE  | 2.56                     | 0.52              |
| 14:AN:23:ARG:HD2   | 14:AN:28:GLY:O    | 2.10                     | 0.52              |
| 17:AQ:34:LYS:HG2   | 17:AQ:35:VAL:N    | 2.23                     | 0.52              |
| 19:AS:61:TYR:CG    | 19:AS:62:ILE:N    | 2.72                     | 0.52              |
| 23:AW:34:G:O6      | 24:AX:14:A:C4     | 2.62                     | 0.52              |
| 25:BA:811:U:C4     | 36:BP:21:ARG:NH2  | 2.75                     | 0.52              |
| 25:BA:1578:U:H2'   | 25:BA:1579:A:H5'  | 1.91                     | 0.52              |
| 25:BA:1899:G:N2    | 25:BA:1902:C:H41  | 2.08                     | 0.52              |
| 25:BA:2058:A:H5''  | 25:BA:2059:A:OP2  | 2.10                     | 0.52              |
| 25:BA:2696:U:H2'   | 25:BA:2697:G:C8   | 2.44                     | 0.52              |
| 28:BD:34:VAL:O     | 28:BD:34:VAL:HG13 | 2.09                     | 0.52              |
| 28:BD:126:GLN:HG3  | 28:BD:129:ASN:ND2 | 2.25                     | 0.52              |
| 31:BG:5:VAL:HG12   | 51:B4:51:TYR:CE1  | 2.43                     | 0.52              |
| 34:BN:134:ARG:H    | 34:BN:135:PRO:CD  | 2.16                     | 0.52              |
| 35:BO:4:PRO:O      | 35:BO:5:GLN:CB    | 2.51                     | 0.52              |
| 41:BU:92:ARG:HE    | 41:BU:94:ASN:HB3  | 1.74                     | 0.52              |
| 41:BU:101:ARG:C    | 41:BU:102:GLU:HG2 | 2.33                     | 0.52              |
| 44:BX:10:ALA:HB1   | 44:BX:11:PRO:CD   | 2.39                     | 0.52              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 45:BY:27:VAL:HA    | 45:BY:28:LYS:NZ   | 2.24                     | 0.52              |
| 55:B8:16:ILE:HG22  | 55:B8:64:TYR:HD2  | 1.71                     | 0.52              |
| 1:CA:119:A:O4'     | 1:CA:120:A:C5     | 2.63                     | 0.52              |
| 1:CA:129(A):G:H5'' | 1:CA:130:A:P      | 2.49                     | 0.52              |
| 1:CA:380:G:N2      | 1:CA:383:A:OP2    | 2.41                     | 0.52              |
| 2:CB:105:PHE:O     | 2:CB:107:THR:N    | 2.42                     | 0.52              |
| 2:CB:109:SER:C     | 2:CB:111:ARG:N    | 2.67                     | 0.52              |
| 4:CD:9:CYS:SG      | 4:CD:22:LYS:CD    | 2.98                     | 0.52              |
| 7:CG:60:LYS:NZ     | 7:CG:63:LYS:HB3   | 2.23                     | 0.52              |
| 8:CH:39:LEU:CD1    | 8:CH:111:ILE:HD11 | 2.39                     | 0.52              |
| 9:CI:118:LYS:O     | 9:CI:119:ALA:HB3  | 2.09                     | 0.52              |
| 14:CN:15:LYS:O     | 14:CN:16:PHE:C    | 2.52                     | 0.52              |
| 15:CO:25:THR:O     | 15:CO:26:GLU:C    | 2.52                     | 0.52              |
| 15:CO:39:LEU:O     | 15:CO:42:HIS:N    | 2.39                     | 0.52              |
| 25:DA:2330:G:H1'   | 47:D0:41:ARG:CB   | 2.39                     | 0.52              |
| 25:DA:2875:C:O2'   | 40:DT:5:ALA:HB3   | 2.10                     | 0.52              |
| 28:DD:155:LEU:O    | 28:DD:156:ALA:HB3 | 2.10                     | 0.52              |
| 29:DE:71:GLY:O     | 29:DE:72:VAL:C    | 2.52                     | 0.52              |
| 31:DG:16:ARG:HH11  | 31:DG:16:ARG:CG   | 2.14                     | 0.52              |
| 31:DG:106:LEU:HD12 | 31:DG:110:ALA:HB3 | 1.92                     | 0.52              |
| 33:DI:82:ARG:HG3   | 33:DI:82:ARG:NH1  | 2.24                     | 0.52              |
| 34:DN:42:TRP:HA    | 34:DN:42:TRP:HE3  | 1.75                     | 0.52              |
| 34:DN:55:VAL:HG22  | 34:DN:126:PRO:HA  | 1.92                     | 0.52              |
| 37:DQ:109:VAL:HG13 | 37:DQ:113:GLN:OE1 | 2.10                     | 0.52              |
| 40:DT:68:TYR:N     | 40:DT:68:TYR:CD2  | 2.77                     | 0.52              |
| 46:DZ:19:ARG:NH1   | 46:DZ:84:GLU:O    | 2.43                     | 0.52              |
| 48:D1:64:ALA:HA    | 48:D1:67:ILE:CG1  | 2.39                     | 0.52              |
| 1:AA:242:C:C6      | 1:AA:242:C:C3'    | 2.92                     | 0.52              |
| 1:AA:501:C:H2'     | 1:AA:502:G:C8     | 2.45                     | 0.52              |
| 1:AA:1066:C:C2'    | 1:AA:1067:A:O5'   | 2.58                     | 0.52              |
| 1:AA:1265:G:H2'    | 1:AA:1266:G:C8    | 2.44                     | 0.52              |
| 6:AF:86:ARG:O      | 6:AF:87:ARG:HG2   | 2.09                     | 0.52              |
| 9:AI:63:ILE:HD11   | 9:AI:81:ILE:HD11  | 1.90                     | 0.52              |
| 10:AJ:8:LEU:HD12   | 10:AJ:20:ALA:HA   | 1.91                     | 0.52              |
| 11:AK:57:THR:HG22  | 11:AK:59:TYR:N    | 2.24                     | 0.52              |
| 11:AK:87:THR:HG22  | 11:AK:88:GLY:N    | 2.24                     | 0.52              |
| 15:AO:39:LEU:O     | 15:AO:40:SER:C    | 2.53                     | 0.52              |
| 20:AT:44:ALA:HB3   | 20:AT:91:LEU:HD12 | 1.91                     | 0.52              |
| 23:AW:56:C:O4'     | 25:BA:2169:A:H1'  | 2.09                     | 0.52              |
| 23:AY:34:G:C2'     | 23:AY:35:A:H5'    | 2.39                     | 0.52              |
| 25:BA:99:U:H1'     | 25:BA:102:G:C2    | 2.44                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:BA:519:U:H2'    | 25:BA:520:G:H8     | 1.74                     | 0.52              |
| 25:BA:671:C:OP1    | 36:BP:42:SER:O     | 2.27                     | 0.52              |
| 25:BA:1024:G:C6    | 25:BA:1025:G:C6    | 2.97                     | 0.52              |
| 25:BA:2031:A:C6    | 25:BA:2498:C:H1'   | 2.44                     | 0.52              |
| 25:BA:2391:G:O2'   | 25:BA:2424:C:N4    | 2.42                     | 0.52              |
| 25:BA:2791:C:H1'   | 25:BA:2792:G:N7    | 2.25                     | 0.52              |
| 28:BD:165:ILE:HG12 | 28:BD:175:LEU:CD2  | 2.39                     | 0.52              |
| 30:BF:31:HIS:HB2   | 36:BP:9:ASN:ND2    | 2.24                     | 0.52              |
| 31:BG:126:ASP:C    | 31:BG:128:ARG:H    | 2.18                     | 0.52              |
| 32:BH:26:VAL:HG11  | 32:BH:76:VAL:HA    | 1.91                     | 0.52              |
| 34:BN:117:PHE:CD2  | 34:BN:117:PHE:C    | 2.87                     | 0.52              |
| 37:BQ:110:THR:O    | 37:BQ:111:GLU:C    | 2.53                     | 0.52              |
| 38:BR:45:ARG:HG3   | 38:BR:46:GLY:N     | 2.25                     | 0.52              |
| 43:BW:22:ASP:HA    | 43:BW:25:ARG:HH12  | 1.75                     | 0.52              |
| 45:BY:47:LYS:HD2   | 45:BY:47:LYS:N     | 2.25                     | 0.52              |
| 46:BZ:29:TYR:HA    | 46:BZ:33:LEU:O     | 2.09                     | 0.52              |
| 54:B7:12:ARG:NH2   | 54:B7:44:PRO:HB3   | 2.25                     | 0.52              |
| 1:CA:17:U:H2'      | 1:CA:18:C:C6       | 2.43                     | 0.52              |
| 1:CA:1148:U:H2'    | 1:CA:1149:C:O4'    | 2.09                     | 0.52              |
| 1:CA:1412:C:H2'    | 1:CA:1413:A:C8     | 2.45                     | 0.52              |
| 2:CB:62:ALA:O      | 2:CB:65:GLY:N      | 2.39                     | 0.52              |
| 2:CB:168:THR:O     | 2:CB:170:GLU:N     | 2.43                     | 0.52              |
| 4:CD:162:LEU:O     | 4:CD:165:MET:HB2   | 2.10                     | 0.52              |
| 6:CF:8:ILE:HA      | 6:CF:87:ARG:O      | 2.08                     | 0.52              |
| 11:CK:17:GLY:C     | 11:CK:80:VAL:HG12  | 2.35                     | 0.52              |
| 11:CK:21:ILE:HA    | 11:CK:30:VAL:HG12  | 1.91                     | 0.52              |
| 16:CP:11:SER:HB2   | 16:CP:14:ASN:HB3   | 1.90                     | 0.52              |
| 22:CV:42:C:C2'     | 22:CV:43:G:O5'     | 2.57                     | 0.52              |
| 25:DA:85:G:OP1     | 45:DY:8:LYS:HA     | 2.10                     | 0.52              |
| 28:DD:65:ILE:HD11  | 28:DD:67:PHE:CD1   | 2.45                     | 0.52              |
| 28:DD:243:GLY:O    | 28:DD:244:ARG:CB   | 2.57                     | 0.52              |
| 30:DF:155:LEU:HD13 | 30:DF:174:VAL:HG22 | 1.92                     | 0.52              |
| 31:DG:104:GLU:O    | 31:DG:108:ASN:HB2  | 2.09                     | 0.52              |
| 33:DI:79:ILE:HB    | 33:DI:141:LYS:O    | 2.09                     | 0.52              |
| 34:DN:58:ASP:O     | 34:DN:60:ILE:HG13  | 2.10                     | 0.52              |
| 35:DO:98:VAL:HG12  | 35:DO:117:LEU:HD22 | 1.91                     | 0.52              |
| 38:DR:8:ARG:HG3    | 38:DR:43:GLU:OE2   | 2.10                     | 0.52              |
| 38:DR:60:LEU:O     | 38:DR:63:ARG:HB3   | 2.09                     | 0.52              |
| 40:DT:30:VAL:HG11  | 40:DT:84:GLN:HG3   | 1.92                     | 0.52              |
| 43:DW:22:ASP:HA    | 43:DW:25:ARG:HH12  | 1.74                     | 0.52              |
| 46:DZ:9:TYR:HE1    | 46:DZ:61:LEU:HD13  | 1.74                     | 0.52              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 53:D6:10:LEU:H      | 53:D6:10:LEU:HD22  | 1.73                     | 0.52              |
| 53:D6:15:GLU:C      | 53:D6:47:THR:HG21  | 2.33                     | 0.52              |
| 1:AA:625:G:H4'      | 16:AP:16:HIS:HD2   | 1.75                     | 0.52              |
| 1:AA:929:G:N2       | 1:AA:1388:C:O2     | 2.38                     | 0.52              |
| 2:AB:71:VAL:HB      | 2:AB:164:VAL:HG13  | 1.92                     | 0.52              |
| 3:AC:151:VAL:C      | 3:AC:152:ILE:HG12  | 2.35                     | 0.52              |
| 4:AD:9:CYS:SG       | 4:AD:22:LYS:CE     | 2.98                     | 0.52              |
| 8:AH:86:ILE:HG22    | 8:AH:87:SER:N      | 2.23                     | 0.52              |
| 9:AI:50:LEU:O       | 9:AI:53:VAL:HG22   | 2.10                     | 0.52              |
| 12:AL:8:ASN:OD1     | 17:AQ:34:LYS:HE2   | 2.10                     | 0.52              |
| 17:AQ:59:ILE:HG22   | 17:AQ:60:ILE:N     | 2.24                     | 0.52              |
| 20:AT:86:ARG:O      | 20:AT:90:GLN:HG3   | 2.08                     | 0.52              |
| 25:BA:345:A:O2'     | 25:BA:347:A:N7     | 2.42                     | 0.52              |
| 25:BA:555:U:O2'     | 25:BA:556:G:C8     | 2.62                     | 0.52              |
| 25:BA:1450(A):C:O5' | 25:BA:1450(A):C:H6 | 1.92                     | 0.52              |
| 25:BA:2422:A:H4'    | 25:BA:2423:U:OP1   | 2.10                     | 0.52              |
| 28:BD:26:LYS:HZ1    | 28:BD:82:ILE:H     | 1.58                     | 0.52              |
| 31:BG:51:ARG:HA     | 31:BG:51:ARG:NE    | 2.24                     | 0.52              |
| 32:BH:109:PHE:CE1   | 32:BH:152:ARG:NE   | 2.77                     | 0.52              |
| 33:BI:83:ALA:HB1    | 33:BI:88:ILE:HA    | 1.87                     | 0.52              |
| 33:BI:119:PRO:O     | 33:BI:120:ILE:C    | 2.53                     | 0.52              |
| 36:BP:9:ASN:CB      | 36:BP:10:PRO:HD2   | 2.40                     | 0.52              |
| 36:BP:83:VAL:O      | 36:BP:83:VAL:HG13  | 2.09                     | 0.52              |
| 41:BU:39:LEU:O      | 41:BU:40:PHE:C     | 2.53                     | 0.52              |
| 1:CA:100:C:H2'      | 1:CA:101:A:N9      | 2.24                     | 0.52              |
| 1:CA:1059:C:OP2     | 3:CC:199:LYS:NZ    | 2.35                     | 0.52              |
| 4:CD:10:ARG:HG3     | 4:CD:10:ARG:NH1    | 2.20                     | 0.52              |
| 4:CD:25:ARG:C       | 4:CD:27:TYR:N      | 2.66                     | 0.52              |
| 5:CE:110:LEU:CD2    | 5:CE:139:LEU:HD21  | 2.37                     | 0.52              |
| 6:CF:21:LEU:O       | 6:CF:24:GLU:HG2    | 2.09                     | 0.52              |
| 7:CG:69:VAL:O       | 7:CG:69:VAL:CG1    | 2.57                     | 0.52              |
| 7:CG:102:ARG:HG2    | 7:CG:106:GLN:OE1   | 2.09                     | 0.52              |
| 8:CH:84:ARG:HG3     | 8:CH:85:ARG:N      | 2.21                     | 0.52              |
| 10:CJ:58:ASP:O      | 10:CJ:60:ARG:CG    | 2.58                     | 0.52              |
| 11:CK:67:ASP:O      | 11:CK:71:LYS:HG3   | 2.08                     | 0.52              |
| 13:CM:15:VAL:HG12   | 13:CM:19:LEU:HD21  | 1.92                     | 0.52              |
| 14:CN:15:LYS:HD2    | 14:CN:16:PHE:CE2   | 2.44                     | 0.52              |
| 20:CT:53:LEU:HG     | 20:CT:102:GLY:H    | 1.75                     | 0.52              |
| 22:CV:20:G:C4       | 22:CV:58:A:H2      | 2.27                     | 0.52              |
| 25:DA:9273:G:C2'    | 25:DA:9274:U:H5'   | 2.39                     | 0.52              |
| 25:DA:340:A:H2'     | 25:DA:341:G:O5'    | 2.10                     | 0.52              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 25:DA:857:C:OP2    | 47:D0:77:ARG:NH2  | 2.42                     | 0.52              |
| 25:DA:1819:A:H5''  | 25:DA:1820:U:H5'' | 1.91                     | 0.52              |
| 25:DA:2287:A:HO2'  | 25:DA:2288:A:P    | 2.32                     | 0.52              |
| 27:DC:83:ILE:HD11  | 27:DC:95:GLY:O    | 2.09                     | 0.52              |
| 34:DN:90:MET:HE2   | 34:DN:90:MET:HA   | 1.91                     | 0.52              |
| 35:DO:87:ILE:HG22  | 35:DO:88:ASN:O    | 2.09                     | 0.52              |
| 41:DU:12:ARG:C     | 41:DU:14:HIS:N    | 2.65                     | 0.52              |
| 41:DU:92:ARG:NE    | 42:DV:11:GLN:HB2  | 2.24                     | 0.52              |
| 45:DY:44:ILE:CD1   | 45:DY:45:VAL:HG23 | 2.40                     | 0.52              |
| 46:DZ:13:GLU:HA    | 46:DZ:13:GLU:OE2  | 2.10                     | 0.52              |
| 55:D8:51:ALA:HA    | 55:D8:54:GLU:OE2  | 2.10                     | 0.52              |
| 1:AA:511:C:O2'     | 1:AA:512:U:OP2    | 2.23                     | 0.52              |
| 2:AB:42:ILE:HD11   | 2:AB:202:PRO:C    | 2.35                     | 0.52              |
| 3:AC:58:GLU:N      | 3:AC:65:ALA:HB3   | 2.20                     | 0.52              |
| 3:AC:77:ILE:O      | 3:AC:83:ARG:HB3   | 2.08                     | 0.52              |
| 5:AE:79:GLU:CD     | 8:AH:104:ARG:HA   | 2.34                     | 0.52              |
| 8:AH:119:LEU:HD12  | 8:AH:124:ALA:HA   | 1.92                     | 0.52              |
| 9:AI:29:ASN:OD1    | 9:AI:64:THR:HA    | 2.08                     | 0.52              |
| 13:AM:67:GLU:CD    | 13:AM:67:GLU:C    | 2.77                     | 0.52              |
| 23:AW:49:C:N4      | 23:AW:65:G:H1     | 2.08                     | 0.52              |
| 25:BA:443:A:N7     | 30:BF:45:ARG:HD2  | 2.24                     | 0.52              |
| 25:BA:1441:G:H2'   | 25:BA:1442:G:H8   | 1.74                     | 0.52              |
| 25:BA:1943:U:H1'   | 25:BA:1945:G:H5'  | 1.90                     | 0.52              |
| 25:BA:2078:C:C4    | 25:BA:2079:U:C4   | 2.98                     | 0.52              |
| 36:BP:148:LEU:HD23 | 36:BP:148:LEU:N   | 2.24                     | 0.52              |
| 37:BQ:26:TYR:CD1   | 37:BQ:28:ALA:HB2  | 2.45                     | 0.52              |
| 39:BS:15:ARG:N     | 39:BS:15:ARG:CD   | 2.68                     | 0.52              |
| 40:BT:92:GLY:C     | 40:BT:94:ALA:N    | 2.61                     | 0.52              |
| 42:BV:20:LEU:H     | 42:BV:20:LEU:HD12 | 1.74                     | 0.52              |
| 45:BY:7:VAL:HB     | 45:BY:8:LYS:HD2   | 1.91                     | 0.52              |
| 54:B7:31:LEU:O     | 54:B7:35:ARG:HB2  | 2.10                     | 0.52              |
| 1:CA:872:A:C4      | 1:CA:874:G:N7     | 2.78                     | 0.52              |
| 1:CA:1014:A:H4'    | 19:CS:14:HIS:CD2  | 2.45                     | 0.52              |
| 2:CB:19:HIS:CE1    | 2:CB:189:ASP:OD2  | 2.62                     | 0.52              |
| 3:CC:15:THR:HG21   | 3:CC:181:ASN:HA   | 1.91                     | 0.52              |
| 3:CC:85:ARG:C      | 3:CC:87:LEU:H     | 2.17                     | 0.52              |
| 9:CI:71:SER:O      | 9:CI:74:ILE:HB    | 2.09                     | 0.52              |
| 10:CJ:40:LEU:CD2   | 10:CJ:69:ASN:HB3  | 2.39                     | 0.52              |
| 12:CL:20:LYS:C     | 12:CL:21:LYS:HD2  | 2.34                     | 0.52              |
| 19:CS:16:LEU:H     | 19:CS:16:LEU:HD13 | 1.75                     | 0.52              |
| 25:DA:614(A):U:H3' | 25:DA:614(A):U:H6 | 1.74                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:DA:792:G:H5''   | 25:DA:793:A:H5'    | 1.91                     | 0.52              |
| 25:DA:889:C:H1'    | 25:DA:890:A:O4'    | 2.09                     | 0.52              |
| 25:DA:2000:G:HO2'  | 25:DA:2689:U:H5    | 1.57                     | 0.52              |
| 25:DA:2751:G:O5'   | 25:DA:2751:G:C8    | 2.57                     | 0.52              |
| 27:DC:86:ALA:CB    | 27:DC:94:VAL:HG11  | 2.40                     | 0.52              |
| 28:DD:33:LEU:O     | 28:DD:34:VAL:C     | 2.52                     | 0.52              |
| 28:DD:248:SER:OG   | 28:DD:252:TRP:CE2  | 2.61                     | 0.52              |
| 28:DD:267:SER:HA   | 28:DD:270:ILE:HG13 | 1.92                     | 0.52              |
| 29:DE:36:ARG:NH1   | 29:DE:86:PRO:HD2   | 2.24                     | 0.52              |
| 30:DF:107:LYS:O    | 30:DF:108:LYS:C    | 2.53                     | 0.52              |
| 31:DG:33:ARG:O     | 31:DG:162:THR:HG23 | 2.10                     | 0.52              |
| 34:DN:18:ALA:HB1   | 34:DN:21:LYS:HB2   | 1.92                     | 0.52              |
| 37:DQ:51:ARG:HH11  | 37:DQ:51:ARG:CB    | 2.21                     | 0.52              |
| 40:DT:80:SER:O     | 40:DT:81:PRO:C     | 2.52                     | 0.52              |
| 41:DU:61:TRP:CZ3   | 41:DU:94:ASN:HB2   | 2.45                     | 0.52              |
| 48:D1:45:ASN:ND2   | 48:D1:47:GLN:NE2   | 2.57                     | 0.52              |
| 50:D3:31:LEU:C     | 50:D3:33:GLN:H     | 2.18                     | 0.52              |
| 51:D4:20:ASN:ND2   | 51:D4:21:VAL:N     | 2.56                     | 0.52              |
| 1:AA:1503:A:HO2'   | 1:AA:1504:G:P      | 2.33                     | 0.52              |
| 3:AC:84:ILE:O      | 3:AC:88:ARG:HG3    | 2.10                     | 0.52              |
| 4:AD:20:TYR:HA     | 4:AD:26:CYS:SG     | 2.50                     | 0.52              |
| 4:AD:79:PHE:C      | 4:AD:79:PHE:CD2    | 2.88                     | 0.52              |
| 7:AG:155:ARG:O     | 7:AG:156:TRP:O     | 2.28                     | 0.52              |
| 11:AK:33:THR:CB    | 11:AK:38:ASN:O     | 2.54                     | 0.52              |
| 11:AK:44:SER:H     | 11:AK:47:VAL:HG23  | 1.74                     | 0.52              |
| 16:AP:21:VAL:CG1   | 16:AP:34:GLU:HB3   | 2.40                     | 0.52              |
| 20:AT:50:GLU:N     | 20:AT:100:ILE:HG12 | 2.25                     | 0.52              |
| 25:BA:29:U:H2'     | 25:BA:30:G:C8      | 2.45                     | 0.52              |
| 25:BA:1494:A:N3    | 25:BA:1494:A:H3'   | 2.25                     | 0.52              |
| 25:BA:1548:C:C4    | 25:BA:1549:C:N4    | 2.77                     | 0.52              |
| 25:BA:1929:G:C4'   | 25:BA:1930:G:OP1   | 2.48                     | 0.52              |
| 25:BA:2011:U:OP1   | 43:BW:42:ARG:NH1   | 2.43                     | 0.52              |
| 28:BD:33:LEU:HD12  | 28:BD:33:LEU:N     | 2.21                     | 0.52              |
| 31:BG:13:GLU:O     | 31:BG:13:GLU:HG3   | 2.10                     | 0.52              |
| 31:BG:138:GLN:OE1  | 31:BG:153:ARG:N    | 2.42                     | 0.52              |
| 31:BG:138:GLN:HB3  | 31:BG:153:ARG:O    | 2.10                     | 0.52              |
| 33:BI:77:LEU:CD1   | 33:BI:104:GLN:CD   | 2.83                     | 0.52              |
| 35:BO:93:PRO:HB3   | 35:BO:114:ILE:CD1  | 2.39                     | 0.52              |
| 36:BP:101:VAL:HG13 | 36:BP:102:ARG:N    | 2.25                     | 0.52              |
| 39:BS:16:ASN:O     | 39:BS:19:LYS:HB3   | 2.10                     | 0.52              |
| 42:BV:39:LEU:HB3   | 42:BV:40:LEU:HD23  | 1.91                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 43:BW:12:ILE:O    | 43:BW:12:ILE:HG23 | 2.10                     | 0.52              |
| 1:CA:977:A:H2'    | 1:CA:978:A:H5''   | 1.92                     | 0.52              |
| 1:CA:1063:C:N3    | 1:CA:1064:G:C6    | 2.78                     | 0.52              |
| 5:CE:51:VAL:O     | 5:CE:54:ALA:HB3   | 2.09                     | 0.52              |
| 7:CG:43:PHE:HD1   | 7:CG:43:PHE:O     | 1.92                     | 0.52              |
| 17:CQ:48:GLU:O    | 17:CQ:49:GLU:C    | 2.52                     | 0.52              |
| 18:CR:70:ILE:HG23 | 18:CR:79:LEU:HD12 | 1.91                     | 0.52              |
| 21:CU:24:ARG:O    | 21:CU:25:LYS:O    | 2.28                     | 0.52              |
| 25:DA:603:A:O2'   | 25:DA:604:G:O5'   | 2.21                     | 0.52              |
| 25:DA:605:C:H1'   | 25:DA:657:U:O2'   | 2.10                     | 0.52              |
| 25:DA:671:C:OP1   | 36:DP:42:SER:O    | 2.27                     | 0.52              |
| 25:DA:1754:C:P    | 40:DT:96:ARG:HH12 | 2.33                     | 0.52              |
| 25:DA:2055:C:OP1  | 52:D5:8:LYS:NZ    | 2.38                     | 0.52              |
| 25:DA:2611:U:O2'  | 52:D5:3:LYS:HE2   | 2.10                     | 0.52              |
| 27:DC:23:ASP:C    | 27:DC:25:ALA:H    | 2.17                     | 0.52              |
| 30:DF:89:VAL:HG12 | 30:DF:90:PHE:N    | 2.25                     | 0.52              |
| 32:DH:10:PRO:O    | 32:DH:11:VAL:CG1  | 2.56                     | 0.52              |
| 32:DH:161:GLY:O   | 32:DH:163:TYR:HD1 | 1.93                     | 0.52              |
| 34:DN:48:MET:HE3  | 34:DN:48:MET:H    | 1.75                     | 0.52              |
| 36:DP:79:ARG:CD   | 36:DP:109:GLY:O   | 2.57                     | 0.52              |
| 39:DS:7:TYR:CE2   | 39:DS:91:PRO:HG3  | 2.44                     | 0.52              |
| 39:DS:60:GLY:O    | 39:DS:61:ASN:CB   | 2.58                     | 0.52              |
| 40:DT:28:VAL:HG13 | 40:DT:46:GLU:CA   | 2.34                     | 0.52              |
| 41:DU:8:VAL:O     | 41:DU:9:VAL:C     | 2.52                     | 0.52              |
| 46:DZ:31:ARG:HB3  | 46:DZ:31:ARG:NH1  | 2.25                     | 0.52              |
| 49:D2:5:GLU:HB3   | 49:D2:9:GLN:HE22  | 1.75                     | 0.52              |
| 49:D2:14:ARG:HH11 | 49:D2:14:ARG:HG3  | 1.75                     | 0.52              |
| 1:AA:407:G:H1     | 1:AA:435:C:N4     | 2.04                     | 0.52              |
| 1:AA:1139:G:H5'   | 1:AA:1140:C:OP1   | 2.09                     | 0.52              |
| 1:AA:1329:A:H5'   | 13:AM:29:ARG:HE   | 1.74                     | 0.52              |
| 2:AB:25:ASN:OD1   | 2:AB:26:PRO:HD2   | 2.08                     | 0.52              |
| 2:AB:75:LYS:C     | 2:AB:75:LYS:CD    | 2.80                     | 0.52              |
| 2:AB:118:LEU:O    | 2:AB:122:PHE:N    | 2.37                     | 0.52              |
| 3:AC:182:ILE:CG1  | 3:AC:203:PHE:HD1  | 2.23                     | 0.52              |
| 6:AF:21:LEU:O     | 6:AF:23:LYS:N     | 2.42                     | 0.52              |
| 7:AG:72:ARG:HB3   | 7:AG:142:GLU:OE2  | 2.10                     | 0.52              |
| 10:AJ:24:VAL:HG12 | 10:AJ:24:VAL:O    | 2.09                     | 0.52              |
| 10:AJ:33:GLN:H    | 10:AJ:75:ILE:HD11 | 1.75                     | 0.52              |
| 13:AM:118:ALA:HB1 | 22:AV:29:C:O3'    | 2.09                     | 0.52              |
| 25:BA:72:U:H1'    | 49:B2:58:ALA:HA   | 1.91                     | 0.52              |
| 25:BA:196:A:N3    | 25:BA:196:A:C2'   | 2.73                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:BA:457:A:H1'    | 25:BA:459:U:C6     | 2.45                     | 0.52              |
| 25:BA:2089:U:H3    | 25:BA:2230:G:H1    | 1.58                     | 0.52              |
| 25:BA:2503:A:N3    | 25:BA:2503:A:C5'   | 2.73                     | 0.52              |
| 25:BA:2581:G:H5''  | 25:BA:2582:G:OP1   | 2.10                     | 0.52              |
| 25:BA:2823:A:OP1   | 29:BE:113:PHE:HB2  | 2.09                     | 0.52              |
| 26:BB:6:C:H4'      | 26:BB:28:C:H5'     | 1.91                     | 0.52              |
| 28:BD:63:ARG:HD3   | 28:BD:63:ARG:N     | 2.24                     | 0.52              |
| 30:BF:2:LYS:H      | 30:BF:2:LYS:CD     | 2.12                     | 0.52              |
| 30:BF:182:ASN:OD1  | 30:BF:185:ASP:N    | 2.42                     | 0.52              |
| 31:BG:39:ILE:HD12  | 31:BG:40:ASN:N     | 2.24                     | 0.52              |
| 32:BH:107:VAL:O    | 32:BH:109:PHE:CE1  | 2.63                     | 0.52              |
| 34:BN:40:PRO:HA    | 41:BU:64:ARG:HG2   | 1.92                     | 0.52              |
| 35:BO:119:PRO:O    | 40:BT:68:TYR:HE1   | 1.93                     | 0.52              |
| 36:BP:47:ASP:OD1   | 36:BP:49:ARG:HG3   | 2.09                     | 0.52              |
| 36:BP:79:ARG:NE    | 36:BP:109:GLY:HA3  | 2.25                     | 0.52              |
| 37:BQ:50:ALA:O     | 37:BQ:51:ARG:C     | 2.53                     | 0.52              |
| 42:BV:19:LYS:CD    | 42:BV:94:LEU:HB2   | 2.39                     | 0.52              |
| 43:BW:75:TYR:CD2   | 43:BW:75:TYR:C     | 2.87                     | 0.52              |
| 46:BZ:141:VAL:HA   | 46:BZ:144:LEU:HD23 | 1.91                     | 0.52              |
| 55:B8:23:VAL:CG1   | 55:B8:46:ARG:HD3   | 2.36                     | 0.52              |
| 1:CA:62:U:O2'      | 1:CA:379:C:O2      | 2.25                     | 0.52              |
| 1:CA:452:A:O2'     | 1:CA:453:A:O5'     | 2.27                     | 0.52              |
| 1:CA:1054:C:O2     | 1:CA:1054:C:H2'    | 2.09                     | 0.52              |
| 2:CB:7:VAL:C       | 2:CB:217:ARG:HH21  | 2.18                     | 0.52              |
| 2:CB:93:VAL:O      | 2:CB:93:VAL:HG23   | 2.10                     | 0.52              |
| 4:CD:13:ARG:O      | 4:CD:15:GLU:N      | 2.42                     | 0.52              |
| 5:CE:107:ARG:HG3   | 5:CE:111:GLU:HG3   | 1.92                     | 0.52              |
| 6:CF:100:ASN:O     | 6:CF:101:ALA:C     | 2.52                     | 0.52              |
| 17:CQ:70:ARG:O     | 17:CQ:71:PHE:HD2   | 1.93                     | 0.52              |
| 20:CT:104:LEU:HD23 | 20:CT:104:LEU:C    | 2.34                     | 0.52              |
| 22:CV:34:U:O2'     | 22:CV:36:A:N7      | 2.41                     | 0.52              |
| 22:CV:51:U:C4      | 22:CV:52:C:N4      | 2.78                     | 0.52              |
| 22:CV:64:G:C2'     | 22:CV:65:G:H5'     | 2.39                     | 0.52              |
| 25:DA:767:U:O5'    | 25:DA:767:U:H6     | 1.92                     | 0.52              |
| 25:DA:995:C:O2     | 25:DA:995:C:C2'    | 2.54                     | 0.52              |
| 25:DA:2576:G:O2'   | 25:DA:2579:C:OP2   | 2.24                     | 0.52              |
| 25:DA:2805:G:N2    | 25:DA:2893:G:O6    | 2.39                     | 0.52              |
| 26:DB:44:G:H1'     | 26:DB:47:C:H42     | 1.74                     | 0.52              |
| 28:DD:37:LEU:O     | 28:DD:38:LYS:C     | 2.50                     | 0.52              |
| 29:DE:81:ILE:O     | 29:DE:81:ILE:CG2   | 2.57                     | 0.52              |
| 31:DG:99:MET:HG3   | 31:DG:100:TRP:N    | 2.25                     | 0.52              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 31:DG:166:ASP:HA  | 31:DG:169:ALA:HB3  | 1.91                     | 0.52              |
| 32:DH:42:ARG:O    | 32:DH:42:ARG:HG3   | 2.09                     | 0.52              |
| 33:DI:110:ASP:HB2 | 33:DI:111:PRO:CA   | 2.40                     | 0.52              |
| 33:DI:112:LYS:O   | 33:DI:113:ARG:HB2  | 2.09                     | 0.52              |
| 34:DN:17:ASP:C    | 34:DN:19:GLU:H     | 2.18                     | 0.52              |
| 36:DP:31:ALA:C    | 36:DP:32:THR:HG23  | 2.35                     | 0.52              |
| 36:DP:52:GLU:CD   | 36:DP:55:ARG:NH2   | 2.66                     | 0.52              |
| 36:DP:108:LYS:C   | 36:DP:110:TYR:H    | 2.17                     | 0.52              |
| 36:DP:115:LEU:CD2 | 36:DP:131:SER:HB2  | 2.40                     | 0.52              |
| 37:DQ:141:GLN:HA  | 46:DZ:53:ILE:HG22  | 1.91                     | 0.52              |
| 38:DR:1:MET:O     | 38:DR:2:ARG:CB     | 2.57                     | 0.52              |
| 40:DT:32:TYR:CB   | 40:DT:81:PRO:HB3   | 2.30                     | 0.52              |
| 45:DY:47:LYS:HG2  | 45:DY:60:PHE:CD1   | 2.45                     | 0.52              |
| 45:DY:48:ALA:H    | 45:DY:60:PHE:HA    | 1.75                     | 0.52              |
| 46:DZ:22:GLY:HA2  | 46:DZ:41:LEU:CD1   | 2.39                     | 0.52              |
| 46:DZ:64:GLY:O    | 46:DZ:65:GLN:C     | 2.52                     | 0.52              |
| 49:D2:53:LEU:O    | 49:D2:56:GLN:HB2   | 2.10                     | 0.52              |
| 1:AA:327:A:N3     | 1:AA:329:A:C8      | 2.78                     | 0.52              |
| 1:AA:693:G:O2'    | 7:AG:82:GLY:HA3    | 2.09                     | 0.52              |
| 1:AA:913:A:O2'    | 1:AA:914:A:OP2     | 2.28                     | 0.52              |
| 1:AA:1054:C:N4    | 23:AY:34:G:N9      | 2.58                     | 0.52              |
| 1:AA:1510:U:H2'   | 1:AA:1511:G:C8     | 2.45                     | 0.52              |
| 6:AF:21:LEU:C     | 6:AF:23:LYS:N      | 2.67                     | 0.52              |
| 6:AF:44:GLY:HA2   | 6:AF:59:TYR:CZ     | 2.45                     | 0.52              |
| 11:AK:62:GLN:HG2  | 11:AK:63:LEU:N     | 2.25                     | 0.52              |
| 13:AM:91:ARG:NH1  | 13:AM:96:LEU:HD22  | 2.25                     | 0.52              |
| 18:AR:36:ASN:O    | 18:AR:39:VAL:HG23  | 2.10                     | 0.52              |
| 19:AS:12:ASP:HB3  | 19:AS:14:HIS:HE1   | 1.68                     | 0.52              |
| 20:AT:56:MET:CE   | 20:AT:85:MET:CE    | 2.87                     | 0.52              |
| 25:BA:243:U:OP2   | 55:B8:8:LYS:HE3    | 2.10                     | 0.52              |
| 25:BA:323:G:H3'   | 30:BF:169:ASN:HD21 | 1.75                     | 0.52              |
| 25:BA:890:A:C5    | 25:BA:892:G:N7     | 2.78                     | 0.52              |
| 25:BA:2119:A:N6   | 25:BA:2171:A:C6    | 2.77                     | 0.52              |
| 25:BA:2418:A:OP2  | 55:B8:29:LYS:CE    | 2.58                     | 0.52              |
| 25:BA:2468:G:H2'  | 25:BA:2476:A:C8    | 2.44                     | 0.52              |
| 26:BB:17:C:H2'    | 26:BB:18:G:O4'     | 2.09                     | 0.52              |
| 29:BE:23:VAL:HA   | 29:BE:184:VAL:O    | 2.09                     | 0.52              |
| 31:BG:39:ILE:HD12 | 31:BG:40:ASN:H     | 1.75                     | 0.52              |
| 31:BG:42:GLY:N    | 31:BG:43:LEU:HD13  | 2.25                     | 0.52              |
| 33:BI:77:LEU:HD12 | 33:BI:104:GLN:HE22 | 1.72                     | 0.52              |
| 33:BI:130:TYR:HB3 | 33:BI:136:VAL:HG13 | 1.92                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 34:BN:134:ARG:N    | 34:BN:135:PRO:CD   | 2.72                     | 0.52              |
| 36:BP:34:GLY:O     | 36:BP:35:HIS:O     | 2.27                     | 0.52              |
| 40:BT:27:THR:O     | 40:BT:88:ILE:HG12  | 2.10                     | 0.52              |
| 41:BU:6:THR:O      | 41:BU:9:VAL:HG23   | 2.10                     | 0.52              |
| 41:BU:12:ARG:HA    | 41:BU:15:LYS:CD    | 2.40                     | 0.52              |
| 45:BY:13:VAL:HB    | 45:BY:72:VAL:HG13  | 1.91                     | 0.52              |
| 50:B3:10:LYS:C     | 50:B3:31:LEU:HD21  | 2.35                     | 0.52              |
| 56:B9:7:VAL:HG13   | 56:B9:34:GLN:NE2   | 2.25                     | 0.52              |
| 1:CA:269:C:H2'     | 1:CA:270:A:C8      | 2.45                     | 0.52              |
| 1:CA:748:C:C4'     | 1:CA:749:C:O5'     | 2.57                     | 0.52              |
| 4:CD:11:LEU:C      | 4:CD:13:ARG:N      | 2.66                     | 0.52              |
| 8:CH:104:ARG:C     | 8:CH:106:GLY:N     | 2.67                     | 0.52              |
| 12:CL:64:TYR:O     | 12:CL:65:GLU:HB2   | 2.10                     | 0.52              |
| 18:CR:19:LYS:O     | 18:CR:20:ALA:HB3   | 2.09                     | 0.52              |
| 19:CS:6:LYS:CG     | 19:CS:7:LYS:HD3    | 2.36                     | 0.52              |
| 22:CV:30:G:C6      | 22:CV:43:G:N1      | 2.78                     | 0.52              |
| 23:CW:36:A:C2      | 23:CW:37:A:N3      | 2.78                     | 0.52              |
| 25:DA:372:G:OP1    | 48:D1:69:LYS:NZ    | 2.44                     | 0.52              |
| 25:DA:1615:C:C6    | 25:DA:1617:C:C4    | 2.98                     | 0.52              |
| 25:DA:1820:U:HO2'  | 25:DA:1821:A:P     | 2.33                     | 0.52              |
| 25:DA:1820:U:O2    | 28:DD:202:LYS:HB3  | 2.10                     | 0.52              |
| 27:DC:40:THR:HG21  | 27:DC:215:THR:CB   | 2.41                     | 0.52              |
| 32:DH:26:VAL:O     | 32:DH:27:LYS:O     | 2.28                     | 0.52              |
| 32:DH:143:GLN:HE22 | 32:DH:147:ASN:ND2  | 2.04                     | 0.52              |
| 37:DQ:115:MET:O    | 37:DQ:119:ARG:HB2  | 2.10                     | 0.52              |
| 38:DR:28:LEU:HA    | 38:DR:34:ILE:HG13  | 1.91                     | 0.52              |
| 38:DR:109:ALA:O    | 38:DR:111:LEU:HD22 | 2.09                     | 0.52              |
| 40:DT:68:TYR:N     | 40:DT:68:TYR:HD2   | 2.08                     | 0.52              |
| 43:DW:18:ARG:HG2   | 43:DW:76:VAL:HG12  | 1.92                     | 0.52              |
| 43:DW:46:PHE:O     | 43:DW:50:VAL:HG12  | 2.10                     | 0.52              |
| 47:D0:46:LYS:HB3   | 47:D0:47:PRO:HD2   | 1.91                     | 0.52              |
| 1:AA:251:G:C4'     | 1:AA:252:U:O5'     | 2.51                     | 0.51              |
| 2:AB:187:LEU:HD22  | 2:AB:187:LEU:C     | 2.35                     | 0.51              |
| 4:AD:15:GLU:HG2    | 4:AD:63:LYS:HG3    | 1.92                     | 0.51              |
| 4:AD:168:ARG:HH21  | 6:CF:18:GLN:NE2    | 2.09                     | 0.51              |
| 8:AH:48:TYR:HD1    | 8:AH:49:GLU:N      | 2.08                     | 0.51              |
| 11:AK:125:PHE:CD1  | 11:AK:125:PHE:N    | 2.75                     | 0.51              |
| 19:AS:6:LYS:CD     | 19:AS:7:LYS:CD     | 2.86                     | 0.51              |
| 23:AW:17:C:N4      | 25:BA:2181:G:H5'   | 2.19                     | 0.51              |
| 25:BA:1364:G:N7    | 48:B1:3:LYS:HE2    | 2.25                     | 0.51              |
| 25:BA:1542:A:O2'   | 25:BA:1543:C:O2    | 2.28                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:BA:2030:A:H5'   | 25:BA:2031:A:OP1   | 2.10                     | 0.51              |
| 25:BA:2712:U:O2'   | 25:BA:2712(A):A:P  | 2.68                     | 0.51              |
| 25:BA:2873:A:H1'   | 38:BR:6:SER:HB3    | 1.90                     | 0.51              |
| 28:BD:13:ARG:HG2   | 28:BD:13:ARG:O     | 2.10                     | 0.51              |
| 28:BD:73:VAL:C     | 28:BD:75:ILE:H     | 2.18                     | 0.51              |
| 31:BG:33:ARG:H     | 31:BG:162:THR:HG23 | 1.75                     | 0.51              |
| 31:BG:133:LEU:HD11 | 31:BG:157:ILE:HD11 | 1.92                     | 0.51              |
| 36:BP:31:ALA:C     | 36:BP:32:THR:HG23  | 2.35                     | 0.51              |
| 37:BQ:10:ARG:HH11  | 37:BQ:10:ARG:HG2   | 1.75                     | 0.51              |
| 37:BQ:16:ARG:HG2   | 37:BQ:18:LYS:HD3   | 1.90                     | 0.51              |
| 39:BS:101:LEU:HD22 | 39:BS:101:LEU:O    | 2.10                     | 0.51              |
| 40:BT:31:SER:O     | 40:BT:32:TYR:CB    | 2.58                     | 0.51              |
| 41:BU:113:ALA:C    | 41:BU:115:ALA:N    | 2.68                     | 0.51              |
| 45:BY:89:PHE:O     | 45:BY:90:LEU:HB3   | 2.10                     | 0.51              |
| 46:BZ:38:TYR:C     | 46:BZ:38:TYR:CD1   | 2.88                     | 0.51              |
| 46:BZ:111:VAL:O    | 46:BZ:111:VAL:HG13 | 2.09                     | 0.51              |
| 48:B1:29:GLY:O     | 48:B1:30:VAL:CG2   | 2.58                     | 0.51              |
| 1:CA:624:C:O3'     | 16:CP:10:GLY:HA2   | 2.10                     | 0.51              |
| 1:CA:950:U:O4'     | 1:CA:971:G:C6      | 2.63                     | 0.51              |
| 7:CG:121:ALA:O     | 7:CG:122:HIS:C     | 2.53                     | 0.51              |
| 11:CK:124:LYS:HD2  | 11:CK:125:PHE:HE1  | 1.75                     | 0.51              |
| 23:CW:16:U:C4      | 23:CW:18:G:H3'     | 2.44                     | 0.51              |
| 25:DA:247:G:H4'    | 25:DA:386:G:C5     | 2.45                     | 0.51              |
| 25:DA:674:G:H1'    | 30:DF:74:ARG:HD3   | 1.92                     | 0.51              |
| 25:DA:1049:C:H2'   | 25:DA:1050:A:H5''  | 1.92                     | 0.51              |
| 25:DA:1578:U:H2'   | 25:DA:1579:A:H5'   | 1.92                     | 0.51              |
| 25:DA:1786:A:O2'   | 25:DA:1938:A:N6    | 2.44                     | 0.51              |
| 25:DA:2562:U:H1'   | 35:DO:23:ARG:NH1   | 2.26                     | 0.51              |
| 27:DC:82:LYS:O     | 27:DC:83:ILE:HD13  | 2.10                     | 0.51              |
| 29:DE:101:ARG:HB2  | 29:DE:201:THR:HG22 | 1.92                     | 0.51              |
| 32:DH:25:LYS:HG2   | 32:DH:34:GLU:HG2   | 1.92                     | 0.51              |
| 32:DH:123:PHE:HE2  | 32:DH:133:VAL:HG22 | 1.75                     | 0.51              |
| 33:DI:114:LEU:O    | 33:DI:115:ALA:HB2  | 2.10                     | 0.51              |
| 34:DN:24:GLY:O     | 34:DN:28:THR:HB    | 2.09                     | 0.51              |
| 37:DQ:141:GLN:HA   | 46:DZ:53:ILE:CG2   | 2.41                     | 0.51              |
| 40:DT:40:THR:O     | 40:DT:41:ARG:CB    | 2.56                     | 0.51              |
| 1:AA:255:G:H1'     | 17:AQ:16:GLN:OE1   | 2.10                     | 0.51              |
| 15:AO:55:GLY:O     | 15:AO:58:MET:HB2   | 2.11                     | 0.51              |
| 19:AS:14:HIS:CD2   | 19:AS:15:LEU:CD2   | 2.93                     | 0.51              |
| 25:BA:396:G:O2'    | 48:B1:43:TYR:O     | 2.28                     | 0.51              |
| 25:BA:811:U:O4'    | 25:BA:1251:C:O4'   | 2.29                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:BA:1109:C:H3'   | 25:BA:1110:G:O4'   | 2.10                     | 0.51              |
| 25:BA:1452:A:N6    | 25:BA:2703:C:C5    | 2.78                     | 0.51              |
| 25:BA:1601:G:C5    | 25:BA:1602:U:C4    | 2.98                     | 0.51              |
| 25:BA:2073:C:H5''  | 28:BD:229:VAL:HG22 | 1.92                     | 0.51              |
| 25:BA:2562:U:H1'   | 35:BO:23:ARG:HH11  | 1.73                     | 0.51              |
| 25:BA:2691:C:N4    | 25:BA:2719:G:N2    | 2.58                     | 0.51              |
| 28:BD:253:GLN:HB2  | 28:BD:257:LEU:HB2  | 1.92                     | 0.51              |
| 30:BF:180:GLY:O    | 30:BF:182:ASN:ND2  | 2.43                     | 0.51              |
| 31:BG:43:LEU:HD23  | 31:BG:88:ILE:HD11  | 1.92                     | 0.51              |
| 34:BN:125:GLY:CA   | 34:BN:126:PRO:O    | 2.58                     | 0.51              |
| 38:BR:20:LEU:HD21  | 38:BR:40:LYS:HD3   | 1.92                     | 0.51              |
| 41:BU:14:HIS:NE2   | 41:BU:32:PHE:CD2   | 2.78                     | 0.51              |
| 41:BU:92:ARG:HH21  | 41:BU:94:ASN:CB    | 2.23                     | 0.51              |
| 42:BV:5:VAL:HG21   | 42:BV:35:LEU:HB3   | 1.92                     | 0.51              |
| 45:BY:20:TYR:HE1   | 45:BY:42:VAL:CA    | 2.23                     | 0.51              |
| 46:BZ:6:LYS:NZ     | 46:BZ:43:GLU:OE1   | 2.43                     | 0.51              |
| 47:B0:25:ARG:HD2   | 47:B0:29:GLN:HE22  | 1.75                     | 0.51              |
| 48:B1:45:ASN:ND2   | 48:B1:45:ASN:C     | 2.68                     | 0.51              |
| 55:B8:4:MET:SD     | 55:B8:61:LEU:HD22  | 2.50                     | 0.51              |
| 1:CA:411:A:N7      | 1:CA:429:U:O4      | 2.43                     | 0.51              |
| 2:CB:173:ALA:O     | 2:CB:176:GLU:N     | 2.44                     | 0.51              |
| 2:CB:213:LEU:HD23  | 2:CB:214:ILE:CG1   | 2.32                     | 0.51              |
| 3:CC:84:ILE:O      | 3:CC:84:ILE:HG12   | 2.09                     | 0.51              |
| 7:CG:76:ARG:O      | 7:CG:87:VAL:HB     | 2.10                     | 0.51              |
| 7:CG:107:ALA:CB    | 7:CG:134:ALA:HB2   | 2.40                     | 0.51              |
| 11:CK:41:THR:HG22  | 11:CK:42:TRP:N     | 2.26                     | 0.51              |
| 11:CK:114:VAL:HG22 | 11:CK:114:VAL:O    | 2.09                     | 0.51              |
| 20:CT:29:LYS:HD2   | 20:CT:66:ALA:CA    | 2.40                     | 0.51              |
| 20:CT:45:GLN:O     | 20:CT:47:GLY:N     | 2.42                     | 0.51              |
| 25:DA:464:U:H4'    | 54:D7:5:TRP:CZ3    | 2.45                     | 0.51              |
| 25:DA:775:G:H4'    | 25:DA:776:G:O5'    | 2.10                     | 0.51              |
| 25:DA:914:C:C2'    | 25:DA:915:C:O5'    | 2.58                     | 0.51              |
| 25:DA:1174:A:H5''  | 25:DA:1175:U:H5'   | 1.92                     | 0.51              |
| 25:DA:1287:A:N6    | 25:DA:1288:U:O4    | 2.43                     | 0.51              |
| 25:DA:2689:U:H4'   | 25:DA:2690:C:OP2   | 2.10                     | 0.51              |
| 25:DA:2808:U:H5'   | 25:DA:2891:G:O6    | 2.10                     | 0.51              |
| 27:DC:76:ALA:C     | 27:DC:78:ALA:N     | 2.69                     | 0.51              |
| 28:DD:70:TRP:CD1   | 28:DD:70:TRP:C     | 2.88                     | 0.51              |
| 28:DD:79:VAL:CG2   | 28:DD:111:LEU:HD11 | 2.39                     | 0.51              |
| 28:DD:106:ILE:HD11 | 28:DD:157:ARG:O    | 2.10                     | 0.51              |
| 29:DE:34:VAL:O     | 29:DE:35:GLN:CB    | 2.57                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 33:DI:110:ASP:HB3  | 33:DI:112:LYS:HG3  | 1.91                     | 0.51              |
| 39:DS:26:LEU:HG    | 39:DS:39:ILE:HD13  | 1.92                     | 0.51              |
| 46:DZ:48:PHE:O     | 46:DZ:49:ARG:C     | 2.53                     | 0.51              |
| 53:D6:25:LYS:HD3   | 55:D8:34:TRP:CZ2   | 2.46                     | 0.51              |
| 55:D8:50:LEU:CD1   | 55:D8:51:ALA:H     | 2.16                     | 0.51              |
| 1:AA:1299:A:N7     | 1:AA:1301:U:O2     | 2.43                     | 0.51              |
| 1:AA:1320:C:H42    | 19:AS:36:ARG:HG3   | 1.74                     | 0.51              |
| 1:AA:1435:G:H2'    | 1:AA:1436:U:C6     | 2.45                     | 0.51              |
| 2:AB:87:ARG:NH2    | 2:AB:233:SER:OG    | 2.43                     | 0.51              |
| 2:AB:171:ALA:HA    | 2:AB:174:VAL:HG23  | 1.91                     | 0.51              |
| 2:AB:180:LEU:O     | 2:AB:181:PHE:HB2   | 2.11                     | 0.51              |
| 3:AC:23:TYR:CD2    | 3:AC:23:TYR:C      | 2.88                     | 0.51              |
| 5:AE:80:ILE:HD11   | 5:AE:91:LEU:HD23   | 1.93                     | 0.51              |
| 5:AE:96:PRO:HA     | 5:AE:117:ASP:OD1   | 2.10                     | 0.51              |
| 6:AF:44:GLY:HA2    | 6:AF:59:TYR:CE2    | 2.46                     | 0.51              |
| 13:AM:13:LYS:HA    | 13:AM:44:ARG:NH1   | 2.26                     | 0.51              |
| 20:AT:44:ALA:HA    | 20:AT:92:LEU:CD2   | 2.40                     | 0.51              |
| 25:BA:749:C:HO2'   | 25:BA:1617:C:HO2'  | 1.57                     | 0.51              |
| 25:BA:2291:U:O2'   | 25:BA:2374:C:O2    | 2.26                     | 0.51              |
| 25:BA:2517:C:O2'   | 25:BA:2518:A:H8    | 1.94                     | 0.51              |
| 31:BG:161:THR:CG2  | 31:BG:162:THR:N    | 2.73                     | 0.51              |
| 32:BH:124:GLU:O    | 32:BH:131:VAL:HG13 | 2.11                     | 0.51              |
| 37:BQ:137:TYR:CZ   | 46:BZ:81:ARG:NH1   | 2.75                     | 0.51              |
| 42:BV:20:LEU:HB3   | 42:BV:21:ARG:HD3   | 1.92                     | 0.51              |
| 48:B1:3:LYS:CG     | 48:B1:4:VAL:N      | 2.73                     | 0.51              |
| 1:CA:490:G:H2'     | 1:CA:491:G:C8      | 2.45                     | 0.51              |
| 2:CB:36:ARG:HE     | 2:CB:36:ARG:N      | 2.09                     | 0.51              |
| 3:CC:140:ARG:CG    | 3:CC:140:ARG:NH1   | 2.71                     | 0.51              |
| 9:CI:91:ASP:C      | 9:CI:93:ARG:H      | 2.18                     | 0.51              |
| 10:CJ:47:PHE:CE2   | 14:CN:37:PHE:HE2   | 2.28                     | 0.51              |
| 11:CK:12:ARG:HD3   | 11:CK:13:GLN:N     | 2.25                     | 0.51              |
| 11:CK:21:ILE:HA    | 11:CK:30:VAL:HA    | 1.92                     | 0.51              |
| 11:CK:21:ILE:HG13  | 11:CK:30:VAL:CG1   | 2.40                     | 0.51              |
| 13:CM:115:LYS:O    | 13:CM:117:VAL:CG1  | 2.58                     | 0.51              |
| 14:CN:9:LYS:C      | 14:CN:11:LYS:N     | 2.67                     | 0.51              |
| 15:CO:33:THR:O     | 15:CO:34:LEU:C     | 2.53                     | 0.51              |
| 20:CT:96:GLY:O     | 20:CT:97:ALA:O     | 2.29                     | 0.51              |
| 25:DA:474:G:O2'    | 25:DA:475:U:OP1    | 2.25                     | 0.51              |
| 26:DB:12:C:N4      | 47:D0:75:LEU:HD12  | 2.24                     | 0.51              |
| 27:DC:169:GLY:O    | 27:DC:170:ALA:HB3  | 2.09                     | 0.51              |
| 30:DF:155:LEU:HD12 | 30:DF:174:VAL:O    | 2.10                     | 0.51              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 31:DG:41:GLN:HB3   | 31:DG:43:LEU:HD13 | 1.93                     | 0.51              |
| 33:DI:1:MET:HG3    | 33:DI:23:PRO:CB   | 2.41                     | 0.51              |
| 33:DI:127:VAL:HG13 | 33:DI:139:GLN:HB3 | 1.92                     | 0.51              |
| 34:DN:103:VAL:O    | 34:DN:106:MET:N   | 2.34                     | 0.51              |
| 36:DP:47:ASP:OD1   | 36:DP:49:ARG:HG3  | 2.09                     | 0.51              |
| 41:DU:97:ASP:O     | 41:DU:98:LEU:C    | 2.52                     | 0.51              |
| 46:DZ:57:ILE:CG2   | 46:DZ:58:VAL:N    | 2.74                     | 0.51              |
| 46:DZ:166:SER:CB   | 46:DZ:168:GLU:HB2 | 2.40                     | 0.51              |
| 48:D1:78:LYS:C     | 48:D1:80:LEU:H    | 2.17                     | 0.51              |
| 52:D5:45:VAL:HG13  | 52:D5:50:GLY:HA2  | 1.93                     | 0.51              |
| 1:AA:251:G:C2      | 1:AA:266:G:C6     | 2.98                     | 0.51              |
| 1:AA:585:G:H4'     | 12:AL:8:ASN:OD1   | 2.11                     | 0.51              |
| 1:AA:674:G:H2'     | 1:AA:675:A:H8     | 1.76                     | 0.51              |
| 5:AE:20:GLN:HG2    | 5:AE:21:ALA:N     | 2.23                     | 0.51              |
| 6:AF:97:PHE:HD2    | 18:AR:31:LEU:HD21 | 1.74                     | 0.51              |
| 7:AG:15:ASP:O      | 7:AG:19:GLY:N     | 2.43                     | 0.51              |
| 9:AI:36:TYR:CD2    | 9:AI:37:PHE:CE2   | 2.99                     | 0.51              |
| 9:AI:99:LEU:HD13   | 9:AI:99:LEU:O     | 2.10                     | 0.51              |
| 22:AV:57:C:O5'     | 22:AV:57:C:H6     | 1.93                     | 0.51              |
| 23:AW:35:A:H8      | 23:AW:35:A:O5'    | 1.93                     | 0.51              |
| 25:BA:74:A:H4'     | 25:BA:75:G:OP2    | 2.10                     | 0.51              |
| 25:BA:614:U:O2'    | 25:BA:614(C):A:C8 | 2.62                     | 0.51              |
| 25:BA:974:G:N1     | 25:BA:989:G:C4    | 2.78                     | 0.51              |
| 25:BA:1275:A:C4    | 38:BR:16:HIS:HD2  | 2.28                     | 0.51              |
| 25:BA:1453:U:C6    | 38:BR:63:ARG:HD3  | 2.46                     | 0.51              |
| 25:BA:1965:C:N3    | 25:BA:1966:A:N6   | 2.58                     | 0.51              |
| 25:BA:2365:G:H4'   | 47:B0:60:PHE:CZ   | 2.45                     | 0.51              |
| 27:BC:47:LEU:HD13  | 27:BC:207:THR:CB  | 2.40                     | 0.51              |
| 28:BD:156:ALA:C    | 28:BD:157:ARG:HG2 | 2.36                     | 0.51              |
| 30:BF:34:TRP:CE3   | 30:BF:35:GLU:HG2  | 2.45                     | 0.51              |
| 31:BG:44:GLY:HA2   | 31:BG:88:ILE:CG2  | 2.28                     | 0.51              |
| 33:BI:56:LYS:CG    | 33:BI:57:ARG:N    | 2.74                     | 0.51              |
| 34:BN:45:ASN:HD22  | 34:BN:45:ASN:C    | 2.19                     | 0.51              |
| 34:BN:97:ARG:O     | 34:BN:100:GLU:HB2 | 2.10                     | 0.51              |
| 35:BO:107:ARG:HD3  | 35:BO:112:MET:HE1 | 1.91                     | 0.51              |
| 37:BQ:134:ARG:C    | 37:BQ:137:TYR:CD2 | 2.88                     | 0.51              |
| 38:BR:9:LYS:C      | 38:BR:10:LEU:CG   | 2.68                     | 0.51              |
| 46:BZ:25:PRO:HA    | 46:BZ:38:TYR:HB2  | 1.93                     | 0.51              |
| 48:B1:58:ILE:HD11  | 48:B1:60:PHE:CE2  | 2.45                     | 0.51              |
| 49:B2:65:ASN:HB3   | 49:B2:69:ARG:HH22 | 1.74                     | 0.51              |
| 53:B6:28:ARG:HA    | 53:B6:32:ASN:CB   | 2.36                     | 0.51              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:CA:100:C:C2      | 1:CA:101:A:C5     | 2.98                     | 0.51              |
| 1:CA:667:G:H4'     | 15:CO:51:HIS:CE1  | 2.45                     | 0.51              |
| 1:CA:1085:U:H4'    | 1:CA:1086:U:OP1   | 2.10                     | 0.51              |
| 12:CL:8:ASN:OD1    | 17:CQ:34:LYS:HE2  | 2.11                     | 0.51              |
| 13:CM:14:ARG:CA    | 13:CM:44:ARG:HA   | 2.37                     | 0.51              |
| 13:CM:44:ARG:O     | 13:CM:46:LYS:N    | 2.42                     | 0.51              |
| 18:CR:40:LEU:C     | 18:CR:42:ARG:N    | 2.67                     | 0.51              |
| 18:CR:56:THR:OG1   | 18:CR:58:LEU:CD1  | 2.59                     | 0.51              |
| 20:CT:74:LYS:C     | 20:CT:76:ALA:N    | 2.69                     | 0.51              |
| 23:CW:9:A:O4'      | 23:CW:46:G:N2     | 2.43                     | 0.51              |
| 25:DA:1175:U:H4'   | 25:DA:1176:G:O5'  | 2.10                     | 0.51              |
| 25:DA:1418:G:OP1   | 25:DA:1588:C:O2'  | 2.29                     | 0.51              |
| 25:DA:2610:C:H4'   | 25:DA:2611:U:OP2  | 2.09                     | 0.51              |
| 26:DB:48:A:H4'     | 39:DS:95:HIS:CD2  | 2.46                     | 0.51              |
| 29:DE:52:LEU:HD23  | 29:DE:76:ARG:HB2  | 1.92                     | 0.51              |
| 29:DE:174:ASP:O    | 29:DE:183:LEU:HB2 | 2.11                     | 0.51              |
| 30:DF:118:ALA:HA   | 30:DF:123:LEU:HB3 | 1.92                     | 0.51              |
| 32:DH:109:PHE:HB2  | 32:DH:111:HIS:O   | 2.10                     | 0.51              |
| 33:DI:31:LEU:HB2   | 33:DI:32:PRO:HD3  | 1.93                     | 0.51              |
| 36:DP:101:VAL:HG23 | 36:DP:107:LYS:H   | 1.76                     | 0.51              |
| 41:DU:11:ARG:O     | 41:DU:11:ARG:HG2  | 2.10                     | 0.51              |
| 52:D5:36:CYS:SG    | 52:D5:37:LYS:N    | 2.83                     | 0.51              |
| 55:D8:49:VAL:C     | 55:D8:53:PRO:HG3  | 2.34                     | 0.51              |
| 56:D9:14:CYS:SG    | 56:D9:25:VAL:HG13 | 2.50                     | 0.51              |
| 1:AA:473:G:H5''    | 16:AP:81:ARG:HH21 | 1.75                     | 0.51              |
| 1:AA:532:A:H2'     | 1:AA:533:A:OP1    | 2.10                     | 0.51              |
| 1:AA:1402:C:H2'    | 1:AA:1403:C:O4'   | 2.10                     | 0.51              |
| 2:AB:178:ARG:HH22  | 2:AB:196:LEU:HA   | 1.75                     | 0.51              |
| 3:AC:50:ALA:HB2    | 3:AC:75:VAL:HB    | 1.92                     | 0.51              |
| 3:AC:79:ARG:HH22   | 11:CK:100:ALA:HB2 | 1.76                     | 0.51              |
| 3:AC:91:LEU:C      | 3:AC:99:VAL:HG11  | 2.36                     | 0.51              |
| 4:AD:170:VAL:HG12  | 4:AD:174:LEU:HB2  | 1.93                     | 0.51              |
| 4:AD:177:ASP:O     | 4:AD:179:GLU:N    | 2.43                     | 0.51              |
| 16:AP:19:ILE:HG22  | 16:AP:36:ILE:CG1  | 2.40                     | 0.51              |
| 22:AV:40:C:H2'     | 22:AV:41:C:C6     | 2.45                     | 0.51              |
| 22:AV:74:A:O3'     | 22:AV:75:C:H6     | 1.93                     | 0.51              |
| 24:AX:13:A:H3'     | 24:AX:14:A:C5'    | 2.40                     | 0.51              |
| 25:BA:404:C:H1'    | 25:BA:406:G:C8    | 2.45                     | 0.51              |
| 25:BA:1495:A:H2'   | 25:BA:1495:A:N3   | 2.26                     | 0.51              |
| 25:BA:2107:C:H42   | 25:BA:2182:G:H1   | 1.57                     | 0.51              |
| 25:BA:2458:G:C1'   | 25:BA:2490:G:H1   | 2.24                     | 0.51              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 29:BE:134:ILE:N    | 29:BE:134:ILE:CD1 | 2.68                     | 0.51              |
| 30:BF:32:LEU:C     | 30:BF:32:LEU:CD2  | 2.83                     | 0.51              |
| 32:BH:107:VAL:HG22 | 32:BH:109:PHE:CE2 | 2.46                     | 0.51              |
| 34:BN:19:GLU:HG3   | 34:BN:20:GLY:N    | 2.26                     | 0.51              |
| 35:BO:61:VAL:HG12  | 35:BO:87:ILE:HD11 | 1.92                     | 0.51              |
| 36:BP:115:LEU:CD2  | 36:BP:131:SER:HB2 | 2.40                     | 0.51              |
| 41:BU:8:VAL:O      | 41:BU:9:VAL:C     | 2.52                     | 0.51              |
| 42:BV:20:LEU:CA    | 42:BV:21:ARG:HD3  | 2.41                     | 0.51              |
| 43:BW:75:TYR:CE2   | 43:BW:104:THR:HB  | 2.45                     | 0.51              |
| 44:BX:43:VAL:HG11  | 44:BX:81:VAL:HG11 | 1.92                     | 0.51              |
| 48:B1:6:GLU:HG3    | 48:B1:61:ARG:O    | 2.10                     | 0.51              |
| 49:B2:48:HIS:O     | 49:B2:50:ILE:N    | 2.43                     | 0.51              |
| 1:CA:511:C:N3      | 1:CA:512:U:C4     | 2.79                     | 0.51              |
| 1:CA:890:G:HO2'    | 1:CA:906:G:H1     | 1.58                     | 0.51              |
| 2:CB:86:GLU:C      | 2:CB:88:ALA:N     | 2.68                     | 0.51              |
| 4:CD:53:ASP:O      | 4:CD:57:ARG:HG3   | 2.10                     | 0.51              |
| 5:CE:59:GLY:O      | 5:CE:60:TYR:C     | 2.52                     | 0.51              |
| 5:CE:146:ALA:HB1   | 5:CE:150:ARG:NH2  | 2.24                     | 0.51              |
| 7:CG:32:ARG:O      | 7:CG:33:ASP:HB2   | 2.09                     | 0.51              |
| 7:CG:150:ALA:O     | 11:CK:57:THR:CG2  | 2.59                     | 0.51              |
| 10:CJ:40:LEU:CG    | 10:CJ:69:ASN:HB3  | 2.37                     | 0.51              |
| 14:CN:13:THR:N     | 14:CN:14:PRO:CD   | 2.69                     | 0.51              |
| 14:CN:51:GLY:C     | 14:CN:53:LEU:H    | 2.18                     | 0.51              |
| 25:DA:270:A:N1     | 25:DA:366:C:O2'   | 2.42                     | 0.51              |
| 25:DA:663:G:H5''   | 36:DP:18:ARG:HG3  | 1.92                     | 0.51              |
| 25:DA:818:G:N1     | 25:DA:1188:U:OP2  | 2.35                     | 0.51              |
| 25:DA:1799:G:O4'   | 25:DA:1800:C:H6   | 1.94                     | 0.51              |
| 25:DA:1899:G:N2    | 25:DA:1902:C:N4   | 2.58                     | 0.51              |
| 29:DE:118:LYS:H    | 29:DE:121:ASN:H   | 1.57                     | 0.51              |
| 30:DF:204:ASN:C    | 30:DF:206:ILE:N   | 2.67                     | 0.51              |
| 31:DG:13:GLU:O     | 31:DG:14:GLU:CB   | 2.58                     | 0.51              |
| 31:DG:28:VAL:O     | 31:DG:31:VAL:HG12 | 2.11                     | 0.51              |
| 34:DN:17:ASP:HB2   | 34:DN:55:VAL:HG12 | 1.91                     | 0.51              |
| 34:DN:42:TRP:CE3   | 34:DN:48:MET:HE1  | 2.46                     | 0.51              |
| 34:DN:56:ASN:HA    | 34:DN:125:GLY:N   | 2.04                     | 0.51              |
| 38:DR:50:HIS:O     | 38:DR:54:LEU:HB2  | 2.11                     | 0.51              |
| 44:DX:57:LEU:N     | 44:DX:57:LEU:HD13 | 2.26                     | 0.51              |
| 45:DY:96:ILE:HD11  | 45:DY:99:CYS:SG   | 2.51                     | 0.51              |
| 46:DZ:89:PHE:CE1   | 46:DZ:96:VAL:HG21 | 2.45                     | 0.51              |
| 2:AB:77:ALA:O      | 2:AB:80:ILE:CG2   | 2.48                     | 0.51              |
| 2:AB:190:THR:C     | 2:AB:192:SER:H    | 2.19                     | 0.51              |

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| Atom-1               | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|--------------------|--------------------------|-------------------|
| 3:AC:58:GLU:H        | 3:AC:65:ALA:CB     | 2.19                     | 0.51              |
| 3:AC:113:ALA:C       | 3:AC:115:LEU:N     | 2.66                     | 0.51              |
| 3:AC:182:ILE:HG23    | 3:AC:202:ILE:C     | 2.36                     | 0.51              |
| 5:AE:39:GLY:HA2      | 5:AE:71:LEU:HD12   | 1.92                     | 0.51              |
| 10:AJ:45:ARG:HG3     | 10:AJ:45:ARG:HH11  | 1.74                     | 0.51              |
| 25:BA:390:A:O2'      | 25:BA:391:G:N7     | 2.41                     | 0.51              |
| 25:BA:964:C:O2'      | 25:BA:2273:A:N3    | 2.40                     | 0.51              |
| 25:BA:1266:G:O2'     | 25:BA:1267:U:OP2   | 2.27                     | 0.51              |
| 25:BA:2421:G:OP2     | 55:B8:31:HIS:HE1   | 1.94                     | 0.51              |
| 25:BA:2458:G:H4'     | 25:BA:2459:A:C8    | 2.45                     | 0.51              |
| 25:BA:2563:U:H2'     | 25:BA:2565:A:OP2   | 2.11                     | 0.51              |
| 25:BA:2712(A):A:H5'' | 25:BA:2713:A:OP2   | 2.11                     | 0.51              |
| 26:BB:66:A:N1        | 26:BB:108:U:C2     | 2.78                     | 0.51              |
| 29:BE:47:VAL:HG21    | 29:BE:86:PRO:CD    | 2.36                     | 0.51              |
| 29:BE:64:LYS:C       | 29:BE:66:HIS:N     | 2.65                     | 0.51              |
| 30:BF:155:LEU:HD22   | 30:BF:186:ILE:HD13 | 1.93                     | 0.51              |
| 31:BG:181:ARG:O      | 31:BG:182:LYS:C    | 2.53                     | 0.51              |
| 32:BH:100:GLY:C      | 32:BH:102:ALA:H    | 2.17                     | 0.51              |
| 36:BP:86:LYS:CG      | 36:BP:87:ASP:N     | 2.74                     | 0.51              |
| 37:BQ:79:LEU:HD23    | 37:BQ:80:GLU:H     | 1.76                     | 0.51              |
| 41:BU:91:ASP:C       | 41:BU:93:LYS:N     | 2.66                     | 0.51              |
| 44:BX:44:GLU:HG2     | 44:BX:49:VAL:O     | 2.11                     | 0.51              |
| 49:B2:19:VAL:O       | 49:B2:20:GLU:C     | 2.53                     | 0.51              |
| 1:CA:1226:C:C4       | 13:CM:104:ARG:HB2  | 2.44                     | 0.51              |
| 1:CA:1423:G:H5'      | 35:DO:49:ARG:HH22  | 1.74                     | 0.51              |
| 2:CB:77:ALA:HB2      | 2:CB:211:ILE:CD1   | 2.39                     | 0.51              |
| 2:CB:166:ASP:C       | 2:CB:166:ASP:OD2   | 2.53                     | 0.51              |
| 9:CI:19:LEU:HD21     | 9:CI:61:ALA:HB2    | 1.93                     | 0.51              |
| 25:DA:444:C:H4'      | 30:DF:49:ALA:HB2   | 1.91                     | 0.51              |
| 25:DA:559:G:H22      | 41:DU:49:HIS:CD2   | 2.27                     | 0.51              |
| 25:DA:1416:G:O2'     | 25:DA:1417:C:O5'   | 2.27                     | 0.51              |
| 25:DA:2679:A:H4'     | 29:DE:165:VAL:HG11 | 1.92                     | 0.51              |
| 29:DE:116:VAL:HG21   | 29:DE:122:PHE:CG   | 2.46                     | 0.51              |
| 30:DF:107:LYS:HD2    | 30:DF:206:ILE:CD1  | 2.29                     | 0.51              |
| 31:DG:51:ARG:HH11    | 31:DG:51:ARG:HB3   | 1.74                     | 0.51              |
| 31:DG:55:LYS:HZ2     | 31:DG:148:MET:HG3  | 1.73                     | 0.51              |
| 32:DH:22:GLY:O       | 32:DH:37:VAL:HB    | 2.10                     | 0.51              |
| 33:DI:127:VAL:HG22   | 33:DI:139:GLN:HB3  | 1.93                     | 0.51              |
| 35:DO:105:GLU:HA     | 35:DO:108:GLU:CD   | 2.35                     | 0.51              |
| 38:DR:75:LEU:HD13    | 38:DR:75:LEU:O     | 2.11                     | 0.51              |
| 39:DS:48:LEU:HD23    | 39:DS:82:ILE:HD11  | 1.91                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 40:DT:92:GLY:C    | 40:DT:94:ALA:N    | 2.63                     | 0.51              |
| 43:DW:60:ASN:C    | 43:DW:61:ASN:HD22 | 2.18                     | 0.51              |
| 49:D2:35:LEU:HB3  | 49:D2:50:ILE:CD1  | 2.41                     | 0.51              |
| 1:AA:103:C:O2'    | 1:AA:172:A:N1     | 2.38                     | 0.51              |
| 1:AA:243:A:H61    | 1:AA:281:G:H1'    | 1.75                     | 0.51              |
| 1:AA:1014:A:C2    | 1:AA:1219:U:H1'   | 2.46                     | 0.51              |
| 1:AA:1277:C:H2'   | 1:AA:1278:U:H5'   | 1.91                     | 0.51              |
| 2:AB:121:LEU:HA   | 2:AB:126:GLU:OE1  | 2.11                     | 0.51              |
| 9:AI:14:VAL:HG12  | 9:AI:15:ALA:N     | 2.25                     | 0.51              |
| 10:AJ:32:ALA:HB3  | 10:AJ:75:ILE:HG13 | 1.93                     | 0.51              |
| 16:AP:74:LEU:O    | 16:AP:79:VAL:HG23 | 2.11                     | 0.51              |
| 17:AQ:53:LEU:HG   | 17:AQ:82:MET:CE   | 2.41                     | 0.51              |
| 25:BA:800:A:H1'   | 25:BA:802:A:OP2   | 2.11                     | 0.51              |
| 25:BA:1320:C:O2   | 25:BA:1322:A:N6   | 2.42                     | 0.51              |
| 25:BA:1418:G:OP1  | 25:BA:1588:C:O2'  | 2.29                     | 0.51              |
| 26:BB:15:A:H1'    | 26:BB:110:G:C5    | 2.46                     | 0.51              |
| 26:BB:75:G:H5''   | 46:BZ:36:LYS:HE2  | 1.92                     | 0.51              |
| 30:BF:18:ARG:O    | 30:BF:19:GLU:HB3  | 2.09                     | 0.51              |
| 31:BG:70:VAL:HG23 | 31:BG:70:VAL:O    | 2.11                     | 0.51              |
| 34:BN:123:TYR:OH  | 34:BN:130:HIS:NE2 | 2.36                     | 0.51              |
| 35:BO:48:PRO:CB   | 35:BO:49:ARG:HH11 | 2.24                     | 0.51              |
| 38:BR:103:ARG:HD2 | 43:BW:40:ASN:CG   | 2.36                     | 0.51              |
| 43:BW:51:LEU:HD13 | 43:BW:52:GLU:CA   | 2.40                     | 0.51              |
| 45:BY:96:ILE:HG22 | 45:BY:97:ARG:H    | 1.75                     | 0.51              |
| 45:BY:97:ARG:HE   | 45:BY:98:VAL:HG23 | 1.75                     | 0.51              |
| 46:BZ:10:ARG:HD2  | 46:BZ:36:LYS:HB3  | 1.92                     | 0.51              |
| 46:BZ:54:HIS:HB3  | 46:BZ:101:PRO:HD3 | 1.93                     | 0.51              |
| 46:BZ:63:ASP:O    | 46:BZ:65:GLN:N    | 2.43                     | 0.51              |
| 49:B2:38:GLN:HB3  | 49:B2:44:LEU:O    | 2.10                     | 0.51              |
| 52:B5:56:LYS:HD2  | 52:B5:56:LYS:N    | 2.23                     | 0.51              |
| 1:CA:486:U:H2'    | 1:CA:487:A:H8     | 1.76                     | 0.51              |
| 1:CA:986:A:H1'    | 19:CS:55:LYS:HA   | 1.92                     | 0.51              |
| 1:CA:1452:C:H2'   | 1:CA:1456:G:OP2   | 2.10                     | 0.51              |
| 2:CB:83:MET:HE2   | 2:CB:83:MET:HA    | 1.91                     | 0.51              |
| 7:CG:43:PHE:C     | 7:CG:43:PHE:CD1   | 2.87                     | 0.51              |
| 13:CM:92:HIS:HD2  | 13:CM:110:ARG:NH2 | 2.09                     | 0.51              |
| 22:CV:20:G:C2     | 22:CV:58:A:C2     | 2.99                     | 0.51              |
| 25:DA:888:C:C5'   | 25:DA:889:C:OP2   | 2.52                     | 0.51              |
| 25:DA:2468:G:OP1  | 37:DQ:119:ARG:NH2 | 2.42                     | 0.51              |
| 25:DA:2572:A:OP1  | 29:DE:144:ARG:HB2 | 2.10                     | 0.51              |
| 29:DE:105:THR:OG1 | 29:DE:199:ARG:NH2 | 2.44                     | 0.51              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 30:DF:196:LEU:O    | 30:DF:200:GLU:HG2 | 2.10                     | 0.51              |
| 31:DG:7:LEU:N      | 31:DG:104:GLU:OE2 | 2.33                     | 0.51              |
| 33:DI:120:ILE:HD12 | 33:DI:121:LYS:N   | 2.26                     | 0.51              |
| 40:DT:7:ILE:O      | 40:DT:11:GLU:OE1  | 2.29                     | 0.51              |
| 40:DT:118:ARG:O    | 40:DT:119:LYS:C   | 2.54                     | 0.51              |
| 42:DV:1:MET:HE2    | 42:DV:43:GLU:HB2  | 1.93                     | 0.51              |
| 45:DY:94:LYS:NZ    | 45:DY:101:LYS:NZ  | 2.59                     | 0.51              |
| 48:D1:58:ILE:HG13  | 48:D1:91:LYS:HB2  | 1.92                     | 0.51              |
| 1:AA:251:G:H1'     | 1:AA:252:U:C6     | 2.46                     | 0.51              |
| 1:AA:1139:G:H1'    | 1:AA:1141:C:H41   | 1.76                     | 0.51              |
| 3:AC:14:ILE:CG1    | 3:AC:15:THR:H     | 2.18                     | 0.51              |
| 4:AD:148:VAL:CG1   | 4:AD:149:ALA:N    | 2.74                     | 0.51              |
| 10:AJ:33:GLN:HB2   | 10:AJ:75:ILE:CD1  | 2.41                     | 0.51              |
| 10:AJ:64:GLU:O     | 14:AN:56:VAL:HA   | 2.11                     | 0.51              |
| 19:AS:16:LEU:O     | 19:AS:20:LEU:HG   | 2.10                     | 0.51              |
| 25:BA:1666:G:C3'   | 25:BA:1667:G:H5'  | 2.40                     | 0.51              |
| 29:BE:71:GLY:O     | 29:BE:73:GLU:N    | 2.44                     | 0.51              |
| 31:BG:34:LEU:O     | 31:BG:99:MET:HE1  | 2.10                     | 0.51              |
| 32:BH:156:ALA:CB   | 32:BH:159:GLU:HB3 | 2.40                     | 0.51              |
| 34:BN:2:LYS:CB     | 34:BN:4:TYR:CE2   | 2.94                     | 0.51              |
| 34:BN:45:ASN:ND2   | 34:BN:45:ASN:C    | 2.69                     | 0.51              |
| 34:BN:104:LYS:HB2  | 34:BN:117:PHE:CE1 | 2.46                     | 0.51              |
| 36:BP:62:LEU:HD23  | 36:BP:62:LEU:H    | 1.76                     | 0.51              |
| 37:BQ:10:ARG:HG2   | 37:BQ:10:ARG:NH1  | 2.25                     | 0.51              |
| 38:BR:28:LEU:O     | 38:BR:28:LEU:HD22 | 2.11                     | 0.51              |
| 42:BV:82:ARG:NH1   | 42:BV:82:ARG:CG   | 2.72                     | 0.51              |
| 43:BW:1:MET:HG3    | 43:BW:2:GLU:N     | 2.26                     | 0.51              |
| 45:BY:27:VAL:HG12  | 45:BY:29:GLU:N    | 2.25                     | 0.51              |
| 46:BZ:126:VAL:HA   | 46:BZ:164:ALA:CB  | 2.41                     | 0.51              |
| 47:B0:49:LYS:HB2   | 47:B0:80:HIS:HB3  | 1.93                     | 0.51              |
| 50:B3:8:LEU:HD23   | 50:B3:53:LEU:O    | 2.10                     | 0.51              |
| 52:B5:41:PRO:CG    | 52:B5:44:THR:HG21 | 2.37                     | 0.51              |
| 55:B8:52:LYS:N     | 55:B8:53:PRO:HD2  | 2.25                     | 0.51              |
| 1:CA:128:G:H22     | 1:CA:130:A:H62    | 1.59                     | 0.51              |
| 1:CA:376:G:OP1     | 16:CP:67:THR:HG21 | 2.11                     | 0.51              |
| 1:CA:1422:G:H5''   | 35:DO:48:PRO:HB3  | 1.92                     | 0.51              |
| 1:CA:1492:A:N6     | 1:CA:1493:A:N6    | 2.59                     | 0.51              |
| 2:CB:13:ALA:O      | 2:CB:14:GLY:C     | 2.54                     | 0.51              |
| 4:CD:141:ARG:O     | 4:CD:142:PRO:C    | 2.54                     | 0.51              |
| 4:CD:172:PRO:HB2   | 4:CD:187:ARG:NH2  | 2.26                     | 0.51              |
| 6:CF:25:ILE:HD13   | 6:CF:25:ILE:N     | 2.25                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:CH:19:VAL:O      | 8:CH:19:VAL:HG23   | 2.11                     | 0.51              |
| 13:CM:48:LEU:O     | 13:CM:49:THR:C     | 2.54                     | 0.51              |
| 17:CQ:53:LEU:HG    | 17:CQ:82:MET:HE1   | 1.93                     | 0.51              |
| 22:CV:35:C:C2'     | 22:CV:36:A:O5'     | 2.59                     | 0.51              |
| 23:CW:8:U:O2'      | 23:CW:21:A:N1      | 2.44                     | 0.51              |
| 25:DA:372:G:O2'    | 25:DA:400:G:N1     | 2.43                     | 0.51              |
| 25:DA:534:U:H5'    | 41:DU:42:ALA:HB1   | 1.92                     | 0.51              |
| 25:DA:871:U:H4'    | 37:DQ:69:PHE:CE2   | 2.45                     | 0.51              |
| 25:DA:1231:G:H2'   | 25:DA:1232:G:C8    | 2.46                     | 0.51              |
| 28:DD:181:GLU:OE2  | 28:DD:270:ILE:HG22 | 2.10                     | 0.51              |
| 34:DN:1:MET:HG2    | 34:DN:2:LYS:H      | 1.75                     | 0.51              |
| 34:DN:25:ARG:NH1   | 34:DN:25:ARG:CG    | 2.73                     | 0.51              |
| 35:DO:24:VAL:CG2   | 35:DO:33:ALA:HB2   | 2.40                     | 0.51              |
| 40:DT:62:THR:HG22  | 40:DT:75:ILE:HG12  | 1.92                     | 0.51              |
| 40:DT:81:PRO:O     | 40:DT:82:LEU:CB    | 2.59                     | 0.51              |
| 41:DU:115:ALA:C    | 41:DU:117:GLN:H    | 2.18                     | 0.51              |
| 45:DY:86:ARG:O     | 45:DY:92:ASN:HA    | 2.11                     | 0.51              |
| 1:AA:501:C:O2      | 1:AA:549:C:O2'     | 2.25                     | 0.51              |
| 1:AA:530:G:O6      | 24:AX:21:C:H1'     | 2.11                     | 0.51              |
| 1:AA:960:U:O2'     | 1:AA:1223:C:H5'    | 2.11                     | 0.51              |
| 1:AA:1032:G:H2'    | 1:AA:1033:G:C8     | 2.46                     | 0.51              |
| 1:AA:1151:A:H2'    | 1:AA:1152:A:C8     | 2.45                     | 0.51              |
| 3:AC:92:ALA:HB2    | 3:AC:99:VAL:CG1    | 2.41                     | 0.51              |
| 3:AC:139:GLN:OE1   | 3:AC:139:GLN:HA    | 2.10                     | 0.51              |
| 8:AH:39:LEU:HD22   | 8:AH:39:LEU:H      | 1.76                     | 0.51              |
| 9:AI:5:TYR:CE2     | 9:AI:16:ARG:HB3    | 2.46                     | 0.51              |
| 10:AJ:47:PHE:CZ    | 14:AN:37:PHE:HE2   | 2.28                     | 0.51              |
| 10:AJ:61:GLU:HG3   | 14:AN:58:LYS:HZ3   | 1.74                     | 0.51              |
| 12:AL:22:SER:O     | 12:AL:24:VAL:N     | 2.44                     | 0.51              |
| 14:AN:3:ARG:HG2    | 14:AN:3:ARG:O      | 2.10                     | 0.51              |
| 25:BA:459:U:H4'    | 54:B7:40:TRP:CZ3   | 2.45                     | 0.51              |
| 25:BA:2611:U:O2    | 52:B5:3:LYS:HE3    | 2.11                     | 0.51              |
| 28:BD:118:VAL:CG2  | 28:BD:119:ALA:N    | 2.74                     | 0.51              |
| 28:BD:145:VAL:HG12 | 28:BD:146:GLU:O    | 2.11                     | 0.51              |
| 30:BF:152:GLU:O    | 30:BF:154:VAL:HG23 | 2.11                     | 0.51              |
| 43:BW:20:VAL:O     | 43:BW:23:LEU:N     | 2.37                     | 0.51              |
| 47:B0:48:GLY:HA3   | 47:B0:80:HIS:ND1   | 2.25                     | 0.51              |
| 1:CA:129(A):G:H1'  | 1:CA:189(G):G:H5'' | 1.93                     | 0.51              |
| 1:CA:736:C:H2'     | 1:CA:737:A:C8      | 2.46                     | 0.51              |
| 1:CA:797:C:OP1     | 11:CK:124:LYS:HE2  | 2.11                     | 0.51              |
| 1:CA:913:A:HO2'    | 1:CA:914:A:P       | 2.34                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 5:CE:120:THR:HG22  | 5:CE:121:LYS:N     | 2.26                     | 0.51              |
| 7:CG:75:VAL:HG23   | 7:CG:75:VAL:O      | 2.11                     | 0.51              |
| 7:CG:102:ARG:O     | 7:CG:106:GLN:HG3   | 2.11                     | 0.51              |
| 7:CG:113:GLU:HG2   | 7:CG:119:ARG:HG2   | 1.93                     | 0.51              |
| 8:CH:91:ARG:HG2    | 8:CH:91:ARG:NH1    | 2.02                     | 0.51              |
| 13:CM:65:LYS:HB2   | 13:CM:69:GLU:HB3   | 1.93                     | 0.51              |
| 18:CR:66:LEU:O     | 18:CR:70:ILE:HG12  | 2.11                     | 0.51              |
| 25:DA:620:G:H4'    | 25:DA:621:A:C5'    | 2.40                     | 0.51              |
| 25:DA:816:C:O2'    | 25:DA:932:G:O6     | 2.22                     | 0.51              |
| 25:DA:2051:A:N6    | 25:DA:2614:A:C8    | 2.79                     | 0.51              |
| 28:DD:71:ASP:CB    | 28:DD:103:ARG:HH22 | 2.23                     | 0.51              |
| 28:DD:83:GLU:HB2   | 28:DD:92:ILE:HD11  | 1.91                     | 0.51              |
| 29:DE:77:ILE:HG22  | 29:DE:78:LEU:HG    | 1.93                     | 0.51              |
| 32:DH:12:PRO:O     | 32:DH:13:LYS:HB2   | 2.10                     | 0.51              |
| 32:DH:16:SER:O     | 32:DH:17:VAL:CB    | 2.59                     | 0.51              |
| 37:DQ:141:GLN:NE2  | 46:DZ:72:ARG:HA    | 2.25                     | 0.51              |
| 40:DT:33:LYS:CE    | 40:DT:43:GLN:OE1   | 2.57                     | 0.51              |
| 41:DU:76:TYR:O     | 41:DU:78:THR:N     | 2.44                     | 0.51              |
| 43:DW:14:PRO:O     | 43:DW:17:VAL:N     | 2.43                     | 0.51              |
| 43:DW:43:GLY:O     | 43:DW:44:ALA:C     | 2.54                     | 0.51              |
| 53:D6:26:ASN:O     | 53:D6:27:LYS:HG2   | 2.11                     | 0.51              |
| 55:D8:50:LEU:HD12  | 55:D8:54:GLU:OE2   | 2.11                     | 0.51              |
| 1:AA:250:A:O2'     | 1:AA:251:G:P       | 2.69                     | 0.51              |
| 1:AA:1281:U:C4'    | 1:AA:1282:C:OP1    | 2.55                     | 0.51              |
| 4:AD:118:ARG:O     | 4:AD:119:GLN:C     | 2.53                     | 0.51              |
| 5:AE:55:VAL:O      | 5:AE:58:ALA:HB3    | 2.11                     | 0.51              |
| 13:AM:15:VAL:HG12  | 13:AM:45:VAL:CG2   | 2.39                     | 0.51              |
| 13:AM:81:LEU:HD11  | 13:AM:88:ARG:NH2   | 2.26                     | 0.51              |
| 19:AS:29:ARG:O     | 19:AS:31:ILE:N     | 2.44                     | 0.51              |
| 23:AW:48:C:H2'     | 23:AW:59:U:H4'     | 1.93                     | 0.51              |
| 25:BA:34:C:H6      | 25:BA:34:C:H3'     | 1.75                     | 0.51              |
| 25:BA:1301:A:H2'   | 25:BA:1302:A:H5''  | 1.89                     | 0.51              |
| 25:BA:2494:G:O2'   | 37:BQ:80:GLU:HA    | 2.10                     | 0.51              |
| 30:BF:150:GLY:HA2  | 30:BF:172:TRP:CD2  | 2.46                     | 0.51              |
| 32:BH:170:ARG:HG2  | 32:BH:171:LEU:N    | 2.26                     | 0.51              |
| 33:BI:127:VAL:HG23 | 33:BI:139:GLN:HG3  | 1.93                     | 0.51              |
| 36:BP:93:GLY:O     | 36:BP:94:GLU:HB2   | 2.11                     | 0.51              |
| 37:BQ:134:ARG:HG3  | 37:BQ:134:ARG:HH11 | 1.76                     | 0.51              |
| 38:BR:92:GLY:O     | 38:BR:94:TYR:CD2   | 2.64                     | 0.51              |
| 41:BU:111:GLU:O    | 41:BU:112:ARG:C    | 2.54                     | 0.51              |
| 43:BW:84:ARG:HB2   | 43:BW:96:ILE:CG2   | 2.41                     | 0.51              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 45:BY:13:VAL:HB    | 45:BY:72:VAL:CG1  | 2.41                     | 0.51              |
| 46:BZ:6:LYS:HE2    | 46:BZ:8:TYR:OH    | 2.10                     | 0.51              |
| 46:BZ:17:ALA:O     | 46:BZ:20:ARG:HB2  | 2.11                     | 0.51              |
| 1:CA:1281:U:H5''   | 1:CA:1282:C:OP2   | 2.10                     | 0.51              |
| 1:CA:1305:G:H5''   | 21:CU:4:GLY:C     | 2.36                     | 0.51              |
| 2:CB:20:GLU:O      | 2:CB:40:HIS:HB2   | 2.11                     | 0.51              |
| 5:CE:104:ALA:N     | 5:CE:106:PRO:HD2  | 2.26                     | 0.51              |
| 5:CE:106:PRO:O     | 5:CE:107:ARG:C    | 2.53                     | 0.51              |
| 9:CI:82:ALA:HA     | 9:CI:85:LEU:CD1   | 2.41                     | 0.51              |
| 11:CK:62:GLN:HG2   | 11:CK:63:LEU:N    | 2.25                     | 0.51              |
| 13:CM:49:THR:C     | 13:CM:51:ALA:N    | 2.67                     | 0.51              |
| 16:CP:68:ASP:O     | 16:CP:71:ARG:HG2  | 2.11                     | 0.51              |
| 18:CR:70:ILE:O     | 18:CR:71:LYS:C    | 2.53                     | 0.51              |
| 20:CT:29:LYS:CD    | 20:CT:66:ALA:CA   | 2.89                     | 0.51              |
| 20:CT:41:ILE:C     | 20:CT:43:LEU:H    | 2.19                     | 0.51              |
| 20:CT:56:MET:HG3   | 20:CT:84:LEU:HD11 | 1.86                     | 0.51              |
| 20:CT:100:ILE:HD12 | 20:CT:100:ILE:N   | 2.25                     | 0.51              |
| 22:CV:20:G:C5      | 22:CV:58:A:H2     | 2.28                     | 0.51              |
| 25:DA:48:G:H2'     | 25:DA:49:A:H2     | 1.76                     | 0.51              |
| 25:DA:1155:A:H4'   | 41:DU:55:ARG:NH1  | 2.26                     | 0.51              |
| 25:DA:1495:A:H2'   | 25:DA:1496:A:O4'  | 2.11                     | 0.51              |
| 25:DA:1693:U:O5'   | 25:DA:1693:U:H6   | 1.93                     | 0.51              |
| 25:DA:2001:A:H5''  | 25:DA:2689:U:H2'  | 1.92                     | 0.51              |
| 25:DA:2311:A:C8    | 31:DG:82:LEU:HD11 | 2.46                     | 0.51              |
| 25:DA:2489:G:N2    | 25:DA:2491:U:O4   | 2.40                     | 0.51              |
| 25:DA:2712:U:O2'   | 25:DA:2712(A):A:P | 2.68                     | 0.51              |
| 27:DC:82:LYS:HE3   | 27:DC:151:GLU:O   | 2.11                     | 0.51              |
| 30:DF:75:HIS:CE1   | 30:DF:82:ILE:HD12 | 2.46                     | 0.51              |
| 32:DH:98:LEU:HD22  | 32:DH:125:VAL:CG2 | 2.41                     | 0.51              |
| 34:DN:12:ARG:HB3   | 34:DN:50:ASP:OD1  | 2.10                     | 0.51              |
| 34:DN:41:ASP:O     | 34:DN:42:TRP:C    | 2.53                     | 0.51              |
| 39:DS:108:GLY:O    | 39:DS:110:LEU:HG  | 2.11                     | 0.51              |
| 46:DZ:58:VAL:HG13  | 46:DZ:67:LEU:H    | 1.76                     | 0.51              |
| 1:AA:222:U:H2'     | 1:AA:223:U:C6     | 2.45                     | 0.50              |
| 1:AA:363:A:C2      | 12:AL:31:PRO:HG2  | 2.46                     | 0.50              |
| 1:AA:501:C:H2'     | 1:AA:502:G:H8     | 1.77                     | 0.50              |
| 1:AA:533:A:O2'     | 1:AA:535:A:OP2    | 2.29                     | 0.50              |
| 1:AA:1192:C:OP2    | 3:AC:4:LYS:NZ     | 2.43                     | 0.50              |
| 4:AD:34:GLU:C      | 4:AD:35:ARG:HG3   | 2.36                     | 0.50              |
| 5:AE:101:ILE:CG1   | 5:AE:119:LEU:CD2  | 2.81                     | 0.50              |
| 8:AH:39:LEU:HD22   | 8:AH:39:LEU:N     | 2.25                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:AJ:30:SER:OG    | 10:AJ:81:THR:HG22  | 2.11                     | 0.50              |
| 13:AM:74:VAL:O     | 13:AM:78:ILE:HG13  | 2.11                     | 0.50              |
| 13:AM:112:GLY:O    | 13:AM:113:PRO:O    | 2.30                     | 0.50              |
| 15:AO:23:GLY:O     | 15:AO:27:VAL:HB    | 2.11                     | 0.50              |
| 20:AT:49:ALA:CA    | 20:AT:100:ILE:HD11 | 2.41                     | 0.50              |
| 22:AV:34:U:N3      | 22:AV:36:A:H5''    | 2.27                     | 0.50              |
| 25:BA:311:A:N9     | 25:BA:332:A:C8     | 2.80                     | 0.50              |
| 25:BA:526:A:O2'    | 25:BA:2043:C:O2    | 2.21                     | 0.50              |
| 25:BA:659:C:H2'    | 25:BA:660:G:C8     | 2.46                     | 0.50              |
| 25:BA:1836:C:H2'   | 25:BA:1837:C:H6    | 1.76                     | 0.50              |
| 25:BA:2519:U:H5''  | 25:BA:2520:C:OP1   | 2.10                     | 0.50              |
| 28:BD:26:LYS:NZ    | 28:BD:81:ALA:HB1   | 2.22                     | 0.50              |
| 28:BD:81:ALA:HA    | 28:BD:113:VAL:CG1  | 2.42                     | 0.50              |
| 28:BD:248:SER:C    | 28:BD:250:TRP:N    | 2.69                     | 0.50              |
| 30:BF:65:TRP:CZ3   | 30:BF:72:ARG:HB2   | 2.47                     | 0.50              |
| 30:BF:117:ARG:HH21 | 30:BF:187:VAL:HA   | 1.76                     | 0.50              |
| 31:BG:14:GLU:C     | 31:BG:17:PRO:HD2   | 2.35                     | 0.50              |
| 31:BG:135:LEU:HD11 | 31:BG:157:ILE:HD11 | 1.93                     | 0.50              |
| 33:BI:131:LYS:HG3  | 33:BI:133:HIS:CE1  | 2.46                     | 0.50              |
| 34:BN:2:LYS:O      | 34:BN:4:TYR:CZ     | 2.64                     | 0.50              |
| 37:BQ:43:THR:O     | 37:BQ:46:GLN:HB2   | 2.10                     | 0.50              |
| 40:BT:31:SER:O     | 40:BT:32:TYR:HB3   | 2.11                     | 0.50              |
| 41:BU:14:HIS:O     | 41:BU:16:LYS:N     | 2.44                     | 0.50              |
| 41:BU:92:ARG:HH21  | 41:BU:94:ASN:HB3   | 1.76                     | 0.50              |
| 42:BV:87:HIS:NE2   | 42:BV:89:GLN:HG2   | 2.27                     | 0.50              |
| 44:BX:18:TYR:N     | 44:BX:18:TYR:CD1   | 2.78                     | 0.50              |
| 46:BZ:85:HIS:C     | 46:BZ:85:HIS:ND1   | 2.68                     | 0.50              |
| 47:B0:53:MET:O     | 47:B0:53:MET:HG3   | 2.06                     | 0.50              |
| 4:CD:80:GLU:C      | 4:CD:82:ALA:N      | 2.69                     | 0.50              |
| 4:CD:96:LEU:HD23   | 4:CD:139:ARG:NH1   | 2.26                     | 0.50              |
| 5:CE:26:PHE:HD1    | 5:CE:26:PHE:H      | 1.58                     | 0.50              |
| 9:CI:18:PHE:HB2    | 9:CI:62:TYR:HB3    | 1.92                     | 0.50              |
| 17:CQ:42:TYR:N     | 17:CQ:42:TYR:CD1   | 2.79                     | 0.50              |
| 20:CT:53:LEU:CD2   | 20:CT:100:ILE:HB   | 2.41                     | 0.50              |
| 23:CW:7:A:O2'      | 23:CW:49:C:OP2     | 2.27                     | 0.50              |
| 24:CX:16:A:C2      | 24:CX:17:U:N1      | 2.79                     | 0.50              |
| 25:DA:1784:A:H4'   | 25:DA:1785:A:O5'   | 2.11                     | 0.50              |
| 25:DA:1799:G:O4'   | 25:DA:1800:C:C6    | 2.63                     | 0.50              |
| 28:DD:211:ARG:O    | 28:DD:215:LEU:HG   | 2.12                     | 0.50              |
| 31:DG:16:ARG:HB3   | 31:DG:17:PRO:HD3   | 1.92                     | 0.50              |
| 31:DG:111:LEU:HB2  | 31:DG:112:PRO:HD3  | 1.93                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 31:DG:129:GLY:HA2 | 31:DG:169:ALA:CB  | 2.41                     | 0.50              |
| 32:DH:127:GLU:HG3 | 32:DH:130:ARG:NE  | 2.26                     | 0.50              |
| 34:DN:39:ARG:HH11 | 34:DN:39:ARG:HG2  | 1.76                     | 0.50              |
| 38:DR:59:ASP:N    | 38:DR:59:ASP:OD2  | 2.44                     | 0.50              |
| 39:DS:65:VAL:O    | 39:DS:69:VAL:HG12 | 2.10                     | 0.50              |
| 41:DU:104:GLN:CD  | 41:DU:104:GLN:H   | 2.18                     | 0.50              |
| 44:DX:39:ILE:O    | 44:DX:40:LYS:C    | 2.52                     | 0.50              |
| 44:DX:63:LYS:HA   | 44:DX:72:LYS:HA   | 1.93                     | 0.50              |
| 1:AA:1279:A:N3    | 1:AA:1279:A:C3'   | 2.71                     | 0.50              |
| 1:AA:1503:A:O2'   | 1:AA:1504:G:P     | 2.69                     | 0.50              |
| 2:AB:18:GLY:H     | 2:AB:42:ILE:HG22  | 1.76                     | 0.50              |
| 4:AD:93:PHE:CD2   | 4:AD:93:PHE:C     | 2.89                     | 0.50              |
| 4:AD:196:LEU:C    | 4:AD:198:VAL:H    | 2.19                     | 0.50              |
| 6:AF:1:MET:HE2    | 6:AF:1:MET:H1     | 1.75                     | 0.50              |
| 8:AH:2:LEU:HD11   | 8:AH:5:PRO:HA     | 1.94                     | 0.50              |
| 8:AH:4:ASP:CG     | 8:AH:85:ARG:HH12  | 2.20                     | 0.50              |
| 9:AI:53:VAL:O     | 9:AI:54:ASP:HB2   | 2.09                     | 0.50              |
| 10:AJ:56:HIS:C    | 10:AJ:58:ASP:H    | 2.19                     | 0.50              |
| 14:AN:3:ARG:O     | 14:AN:7:ILE:HG12  | 2.11                     | 0.50              |
| 14:AN:45:ARG:HG3  | 14:AN:45:ARG:NH1  | 2.22                     | 0.50              |
| 16:AP:58:TYR:CA   | 16:AP:61:SER:HB3  | 2.41                     | 0.50              |
| 20:AT:27:LYS:HD3  | 20:AT:27:LYS:O    | 2.12                     | 0.50              |
| 20:AT:50:GLU:HA   | 20:AT:100:ILE:CG2 | 2.39                     | 0.50              |
| 23:AW:11:C:H2'    | 23:AW:12:U:C6     | 2.46                     | 0.50              |
| 23:AW:57:G:H2'    | 23:AW:57:G:N3     | 2.26                     | 0.50              |
| 25:BA:27:G:HO2'   | 25:BA:28:A:P      | 2.34                     | 0.50              |
| 25:BA:436:C:O5'   | 25:BA:436:C:H6    | 1.94                     | 0.50              |
| 25:BA:482:A:H5'   | 45:BY:47:LYS:HG2  | 1.93                     | 0.50              |
| 25:BA:1299:G:H8   | 25:BA:1299:G:O5'  | 1.95                     | 0.50              |
| 25:BA:2147:G:H2'  | 25:BA:2148:G:O4'  | 2.11                     | 0.50              |
| 25:BA:2171:A:O2'  | 25:BA:2172:U:O5'  | 2.29                     | 0.50              |
| 25:BA:2457:U:C2'  | 25:BA:2458:G:C5'  | 2.86                     | 0.50              |
| 25:BA:2820:A:N6   | 29:BE:192:ASN:HB2 | 2.27                     | 0.50              |
| 29:BE:34:VAL:HG22 | 29:BE:48:GLN:HE21 | 1.76                     | 0.50              |
| 33:BI:10:GLU:C    | 33:BI:12:LEU:H    | 2.19                     | 0.50              |
| 35:BO:68:GLU:CB   | 35:BO:78:ARG:HB2  | 2.39                     | 0.50              |
| 35:BO:88:ASN:O    | 35:BO:91:LEU:N    | 2.37                     | 0.50              |
| 40:BT:61:PHE:CE2  | 40:BT:76:PHE:HB2  | 2.46                     | 0.50              |
| 43:BW:92:ARG:O    | 43:BW:93:ALA:HB3  | 2.11                     | 0.50              |
| 1:CA:332:G:H2'    | 1:CA:333:G:H8     | 1.77                     | 0.50              |
| 1:CA:963:G:H21    | 10:CJ:55:LYS:HZ3  | 1.57                     | 0.50              |

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| Atom-1              | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|-------------------|--------------------------|-------------------|
| 1:CA:1528:U:H4'     | 1:CA:1529:G:O5'   | 2.10                     | 0.50              |
| 2:CB:105:PHE:C      | 2:CB:107:THR:N    | 2.67                     | 0.50              |
| 3:CC:76:VAL:HG23    | 3:CC:77:ILE:N     | 2.26                     | 0.50              |
| 4:CD:9:CYS:SG       | 4:CD:22:LYS:HD2   | 2.51                     | 0.50              |
| 4:CD:25:ARG:C       | 4:CD:27:TYR:H     | 2.19                     | 0.50              |
| 4:CD:138:TYR:HD2    | 4:CD:139:ARG:N    | 2.10                     | 0.50              |
| 5:CE:43:LEU:HD12    | 5:CE:44:GLY:H     | 1.77                     | 0.50              |
| 6:CF:1:MET:HE2      | 6:CF:1:MET:HA     | 1.93                     | 0.50              |
| 11:CK:59:TYR:CZ     | 11:CK:63:LEU:CD1  | 2.93                     | 0.50              |
| 13:CM:70:LEU:O      | 13:CM:74:VAL:HG23 | 2.11                     | 0.50              |
| 25:DA:26:G:OP1      | 43:DW:80:PRO:HB3  | 2.12                     | 0.50              |
| 25:DA:1558:A:C8     | 25:DA:1560:G:C8   | 2.99                     | 0.50              |
| 25:DA:2249:U:H1'    | 25:DA:2275:C:H41  | 1.76                     | 0.50              |
| 25:DA:2571:C:H5''   | 25:DA:2572:A:H5'' | 1.93                     | 0.50              |
| 29:DE:116:VAL:CG2   | 29:DE:117:MET:N   | 2.75                     | 0.50              |
| 31:DG:34:LEU:HD22   | 31:DG:34:LEU:C    | 2.36                     | 0.50              |
| 32:DH:16:SER:O      | 32:DH:17:VAL:HB   | 2.11                     | 0.50              |
| 32:DH:132:ARG:HH11  | 32:DH:132:ARG:CB  | 2.24                     | 0.50              |
| 36:DP:86:LYS:CG     | 36:DP:87:ASP:N    | 2.74                     | 0.50              |
| 36:DP:115:LEU:HD23  | 36:DP:131:SER:HB2 | 1.94                     | 0.50              |
| 42:DV:48:GLY:O      | 42:DV:49:THR:C    | 2.54                     | 0.50              |
| 46:DZ:108:PRO:O     | 46:DZ:143:GLY:HA2 | 2.11                     | 0.50              |
| 1:AA:983:A:N3       | 1:AA:983:A:C3'    | 2.72                     | 0.50              |
| 1:AA:983:A:H61      | 1:AA:1222:G:H22   | 1.59                     | 0.50              |
| 1:AA:1067:A:C4'     | 1:AA:1068:G:O5'   | 2.55                     | 0.50              |
| 1:AA:1279:A:C2      | 1:AA:1279:A:OP2   | 2.64                     | 0.50              |
| 3:AC:175:LEU:HD23   | 3:AC:201:TYR:HE2  | 1.72                     | 0.50              |
| 4:AD:8:VAL:O        | 4:AD:11:LEU:CG    | 2.60                     | 0.50              |
| 4:AD:173:TRP:CA     | 4:AD:187:ARG:HH12 | 2.23                     | 0.50              |
| 10:AJ:49:VAL:CG2    | 14:AN:41:ARG:HB2  | 2.28                     | 0.50              |
| 11:AK:32:ILE:CD1    | 11:AK:68:ALA:O    | 2.59                     | 0.50              |
| 17:AQ:85:VAL:O      | 17:AQ:89:LEU:HB2  | 2.11                     | 0.50              |
| 18:AR:50:ILE:CD1    | 18:AR:70:ILE:HG21 | 2.41                     | 0.50              |
| 19:AS:16:LEU:O      | 19:AS:17:GLU:C    | 2.54                     | 0.50              |
| 22:AV:19:G:C2       | 22:AV:59:A:C4     | 2.99                     | 0.50              |
| 22:AV:30:G:O2'      | 22:AV:31:G:H5'    | 2.11                     | 0.50              |
| 25:BA:1187:G:OP1    | 42:BV:81:TYR:OH   | 2.25                     | 0.50              |
| 25:BA:1525:G:H2'    | 25:BA:1526:G:C8   | 2.46                     | 0.50              |
| 25:BA:1812:A:H2'    | 25:BA:1813:G:C8   | 2.46                     | 0.50              |
| 25:BA:2079:U:H2'    | 25:BA:2080:G:O4'  | 2.12                     | 0.50              |
| 25:BA:2712(A):A:C5' | 38:BR:13:HIS:HD2  | 2.24                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 26:BB:49:C:H2'     | 26:BB:50:G:C8      | 2.46                     | 0.50              |
| 27:BC:22:ILE:HG23  | 27:BC:24:GLU:OE2   | 2.11                     | 0.50              |
| 27:BC:39:GLU:HG2   | 27:BC:180:PHE:CB   | 2.41                     | 0.50              |
| 28:BD:143:HIS:HD2  | 28:BD:144:ALA:CB   | 2.24                     | 0.50              |
| 28:BD:182:LEU:HB2  | 28:BD:271:ILE:O    | 2.12                     | 0.50              |
| 30:BF:23:ASP:C     | 30:BF:24:LEU:HD22  | 2.36                     | 0.50              |
| 31:BG:167:GLU:HA   | 31:BG:170:ARG:HB3  | 1.92                     | 0.50              |
| 33:BI:140:LEU:HD12 | 33:BI:141:LYS:N    | 2.27                     | 0.50              |
| 34:BN:97:ARG:O     | 34:BN:100:GLU:N    | 2.44                     | 0.50              |
| 36:BP:49:ARG:CZ    | 36:BP:50:ARG:HH22  | 2.25                     | 0.50              |
| 39:BS:13:ARG:O     | 39:BS:14:VAL:C     | 2.54                     | 0.50              |
| 40:BT:30:VAL:HG13  | 40:BT:31:SER:H     | 1.76                     | 0.50              |
| 40:BT:129:ARG:NH1  | 40:BT:131:ALA:O    | 2.43                     | 0.50              |
| 53:B6:32:ASN:CG    | 53:B6:33:LYS:N     | 2.66                     | 0.50              |
| 1:CA:61:G:C5       | 1:CA:107:G:C2      | 2.99                     | 0.50              |
| 1:CA:204:U:H4'     | 1:CA:216:G:O5'     | 2.11                     | 0.50              |
| 1:CA:625:G:H4'     | 16:CP:16:HIS:CD2   | 2.45                     | 0.50              |
| 1:CA:666:G:H5'     | 1:CA:726:C:H1'     | 1.93                     | 0.50              |
| 1:CA:817:C:C4      | 1:CA:819:A:H1'     | 2.46                     | 0.50              |
| 1:CA:982:U:H5''    | 14:CN:6:LEU:HD11   | 1.92                     | 0.50              |
| 2:CB:31:TYR:HE2    | 2:CB:46:LYS:HZ3    | 1.60                     | 0.50              |
| 2:CB:44:LEU:O      | 2:CB:47:THR:HB     | 2.10                     | 0.50              |
| 3:CC:64:VAL:HG22   | 3:CC:97:LYS:NZ     | 2.26                     | 0.50              |
| 11:CK:49:GLY:O     | 11:CK:50:TYR:CG    | 2.65                     | 0.50              |
| 15:CO:74:ASP:OD2   | 15:CO:77:ARG:HG2   | 2.11                     | 0.50              |
| 20:CT:26:ASN:HB3   | 20:CT:71:THR:HG23  | 1.92                     | 0.50              |
| 20:CT:84:LEU:O     | 20:CT:84:LEU:HD13  | 2.11                     | 0.50              |
| 21:CU:2:GLY:O      | 21:CU:4:GLY:N      | 2.43                     | 0.50              |
| 23:CW:37:A:C6      | 23:CW:38:A:C6      | 2.99                     | 0.50              |
| 25:DA:283:A:O2'    | 25:DA:284:U:OP1    | 2.28                     | 0.50              |
| 25:DA:637:A:OP2    | 36:DP:115:LEU:HD22 | 2.11                     | 0.50              |
| 25:DA:1019:U:O2'   | 25:DA:1021:A:H2    | 1.93                     | 0.50              |
| 25:DA:1266:G:O2'   | 25:DA:1267:U:OP2   | 2.29                     | 0.50              |
| 25:DA:1428:C:N4    | 25:DA:1569:A:H3'   | 2.26                     | 0.50              |
| 25:DA:1754:C:N3    | 25:DA:2716:U:O2'   | 2.44                     | 0.50              |
| 25:DA:1819:A:C5'   | 25:DA:1820:U:H5'   | 2.42                     | 0.50              |
| 25:DA:1820:U:H1'   | 28:DD:202:LYS:HB3  | 1.91                     | 0.50              |
| 25:DA:2162:G:O3'   | 25:DA:2172:U:O2'   | 2.27                     | 0.50              |
| 25:DA:2391:G:O2'   | 25:DA:2424:C:N4    | 2.44                     | 0.50              |
| 25:DA:2847:U:C3'   | 25:DA:2848:G:C5'   | 2.88                     | 0.50              |
| 28:DD:133:LEU:HD23 | 28:DD:136:ILE:HD12 | 1.93                     | 0.50              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 33:DI:8:PRO:HG3   | 33:DI:14:ASP:HB2   | 1.93                     | 0.50              |
| 33:DI:132:PRO:O   | 33:DI:133:HIS:O    | 2.28                     | 0.50              |
| 38:DR:21:TYR:OH   | 38:DR:43:GLU:HG2   | 2.10                     | 0.50              |
| 39:DS:32:LEU:O    | 39:DS:62:LYS:HE2   | 2.11                     | 0.50              |
| 41:DU:91:ASP:C    | 41:DU:93:LYS:N     | 2.67                     | 0.50              |
| 41:DU:92:ARG:HH21 | 41:DU:94:ASN:ND2   | 2.07                     | 0.50              |
| 44:DX:43:VAL:HG21 | 44:DX:81:VAL:HG11  | 1.93                     | 0.50              |
| 45:DY:43:ASN:HA   | 45:DY:64:GLU:HA    | 1.93                     | 0.50              |
| 46:DZ:96:VAL:HG22 | 46:DZ:97:GLU:N     | 2.27                     | 0.50              |
| 47:D0:82:ARG:HG3  | 47:D0:82:ARG:O     | 2.11                     | 0.50              |
| 48:D1:8:SER:OG    | 48:D1:10:LYS:HG3   | 2.11                     | 0.50              |
| 53:D6:19:ARG:H    | 53:D6:19:ARG:HD2   | 1.77                     | 0.50              |
| 2:AB:21:ARG:HB3   | 2:AB:39:ILE:HA     | 1.92                     | 0.50              |
| 4:AD:82:ALA:O     | 4:AD:83:SER:C      | 2.53                     | 0.50              |
| 4:AD:92:VAL:HG12  | 4:AD:96:LEU:CD1    | 2.41                     | 0.50              |
| 5:AE:80:ILE:CD1   | 5:AE:91:LEU:HD23   | 2.41                     | 0.50              |
| 6:AF:8:ILE:HD11   | 6:AF:79:LEU:HD13   | 1.92                     | 0.50              |
| 10:AJ:13:HIS:CE1  | 10:AJ:14:LYS:HE3   | 2.46                     | 0.50              |
| 12:AL:54:LYS:HD2  | 12:AL:54:LYS:N     | 2.26                     | 0.50              |
| 12:AL:70:ILE:HG12 | 12:AL:100:ILE:HD12 | 1.92                     | 0.50              |
| 12:AL:117:ARG:NH2 | 12:AL:124:LYS:HB2  | 2.26                     | 0.50              |
| 16:AP:14:ASN:N    | 16:AP:15:PRO:HD3   | 2.25                     | 0.50              |
| 19:AS:29:ARG:HD2  | 19:AS:30:LEU:N     | 2.26                     | 0.50              |
| 20:AT:53:LEU:CD1  | 20:AT:102:GLY:CA   | 2.82                     | 0.50              |
| 22:AV:52:C:N3     | 22:AV:53:G:N7      | 2.59                     | 0.50              |
| 25:BA:2287:A:C6   | 25:BA:2289:G:C4    | 2.99                     | 0.50              |
| 25:BA:2320:A:N6   | 25:BA:2333:A:N9    | 2.59                     | 0.50              |
| 25:BA:2500:U:C2   | 25:BA:2504:U:C5    | 2.99                     | 0.50              |
| 25:BA:2776:A:O2'  | 25:BA:2781:A:H4'   | 2.12                     | 0.50              |
| 25:BA:2844:G:H3'  | 25:BA:2845:G:H8    | 1.75                     | 0.50              |
| 25:BA:2848:G:H1'  | 25:BA:2868:A:N6    | 2.26                     | 0.50              |
| 29:BE:15:PHE:CD2  | 29:BE:15:PHE:N     | 2.78                     | 0.50              |
| 30:BF:65:TRP:HH2  | 30:BF:72:ARG:NH2   | 2.05                     | 0.50              |
| 31:BG:83:ARG:HD3  | 31:BG:83:ARG:C     | 2.36                     | 0.50              |
| 34:BN:87:LEU:O    | 34:BN:88:GLU:C     | 2.55                     | 0.50              |
| 36:BP:91:PHE:CD1  | 36:BP:91:PHE:N     | 2.79                     | 0.50              |
| 44:BX:64:LYS:HD3  | 44:BX:73:ARG:NE    | 2.26                     | 0.50              |
| 47:B0:82:ARG:O    | 47:B0:82:ARG:HG3   | 2.11                     | 0.50              |
| 1:CA:128:G:O2'    | 17:CQ:3:LYS:HE2    | 2.11                     | 0.50              |
| 2:CB:116:GLU:HA   | 2:CB:119:GLU:HB2   | 1.93                     | 0.50              |
| 3:CC:191:THR:OG1  | 3:CC:192:THR:N     | 2.44                     | 0.50              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 4:CD:138:TYR:C     | 4:CD:138:TYR:HD2    | 2.19                     | 0.50              |
| 5:CE:8:GLU:CA      | 5:CE:34:VAL:HG22    | 2.40                     | 0.50              |
| 7:CG:31:MET:SD     | 7:CG:34:GLY:HA2     | 2.52                     | 0.50              |
| 11:CK:20:TYR:HB2   | 11:CK:31:THR:O      | 2.12                     | 0.50              |
| 15:CO:56:LEU:O     | 15:CO:59:MET:HB2    | 2.11                     | 0.50              |
| 16:CP:8:ARG:CG     | 16:CP:8:ARG:NH1     | 2.53                     | 0.50              |
| 16:CP:20:VAL:HG23  | 16:CP:34:GLU:O      | 2.10                     | 0.50              |
| 20:CT:16:HIS:O     | 20:CT:17:ARG:C      | 2.54                     | 0.50              |
| 23:CW:5:G:N2       | 23:CW:69:G:C2       | 2.80                     | 0.50              |
| 25:DA:768:G:O2'    | 25:DA:769:G:H5'     | 2.11                     | 0.50              |
| 25:DA:1453:U:C4'   | 25:DA:1455:G:OP1    | 2.30                     | 0.50              |
| 25:DA:1962:C:O2'   | 25:DA:1964:G:OP2    | 2.28                     | 0.50              |
| 25:DA:2576:G:H3'   | 25:DA:2576:G:N3     | 2.27                     | 0.50              |
| 25:DA:2593:U:H2'   | 25:DA:2594:C:C6     | 2.46                     | 0.50              |
| 28:DD:44:ASN:HB3   | 28:DD:49:ILE:CA     | 2.28                     | 0.50              |
| 28:DD:190:TYR:O    | 28:DD:191:ALA:HB2   | 2.12                     | 0.50              |
| 32:DH:16:SER:HB3   | 32:DH:26:VAL:O      | 2.12                     | 0.50              |
| 36:DP:35:HIS:O     | 36:DP:36:LYS:HB2    | 2.11                     | 0.50              |
| 37:DQ:79:LEU:O     | 37:DQ:80:GLU:HB2    | 2.12                     | 0.50              |
| 40:DT:28:VAL:O     | 40:DT:29:ARG:CB     | 2.48                     | 0.50              |
| 46:DZ:128:VAL:HG22 | 46:DZ:129:SER:N     | 2.26                     | 0.50              |
| 47:D0:49:LYS:N     | 47:D0:80:HIS:HB3    | 2.25                     | 0.50              |
| 50:D3:29:ARG:HB2   | 50:D3:33:GLN:NE2    | 2.26                     | 0.50              |
| 1:AA:79:G:H4'      | 1:AA:80:G:OP1       | 2.11                     | 0.50              |
| 1:AA:250:A:HO2'    | 1:AA:251:G:P        | 2.34                     | 0.50              |
| 1:AA:376:G:H5''    | 16:AP:5:ARG:HD2     | 1.94                     | 0.50              |
| 1:AA:595:G:H5''    | 1:AA:596:C:OP1      | 2.12                     | 0.50              |
| 1:AA:1118:C:H5''   | 9:AI:104:ARG:CG     | 2.40                     | 0.50              |
| 1:AA:1346:A:H61    | 1:AA:1374:A:H3'     | 1.76                     | 0.50              |
| 4:AD:133:VAL:HG11  | 4:AD:138:TYR:HD1    | 1.75                     | 0.50              |
| 5:AE:36:ASP:OD1    | 5:AE:40:ARG:HB2     | 2.11                     | 0.50              |
| 9:AI:31:GLN:HG3    | 9:AI:35:GLU:CD      | 2.37                     | 0.50              |
| 13:AM:93:ARG:HA    | 13:AM:93:ARG:NE     | 2.25                     | 0.50              |
| 22:AV:1:C:H3'      | 22:AV:1:C:H6        | 1.76                     | 0.50              |
| 25:BA:221:A:N7     | 25:BA:266:G:O6      | 2.39                     | 0.50              |
| 25:BA:447:A:N1     | 25:BA:454:A:H2'     | 2.26                     | 0.50              |
| 25:BA:2405:G:O2'   | 25:BA:2406:U:P      | 2.70                     | 0.50              |
| 25:BA:2801:A:H5''  | 25:BA:2801(A):A:OP1 | 2.11                     | 0.50              |
| 26:BB:109:C:OP2    | 26:BB:109:C:H6      | 1.94                     | 0.50              |
| 28:BD:142:VAL:HG22 | 28:BD:143:HIS:H     | 1.77                     | 0.50              |
| 28:BD:172:TYR:HD2  | 28:BD:184:LYS:HD2   | 1.75                     | 0.50              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 29:BE:49:LEU:CD1  | 29:BE:81:ILE:HG13  | 2.35                     | 0.50              |
| 30:BF:17:ARG:HG3  | 30:BF:17:ARG:NH1   | 2.18                     | 0.50              |
| 31:BG:33:ARG:HB2  | 31:BG:162:THR:HG21 | 1.91                     | 0.50              |
| 33:BI:30:LEU:HD23 | 33:BI:30:LEU:N     | 2.25                     | 0.50              |
| 33:BI:88:ILE:CG1  | 33:BI:122:GLU:H    | 2.24                     | 0.50              |
| 34:BN:45:ASN:HD22 | 34:BN:46:VAL:N     | 2.06                     | 0.50              |
| 35:BO:9:GLU:OE2   | 35:BO:18:LYS:HE2   | 2.11                     | 0.50              |
| 35:BO:87:ILE:HG22 | 35:BO:88:ASN:N     | 2.26                     | 0.50              |
| 40:BT:3:ARG:HH11  | 40:BT:6:LEU:HD12   | 1.75                     | 0.50              |
| 41:BU:25:TRP:HD1  | 41:BU:26:GLY:CA    | 2.25                     | 0.50              |
| 41:BU:59:ARG:O    | 41:BU:63:VAL:HG23  | 2.11                     | 0.50              |
| 41:BU:93:LYS:O    | 41:BU:96:ALA:HB3   | 2.10                     | 0.50              |
| 42:BV:79:VAL:O    | 42:BV:79:VAL:CG2   | 2.59                     | 0.50              |
| 48:B1:23:LYS:HD3  | 48:B1:28:GLY:HA3   | 1.93                     | 0.50              |
| 53:B6:20:ASN:O    | 53:B6:21:TYR:CG    | 2.65                     | 0.50              |
| 53:B6:42:TRP:HA   | 53:B6:42:TRP:CE3   | 2.46                     | 0.50              |
| 1:CA:60:A:H1'     | 1:CA:61:G:O4'      | 2.12                     | 0.50              |
| 1:CA:274:A:O2'    | 1:CA:275:G:O4'     | 2.30                     | 0.50              |
| 1:CA:872:A:N3     | 1:CA:872:A:C2'     | 2.74                     | 0.50              |
| 1:CA:1456:G:C2    | 1:CA:1457:G:N9     | 2.80                     | 0.50              |
| 3:CC:58:GLU:HB2   | 3:CC:65:ALA:CB     | 2.40                     | 0.50              |
| 3:CC:129:ALA:CB   | 3:CC:132:ARG:HB2   | 2.41                     | 0.50              |
| 5:CE:16:THR:OG1   | 5:CE:17:ALA:N      | 2.41                     | 0.50              |
| 5:CE:83:GLU:HG3   | 5:CE:88:LYS:HG3    | 1.93                     | 0.50              |
| 13:CM:115:LYS:O   | 13:CM:117:VAL:HG13 | 2.11                     | 0.50              |
| 15:CO:57:LEU:O    | 15:CO:58:MET:C     | 2.55                     | 0.50              |
| 25:DA:395:U:O2'   | 25:DA:396:G:C8     | 2.65                     | 0.50              |
| 25:DA:910:A:C5    | 37:DQ:13:GLN:HG3   | 2.46                     | 0.50              |
| 25:DA:1300:U:C5   | 25:DA:1634:A:H1'   | 2.45                     | 0.50              |
| 25:DA:2119:A:H61  | 25:DA:2168:G:H1'   | 1.77                     | 0.50              |
| 28:DD:80:ALA:HB2  | 28:DD:96:HIS:CD2   | 2.46                     | 0.50              |
| 29:DE:131:ALA:O   | 29:DE:132:HIS:CB   | 2.60                     | 0.50              |
| 30:DF:65:TRP:CB   | 30:DF:66:PRO:CD    | 2.87                     | 0.50              |
| 30:DF:197:ASP:C   | 30:DF:199:TRP:H    | 2.20                     | 0.50              |
| 31:DG:7:LEU:HD23  | 31:DG:7:LEU:C      | 2.37                     | 0.50              |
| 33:DI:30:LEU:HB3  | 33:DI:36:ALA:HB3   | 1.92                     | 0.50              |
| 33:DI:71:ILE:C    | 33:DI:74:ASN:HD21  | 2.19                     | 0.50              |
| 33:DI:74:ASN:CG   | 33:DI:75:LEU:H     | 2.18                     | 0.50              |
| 34:DN:133:GLN:C   | 34:DN:134:ARG:HG3  | 2.35                     | 0.50              |
| 36:DP:56:SER:O    | 36:DP:57:THR:HB    | 2.11                     | 0.50              |
| 36:DP:93:GLY:O    | 36:DP:94:GLU:HB2   | 2.11                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 36:DP:101:VAL:HG13 | 36:DP:102:ARG:N    | 2.25                     | 0.50              |
| 40:DT:20:PRO:HD2   | 40:DT:85:LYS:HE3   | 1.93                     | 0.50              |
| 40:DT:129:ARG:C    | 40:DT:129:ARG:CD   | 2.66                     | 0.50              |
| 42:DV:38:LEU:H     | 42:DV:51:VAL:HG13  | 1.76                     | 0.50              |
| 45:DY:97:ARG:H     | 45:DY:97:ARG:CD    | 2.18                     | 0.50              |
| 1:AA:60:A:O2'      | 1:AA:61:G:OP2      | 2.30                     | 0.50              |
| 1:AA:327:A:O2'     | 1:AA:328:C:O4'     | 2.30                     | 0.50              |
| 1:AA:406:G:H1'     | 1:AA:495:A:N1      | 2.27                     | 0.50              |
| 1:AA:436:C:H2'     | 1:AA:437:U:H6      | 1.75                     | 0.50              |
| 1:AA:533:A:O2'     | 1:AA:534:U:OP1     | 2.28                     | 0.50              |
| 1:AA:1067:A:OP2    | 1:AA:1067:A:C8     | 2.65                     | 0.50              |
| 1:AA:1137:C:H4'    | 1:AA:1138:G:C2     | 2.46                     | 0.50              |
| 10:AJ:67:THR:O     | 10:AJ:67:THR:CG2   | 2.60                     | 0.50              |
| 12:AL:24:VAL:HG13  | 12:AL:98:TYR:HE2   | 1.77                     | 0.50              |
| 13:AM:15:VAL:HA    | 13:AM:18:ALA:HB3   | 1.93                     | 0.50              |
| 19:AS:45:VAL:C     | 19:AS:47:HIS:N     | 2.63                     | 0.50              |
| 19:AS:51:VAL:O     | 19:AS:58:VAL:HG13  | 2.12                     | 0.50              |
| 23:AW:15:G:N3      | 23:AW:59:U:O2      | 2.45                     | 0.50              |
| 23:AW:65:G:C6      | 23:AW:66:U:C4      | 3.00                     | 0.50              |
| 25:BA:49:A:H61     | 25:BA:177:G:H2'    | 1.77                     | 0.50              |
| 25:BA:560:C:H4'    | 41:BU:52:ARG:NH2   | 2.26                     | 0.50              |
| 25:BA:976:C:H5'    | 25:BA:1156:A:N6    | 2.27                     | 0.50              |
| 25:BA:1326:U:C5    | 25:BA:1647:G:O2'   | 2.64                     | 0.50              |
| 25:BA:1453:U:O2'   | 25:BA:1455:G:H8    | 1.92                     | 0.50              |
| 25:BA:1930:G:O2'   | 25:BA:1931:U:OP2   | 2.30                     | 0.50              |
| 25:BA:2287:A:N6    | 25:BA:2344:U:H3    | 2.10                     | 0.50              |
| 25:BA:2445:G:OP1   | 30:BF:74:ARG:NH2   | 2.45                     | 0.50              |
| 25:BA:2654:A:H1'   | 25:BA:2656:U:C6    | 2.47                     | 0.50              |
| 28:BD:3:VAL:HG13   | 28:BD:17:THR:HB    | 1.93                     | 0.50              |
| 28:BD:67:PHE:CE1   | 28:BD:157:ARG:NH1  | 2.80                     | 0.50              |
| 28:BD:69:ARG:NH2   | 28:BD:192:THR:HG21 | 2.26                     | 0.50              |
| 28:BD:69:ARG:NH2   | 28:BD:192:THR:CG2  | 2.75                     | 0.50              |
| 28:BD:239:ARG:HH21 | 28:BD:239:ARG:HG2  | 1.76                     | 0.50              |
| 31:BG:36:LYS:HE2   | 31:BG:160:VAL:HG21 | 1.92                     | 0.50              |
| 35:BO:48:PRO:HB3   | 35:BO:49:ARG:NH1   | 2.26                     | 0.50              |
| 37:BQ:48:GLU:OE1   | 37:BQ:48:GLU:HA    | 2.11                     | 0.50              |
| 39:BS:74:ALA:HB1   | 39:BS:103:GLU:HB2  | 1.94                     | 0.50              |
| 43:BW:88:ARG:NH1   | 43:BW:94:ASP:OD1   | 2.45                     | 0.50              |
| 45:BY:2:ARG:N      | 45:BY:5:MET:HE2    | 2.27                     | 0.50              |
| 46:BZ:30:ASN:C     | 46:BZ:32:HIS:H     | 2.20                     | 0.50              |
| 46:BZ:96:VAL:CG1   | 46:BZ:97:GLU:N     | 2.74                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 48:B1:46:LEU:N     | 48:B1:46:LEU:CD2   | 2.75                     | 0.50              |
| 49:B2:13:ALA:HA    | 49:B2:16:LEU:CG    | 2.42                     | 0.50              |
| 8:CH:29:SER:HB3    | 8:CH:32:LYS:HB2    | 1.94                     | 0.50              |
| 9:CI:4:TYR:CE2     | 9:CI:59:PHE:CE2    | 2.97                     | 0.50              |
| 10:CJ:6:ILE:HA     | 10:CJ:97:GLU:O     | 2.12                     | 0.50              |
| 25:DA:614(A):U:O2' | 25:DA:614(B):G:OP1 | 2.30                     | 0.50              |
| 25:DA:873:G:H1     | 25:DA:904:C:H42    | 1.58                     | 0.50              |
| 25:DA:1616:A:N3    | 25:DA:1616:A:H5'   | 2.26                     | 0.50              |
| 25:DA:2119:A:N6    | 25:DA:2168:G:H1'   | 2.27                     | 0.50              |
| 25:DA:2725:A:O2'   | 25:DA:2726:U:O2    | 2.30                     | 0.50              |
| 25:DA:2751:G:OP2   | 32:DH:4:ILE:CG2    | 2.60                     | 0.50              |
| 30:DF:11:VAL:HB    | 30:DF:18:ARG:HG3   | 1.93                     | 0.50              |
| 31:DG:129:GLY:HA2  | 31:DG:169:ALA:HB2  | 1.93                     | 0.50              |
| 32:DH:30:LYS:HB2   | 32:DH:79:VAL:O     | 2.12                     | 0.50              |
| 32:DH:103:LEU:CD2  | 32:DH:115:VAL:HB   | 2.41                     | 0.50              |
| 32:DH:109:PHE:O    | 32:DH:111:HIS:N    | 2.37                     | 0.50              |
| 40:DT:91:ARG:CB    | 40:DT:116:ALA:HA   | 2.42                     | 0.50              |
| 1:AA:1231:G:H5''   | 9:AI:128:ARG:HG3   | 1.93                     | 0.50              |
| 5:AE:68:GLU:O      | 5:AE:68:GLU:OE2    | 2.30                     | 0.50              |
| 5:AE:79:GLU:OE1    | 8:AH:104:ARG:HA    | 2.12                     | 0.50              |
| 5:AE:121:LYS:O     | 5:AE:122:GLU:HG3   | 2.11                     | 0.50              |
| 6:AF:24:GLU:O      | 6:AF:27:GLN:HB2    | 2.12                     | 0.50              |
| 12:AL:75:HIS:ND1   | 12:AL:76:ASN:N     | 2.59                     | 0.50              |
| 18:AR:44:LEU:HB3   | 18:AR:48:GLY:O     | 2.11                     | 0.50              |
| 20:AT:41:ILE:HG22  | 20:AT:88:VAL:HG23  | 1.93                     | 0.50              |
| 22:AV:54:G:C4      | 22:AV:55:U:C5      | 2.99                     | 0.50              |
| 23:AW:53:G:C6      | 23:AW:54:U:C4      | 2.99                     | 0.50              |
| 25:BA:74:A:N3      | 25:BA:74:A:O5'     | 2.44                     | 0.50              |
| 25:BA:340:A:H2'    | 25:BA:341:G:H8     | 1.76                     | 0.50              |
| 25:BA:659:C:H2'    | 25:BA:660:G:H8     | 1.77                     | 0.50              |
| 25:BA:703:U:H2'    | 25:BA:704:G:H5'    | 1.93                     | 0.50              |
| 25:BA:776:G:H4'    | 25:BA:777:A:O5'    | 2.11                     | 0.50              |
| 25:BA:1486:A:N6    | 25:BA:1504:C:H42   | 2.10                     | 0.50              |
| 25:BA:1789:A:H5''  | 28:BD:220:HIS:O    | 2.11                     | 0.50              |
| 25:BA:1826:G:H2'   | 25:BA:1827:C:H6    | 1.74                     | 0.50              |
| 25:BA:2171:A:O2'   | 25:BA:2172:U:C6    | 2.63                     | 0.50              |
| 28:BD:70:TRP:CH2   | 28:BD:150:LYS:HA   | 2.46                     | 0.50              |
| 29:BE:89:ASP:O     | 29:BE:90:THR:HB    | 2.10                     | 0.50              |
| 30:BF:51:THR:HG21  | 30:BF:91:GLY:C     | 2.37                     | 0.50              |
| 36:BP:27:HIS:ND1   | 36:BP:27:HIS:N     | 2.59                     | 0.50              |
| 36:BP:35:HIS:O     | 36:BP:36:LYS:HB2   | 2.11                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 40:BT:106:SER:C    | 40:BT:107:ASP:OD1  | 2.54                     | 0.50              |
| 42:BV:35:LEU:O     | 42:BV:37:VAL:O     | 2.30                     | 0.50              |
| 47:B0:54:GLY:O     | 47:B0:57:PHE:N     | 2.41                     | 0.50              |
| 50:B3:38:GLU:O     | 50:B3:40:THR:HG23  | 2.11                     | 0.50              |
| 51:B4:64:LYS:C     | 51:B4:65:CYS:SG    | 2.95                     | 0.50              |
| 1:CA:1067:A:O2'    | 1:CA:1068:G:O5'    | 2.30                     | 0.50              |
| 1:CA:1137:C:H4'    | 1:CA:1138:G:C2     | 2.47                     | 0.50              |
| 1:CA:1305:G:O4'    | 1:CA:1305:G:OP2    | 2.30                     | 0.50              |
| 1:CA:1431:C:H2'    | 1:CA:1432:G:O4'    | 2.11                     | 0.50              |
| 6:CF:77:ARG:O      | 6:CF:78:GLU:C      | 2.54                     | 0.50              |
| 8:CH:85:ARG:HG3    | 8:CH:85:ARG:HH11   | 1.77                     | 0.50              |
| 10:CJ:5:ARG:O      | 10:CJ:98:ILE:HA    | 2.12                     | 0.50              |
| 13:CM:93:ARG:HD3   | 25:DA:888:C:OP2    | 2.12                     | 0.50              |
| 20:CT:8:ARG:O      | 20:CT:9:ASN:OD1    | 2.30                     | 0.50              |
| 20:CT:25:ARG:HG3   | 20:CT:25:ARG:NH1   | 2.25                     | 0.50              |
| 23:CW:37:A:N6      | 23:CW:38:A:N1      | 2.59                     | 0.50              |
| 25:DA:33:U:O4      | 25:DA:446:G:O2'    | 2.27                     | 0.50              |
| 25:DA:265:A:H1'    | 25:DA:266:G:O4'    | 2.12                     | 0.50              |
| 25:DA:598:G:H4'    | 36:DP:11:GLY:CA    | 2.42                     | 0.50              |
| 25:DA:614(C):A:O2' | 25:DA:615:G:O5'    | 2.30                     | 0.50              |
| 25:DA:969:U:OP1    | 50:D3:17:LYS:HD3   | 2.12                     | 0.50              |
| 25:DA:995:C:O2     | 25:DA:995:C:H2'    | 2.11                     | 0.50              |
| 25:DA:1840:G:H1    | 25:DA:1902:C:H42   | 1.58                     | 0.50              |
| 25:DA:2725:A:O2'   | 25:DA:2726:U:O5'   | 2.30                     | 0.50              |
| 28:DD:31:LYS:HZ1   | 28:DD:102:LYS:NZ   | 2.09                     | 0.50              |
| 30:DF:36:VAL:HG11  | 30:DF:183:VAL:CG1  | 2.41                     | 0.50              |
| 31:DG:95:ARG:O     | 31:DG:96:ARG:O     | 2.30                     | 0.50              |
| 32:DH:7:LEU:N      | 32:DH:8:PRO:CD     | 2.74                     | 0.50              |
| 32:DH:26:VAL:HG13  | 32:DH:27:LYS:N     | 2.26                     | 0.50              |
| 33:DI:92:VAL:O     | 33:DI:120:ILE:HG23 | 2.12                     | 0.50              |
| 35:DO:104:ARG:HH21 | 40:DT:43:GLN:NE2   | 2.07                     | 0.50              |
| 40:DT:39:ARG:HG3   | 40:DT:40:THR:HG22  | 1.93                     | 0.50              |
| 41:DU:76:TYR:C     | 41:DU:78:THR:N     | 2.70                     | 0.50              |
| 44:DX:50:LYS:O     | 44:DX:83:VAL:HA    | 2.12                     | 0.50              |
| 45:DY:43:ASN:CB    | 45:DY:64:GLU:HA    | 2.41                     | 0.50              |
| 51:D4:11:PRO:HA    | 51:D4:25:TYR:CD2   | 2.46                     | 0.50              |
| 1:AA:189(K):U:H2'  | 1:AA:189(L):G:C8   | 2.46                     | 0.50              |
| 1:AA:366:C:O2'     | 1:AA:367:U:OP1     | 2.30                     | 0.50              |
| 1:AA:422:C:O2'     | 1:AA:423:G:N2      | 2.45                     | 0.50              |
| 1:AA:518:C:O2'     | 12:AL:50:SER:HB3   | 2.11                     | 0.50              |
| 1:AA:1067:A:O2'    | 1:AA:1068:G:O5'    | 2.30                     | 0.50              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AA:1321:C:C4    | 1:AA:1322:C:C4     | 3.00                     | 0.50              |
| 2:AB:28:PHE:CZ    | 2:AB:189:ASP:HA    | 2.47                     | 0.50              |
| 2:AB:114:ARG:HH12 | 2:AB:118:LEU:HD21  | 1.76                     | 0.50              |
| 2:AB:228:GLY:O    | 2:AB:230:VAL:HG13  | 2.12                     | 0.50              |
| 3:AC:172:ARG:O    | 3:AC:173:VAL:HG23  | 2.12                     | 0.50              |
| 4:AD:76:ARG:HD2   | 4:AD:207:TYR:CE1   | 2.46                     | 0.50              |
| 4:AD:110:PHE:HD2  | 4:AD:148:VAL:CG2   | 2.25                     | 0.50              |
| 6:AF:23:LYS:O     | 6:AF:27:GLN:HG2    | 2.12                     | 0.50              |
| 8:AH:9:MET:O      | 8:AH:12:ARG:N      | 2.44                     | 0.50              |
| 9:AI:5:TYR:HA     | 9:AI:17:VAL:O      | 2.12                     | 0.50              |
| 11:AK:32:ILE:HD11 | 11:AK:68:ALA:O     | 2.11                     | 0.50              |
| 13:AM:3:ARG:CZ    | 31:BG:113:ARG:NH2  | 2.58                     | 0.50              |
| 13:AM:90:LEU:C    | 13:AM:91:ARG:HG2   | 2.37                     | 0.50              |
| 15:AO:67:LEU:O    | 15:AO:71:GLN:N     | 2.40                     | 0.50              |
| 22:AV:58:A:O2'    | 22:AV:59:A:H5'     | 2.12                     | 0.50              |
| 25:BA:271(A):A:N1 | 25:BA:272(D):G:O2' | 2.43                     | 0.50              |
| 25:BA:301:G:O2'   | 25:BA:302:C:O4'    | 2.25                     | 0.50              |
| 25:BA:527:C:H1'   | 25:BA:528:A:C6     | 2.47                     | 0.50              |
| 25:BA:571:A:H1'   | 25:BA:573:G:C8     | 2.47                     | 0.50              |
| 25:BA:1210:A:O2'  | 25:BA:1211:U:OP2   | 2.29                     | 0.50              |
| 25:BA:1668:A:N6   | 25:BA:1676:A:H61   | 2.09                     | 0.50              |
| 30:BF:64:ILE:O    | 30:BF:65:TRP:CD1   | 2.53                     | 0.50              |
| 30:BF:132:VAL:O   | 30:BF:133:ASN:C    | 2.54                     | 0.50              |
| 36:BP:124:LYS:HG3 | 36:BP:143:GLY:C    | 2.37                     | 0.50              |
| 37:BQ:27:VAL:HG13 | 37:BQ:105:GLU:OE1  | 2.11                     | 0.50              |
| 38:BR:84:ALA:N    | 38:BR:85:PRO:CD    | 2.75                     | 0.50              |
| 39:BS:16:ASN:OD1  | 39:BS:16:ASN:N     | 2.43                     | 0.50              |
| 44:BX:83:VAL:O    | 44:BX:84:ALA:C     | 2.55                     | 0.50              |
| 45:BY:31:LEU:CB   | 45:BY:32:PRO:CA    | 2.90                     | 0.50              |
| 46:BZ:136:PHE:O   | 46:BZ:137:ILE:HG13 | 2.11                     | 0.50              |
| 51:B4:44:CYS:O    | 51:B4:46:ASN:N     | 2.39                     | 0.50              |
| 1:CA:92:C:H2'     | 1:CA:93:G:H8       | 1.75                     | 0.50              |
| 1:CA:266:G:O2'    | 1:CA:267:C:OP2     | 2.26                     | 0.50              |
| 1:CA:344:A:C5'    | 1:CA:345:C:OP2     | 2.48                     | 0.50              |
| 1:CA:429:U:O2'    | 1:CA:430:A:O5'     | 2.30                     | 0.50              |
| 4:CD:98:GLU:OE2   | 4:CD:103:ASN:ND2   | 2.44                     | 0.50              |
| 4:CD:124:GLY:O    | 4:CD:126:ILE:N     | 2.45                     | 0.50              |
| 4:CD:165:MET:O    | 4:CD:167:GLY:N     | 2.44                     | 0.50              |
| 6:CF:14:LEU:HB3   | 6:CF:19:LEU:HB2    | 1.94                     | 0.50              |
| 12:CL:60:LEU:HD23 | 12:CL:64:TYR:CB    | 2.42                     | 0.50              |
| 13:CM:78:ILE:O    | 13:CM:81:LEU:HB2   | 2.11                     | 0.50              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 14:CN:9:LYS:C     | 14:CN:11:LYS:H     | 2.18                     | 0.50              |
| 18:CR:50:ILE:O    | 18:CR:51:LEU:C     | 2.55                     | 0.50              |
| 25:DA:655:A:H2'   | 25:DA:656:G:H5'    | 1.94                     | 0.50              |
| 25:DA:753:C:OP2   | 25:DA:753:C:H5     | 1.87                     | 0.50              |
| 25:DA:2051:A:H61  | 25:DA:2614:A:C2'   | 2.25                     | 0.50              |
| 25:DA:2503:A:H4'  | 25:DA:2504:U:OP1   | 2.11                     | 0.50              |
| 25:DA:2725:A:N6   | 25:DA:2727:G:N3    | 2.60                     | 0.50              |
| 28:DD:161:THR:O   | 28:DD:196:VAL:HG23 | 2.11                     | 0.50              |
| 28:DD:248:SER:HB2 | 28:DD:249:PRO:HD2  | 1.94                     | 0.50              |
| 30:DF:174:VAL:O   | 30:DF:174:VAL:CG2  | 2.60                     | 0.50              |
| 33:DI:33:ARG:HB3  | 33:DI:35:LEU:HG    | 1.94                     | 0.50              |
| 34:DN:25:ARG:O    | 34:DN:28:THR:HG22  | 2.12                     | 0.50              |
| 35:DO:4:PRO:O     | 35:DO:5:GLN:CB     | 2.59                     | 0.50              |
| 36:DP:64:LYS:HB3  | 55:D8:25:MET:CG    | 2.36                     | 0.50              |
| 37:DQ:54:MET:HG2  | 37:DQ:64:ILE:HG21  | 1.93                     | 0.50              |
| 40:DT:61:PHE:CE2  | 40:DT:76:PHE:HB2   | 2.47                     | 0.50              |
| 43:DW:1:MET:HE2   | 43:DW:2:GLU:H      | 1.77                     | 0.50              |
| 45:DY:12:THR:OG1  | 45:DY:26:LYS:HE2   | 2.12                     | 0.50              |
| 46:DZ:29:TYR:HA   | 46:DZ:33:LEU:O     | 2.11                     | 0.50              |
| 53:D6:32:ASN:CG   | 53:D6:33:LYS:N     | 2.69                     | 0.50              |
| 1:AA:79:G:O4'     | 1:AA:80:G:OP1      | 2.30                     | 0.50              |
| 1:AA:262:A:O3'    | 20:AT:75:ASN:ND2   | 2.45                     | 0.50              |
| 1:AA:668:G:O2'    | 15:AO:46:HIS:CD2   | 2.65                     | 0.50              |
| 4:AD:187:ARG:NH1  | 4:AD:187:ARG:HG2   | 2.27                     | 0.50              |
| 4:AD:190:ASP:O    | 4:AD:194:LEU:HD23  | 2.12                     | 0.50              |
| 5:AE:73:ASN:O     | 5:AE:75:THR:HG22   | 2.12                     | 0.50              |
| 12:AL:7:ILE:C     | 12:AL:9:GLN:N      | 2.70                     | 0.50              |
| 14:AN:4:LYS:HD2   | 14:AN:7:ILE:HD11   | 1.93                     | 0.50              |
| 22:AV:35:C:O2'    | 22:AV:36:A:OP1     | 2.30                     | 0.50              |
| 23:AW:34:G:N9     | 24:AX:14:A:C2      | 2.77                     | 0.50              |
| 25:BA:35:G:C4     | 25:BA:454:A:C2     | 3.00                     | 0.50              |
| 25:BA:90:U:O2'    | 25:BA:92:A:H5''    | 2.12                     | 0.50              |
| 25:BA:142:A:C8    | 25:BA:1408:C:H1'   | 2.46                     | 0.50              |
| 25:BA:373:U:H2'   | 25:BA:374:A:C8     | 2.45                     | 0.50              |
| 25:BA:458:G:O2'   | 25:BA:459:U:OP2    | 2.30                     | 0.50              |
| 25:BA:527:C:H5''  | 25:BA:528:A:OP1    | 2.12                     | 0.50              |
| 25:BA:690:G:H2'   | 25:BA:691:C:C6     | 2.47                     | 0.50              |
| 25:BA:870:A:H4'   | 37:BQ:6:ARG:O      | 2.11                     | 0.50              |
| 25:BA:1899:G:H21  | 25:BA:1902:C:N4    | 2.10                     | 0.50              |
| 25:BA:2111:C:H42  | 25:BA:2147:G:N2    | 2.09                     | 0.50              |
| 28:BD:32:SER:O    | 28:BD:33:LEU:C     | 2.55                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 28:BD:89:SER:O     | 28:BD:198:ASN:ND2  | 2.45                     | 0.50              |
| 29:BE:173:VAL:HG12 | 29:BE:174:ASP:N    | 2.26                     | 0.50              |
| 31:BG:66:GLN:O     | 31:BG:67:LYS:C     | 2.54                     | 0.50              |
| 31:BG:101:ILE:CG1  | 31:BG:105:LYS:HE3  | 2.37                     | 0.50              |
| 34:BN:18:ALA:CB    | 34:BN:21:LYS:CB    | 2.89                     | 0.50              |
| 34:BN:24:GLY:H     | 34:BN:27:ALA:H     | 1.59                     | 0.50              |
| 36:BP:118:GLY:O    | 36:BP:119:GLU:C    | 2.55                     | 0.50              |
| 40:BT:36:GLU:C     | 40:BT:38:ASN:H     | 2.20                     | 0.50              |
| 41:BU:94:ASN:C     | 41:BU:94:ASN:HD22  | 2.19                     | 0.50              |
| 42:BV:19:LYS:HG2   | 42:BV:94:LEU:H     | 1.77                     | 0.50              |
| 43:BW:26:GLY:HA2   | 43:BW:71:VAL:O     | 2.11                     | 0.50              |
| 55:B8:22:VAL:HB    | 55:B8:49:VAL:HG23  | 1.94                     | 0.50              |
| 1:CA:79:G:O4'      | 1:CA:80:G:OP1      | 2.30                     | 0.50              |
| 1:CA:950:U:H2'     | 1:CA:951:G:H8      | 1.76                     | 0.50              |
| 2:CB:114:ARG:O     | 2:CB:114:ARG:CG    | 2.59                     | 0.50              |
| 2:CB:194:PRO:O     | 2:CB:196:LEU:N     | 2.45                     | 0.50              |
| 3:CC:11:ARG:HD3    | 3:CC:178:LEU:HD12  | 1.92                     | 0.50              |
| 12:CL:126:LYS:CG   | 12:CL:127:GLU:N    | 2.75                     | 0.50              |
| 16:CP:8:ARG:HB3    | 16:CP:28:ARG:HH12  | 1.76                     | 0.50              |
| 16:CP:67:THR:HB    | 16:CP:70:ALA:HB2   | 1.93                     | 0.50              |
| 19:CS:63:THR:HG23  | 19:CS:66:MET:H     | 1.76                     | 0.50              |
| 22:CV:53:G:O2'     | 22:CV:54:G:OP1     | 2.30                     | 0.50              |
| 25:DA:565:C:H4'    | 25:DA:1253:A:N6    | 2.26                     | 0.50              |
| 25:DA:581:C:H2'    | 25:DA:582:G:C8     | 2.46                     | 0.50              |
| 25:DA:1803:A:O2'   | 28:DD:259:THR:HG21 | 2.12                     | 0.50              |
| 25:DA:2306:C:O5'   | 25:DA:2307:G:H5''  | 2.12                     | 0.50              |
| 25:DA:2437:U:H2'   | 25:DA:2438:U:C6    | 2.47                     | 0.50              |
| 25:DA:2734:A:H5'   | 25:DA:2735:G:OP2   | 2.12                     | 0.50              |
| 25:DA:2848:G:C2    | 25:DA:2867:G:C4    | 3.00                     | 0.50              |
| 26:DB:48:A:H4'     | 39:DS:95:HIS:HD2   | 1.76                     | 0.50              |
| 28:DD:2:ALA:O      | 28:DD:3:VAL:HB     | 2.11                     | 0.50              |
| 31:DG:49:ASP:HB3   | 31:DG:52:ILE:HG12  | 1.94                     | 0.50              |
| 36:DP:49:ARG:CZ    | 36:DP:50:ARG:HH22  | 2.25                     | 0.50              |
| 38:DR:84:ALA:N     | 38:DR:85:PRO:CD    | 2.74                     | 0.50              |
| 39:DS:5:THR:C      | 39:DS:7:TYR:H      | 2.19                     | 0.50              |
| 41:DU:92:ARG:O     | 41:DU:94:ASN:N     | 2.45                     | 0.50              |
| 42:DV:39:LEU:N     | 42:DV:39:LEU:HD13  | 2.27                     | 0.50              |
| 42:DV:75:PHE:CD1   | 42:DV:75:PHE:C     | 2.90                     | 0.50              |
| 1:AA:274:A:O2'     | 1:AA:275:G:O5'     | 2.22                     | 0.49              |
| 1:AA:324:G:OP1     | 20:AT:22:ARG:HD3   | 2.12                     | 0.49              |
| 1:AA:328:C:H4'     | 1:AA:329:A:H5''    | 1.94                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:AB:21:ARG:HD3    | 2:AB:39:ILE:HG13   | 1.94                     | 0.49              |
| 2:AB:204:ASN:HD22  | 2:AB:205:ASP:N     | 2.09                     | 0.49              |
| 3:AC:29:TYR:CD2    | 3:AC:29:TYR:C      | 2.90                     | 0.49              |
| 4:AD:173:TRP:CA    | 4:AD:187:ARG:NH1   | 2.73                     | 0.49              |
| 4:AD:192:GLU:O     | 4:AD:194:LEU:N     | 2.45                     | 0.49              |
| 10:AJ:6:ILE:HG13   | 10:AJ:72:VAL:O     | 2.12                     | 0.49              |
| 10:AJ:72:VAL:O     | 10:AJ:73:ASP:OD1   | 2.30                     | 0.49              |
| 22:AV:57:C:C2'     | 22:AV:58:A:H5'     | 2.42                     | 0.49              |
| 23:AW:38:A:C6      | 23:AW:39:U:C5      | 3.00                     | 0.49              |
| 25:BA:322:A:P      | 30:BF:169:ASN:HB2  | 2.52                     | 0.49              |
| 25:BA:372:G:O2'    | 25:BA:373:U:OP2    | 2.30                     | 0.49              |
| 25:BA:910:A:N7     | 37:BQ:13:GLN:HG3   | 2.26                     | 0.49              |
| 25:BA:1131:G:H1'   | 34:BN:82:LEU:HD12  | 1.94                     | 0.49              |
| 25:BA:1902:C:O2'   | 28:BD:244:ARG:CB   | 2.59                     | 0.49              |
| 25:BA:2123:G:H2'   | 25:BA:2124:G:C8    | 2.47                     | 0.49              |
| 25:BA:2233:U:H2'   | 25:BA:2234:G:C8    | 2.47                     | 0.49              |
| 25:BA:2580:U:H4'   | 29:BE:130:GLY:HA2  | 1.94                     | 0.49              |
| 36:BP:48:PRO:O     | 36:BP:50:ARG:N     | 2.45                     | 0.49              |
| 36:BP:92:GLU:HA    | 36:BP:123:LEU:CD1  | 2.42                     | 0.49              |
| 36:BP:101:VAL:HG23 | 36:BP:107:LYS:H    | 1.76                     | 0.49              |
| 38:BR:67:LEU:O     | 38:BR:67:LEU:HD12  | 2.11                     | 0.49              |
| 40:BT:134:GLU:O    | 40:BT:135:ALA:HB3  | 2.12                     | 0.49              |
| 45:BY:11:ASP:OD1   | 45:BY:12:THR:O     | 2.30                     | 0.49              |
| 45:BY:45:VAL:HA    | 45:BY:62:GLU:HG2   | 1.93                     | 0.49              |
| 46:BZ:150:LEU:O    | 46:BZ:171:ILE:HG12 | 2.11                     | 0.49              |
| 1:CA:652:U:C4      | 1:CA:752:G:N3      | 2.80                     | 0.49              |
| 1:CA:1054:C:OP2    | 1:CA:1054:C:C4'    | 2.60                     | 0.49              |
| 1:CA:1292:U:H2'    | 1:CA:1293:G:C8     | 2.47                     | 0.49              |
| 2:CB:168:THR:HG23  | 2:CB:192:SER:CB    | 2.42                     | 0.49              |
| 4:CD:22:LYS:HD3    | 4:CD:26:CYS:SG     | 2.52                     | 0.49              |
| 4:CD:103:ASN:O     | 4:CD:106:TYR:HB3   | 2.12                     | 0.49              |
| 8:CH:29:SER:HB3    | 8:CH:32:LYS:CD     | 2.42                     | 0.49              |
| 9:CI:89:ASN:O      | 9:CI:91:ASP:N      | 2.44                     | 0.49              |
| 9:CI:95:LYS:HD3    | 9:CI:95:LYS:C      | 2.37                     | 0.49              |
| 16:CP:81:ARG:HG2   | 16:CP:83:GLU:OE2   | 2.12                     | 0.49              |
| 18:CR:86:VAL:C     | 18:CR:87:ARG:HD3   | 2.36                     | 0.49              |
| 25:DA:184:C:H2'    | 25:DA:185:U:C6     | 2.46                     | 0.49              |
| 25:DA:9271:G:N3    | 25:DA:9272:G:H1'   | 2.27                     | 0.49              |
| 25:DA:362(F):A:O2' | 25:DA:364:C:H5     | 1.94                     | 0.49              |
| 25:DA:1162:G:H21   | 42:DV:89:GLN:HE22  | 1.60                     | 0.49              |
| 25:DA:1297:C:O2'   | 25:DA:1302:A:N1    | 2.37                     | 0.49              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:DA:1558:A:O2'  | 25:DA:1559:G:OP2   | 2.30                     | 0.49              |
| 25:DA:2475:C:H42  | 25:DA:2529:G:H22   | 1.60                     | 0.49              |
| 28:DD:12:SER:HB2  | 28:DD:208:LYS:HB3  | 1.93                     | 0.49              |
| 28:DD:31:LYS:HE3  | 28:DD:94:LEU:HD11  | 1.94                     | 0.49              |
| 28:DD:44:ASN:HB2  | 28:DD:48:ARG:O     | 2.12                     | 0.49              |
| 29:DE:107:THR:O   | 29:DE:190:GLY:HA2  | 2.12                     | 0.49              |
| 34:DN:123:TYR:CE2 | 34:DN:129:PRO:HD2  | 2.47                     | 0.49              |
| 36:DP:61:ARG:O    | 36:DP:61:ARG:HD2   | 2.12                     | 0.49              |
| 36:DP:124:LYS:HG3 | 36:DP:143:GLY:C    | 2.37                     | 0.49              |
| 38:DR:45:ARG:CG   | 38:DR:46:GLY:H     | 2.24                     | 0.49              |
| 39:DS:52:SER:O    | 39:DS:56:LEU:CD2   | 2.60                     | 0.49              |
| 40:DT:24:PRO:HA   | 40:DT:49:VAL:HG13  | 1.94                     | 0.49              |
| 43:DW:110:LYS:HG3 | 43:DW:111:HIS:ND1  | 2.26                     | 0.49              |
| 45:DY:39:VAL:CG1  | 45:DY:40:GLU:H     | 2.12                     | 0.49              |
| 45:DY:46:LYS:O    | 45:DY:48:ALA:N     | 2.45                     | 0.49              |
| 45:DY:81:LYS:HZ2  | 45:DY:98:VAL:HG11  | 1.76                     | 0.49              |
| 46:DZ:58:VAL:HG11 | 46:DZ:66:SER:HB3   | 1.93                     | 0.49              |
| 46:DZ:59:LEU:HG   | 46:DZ:69:THR:CG2   | 2.41                     | 0.49              |
| 1:AA:1048:G:H2'   | 1:AA:1049:U:OP2    | 2.13                     | 0.49              |
| 2:AB:25:ASN:OD1   | 2:AB:27:LYS:N      | 2.43                     | 0.49              |
| 2:AB:80:ILE:CD1   | 2:AB:212:GLN:HA    | 2.42                     | 0.49              |
| 4:AD:158:ILE:O    | 4:AD:159:ARG:C     | 2.55                     | 0.49              |
| 5:AE:41:VAL:CG1   | 5:AE:113:ALA:HA    | 2.42                     | 0.49              |
| 8:AH:48:TYR:O     | 8:AH:49:GLU:HB3    | 2.12                     | 0.49              |
| 10:AJ:72:VAL:HG12 | 10:AJ:73:ASP:N     | 2.27                     | 0.49              |
| 22:AV:53:G:O2'    | 22:AV:54:G:H5'     | 2.12                     | 0.49              |
| 23:AY:39:U:C2     | 23:AY:40:C:C5      | 3.00                     | 0.49              |
| 25:BA:142:A:H5'   | 25:BA:142(A):C:OP2 | 2.11                     | 0.49              |
| 25:BA:614:U:O2    | 25:BA:614:U:O4'    | 2.30                     | 0.49              |
| 25:BA:1706:U:H5'' | 25:BA:1707:G:OP2   | 2.11                     | 0.49              |
| 25:BA:1819:A:C1'  | 25:BA:1821:A:C5    | 2.94                     | 0.49              |
| 25:BA:1838:C:N4   | 25:BA:1898:U:H2'   | 2.26                     | 0.49              |
| 25:BA:2078:C:N4   | 25:BA:2079:U:O4    | 2.45                     | 0.49              |
| 33:BI:64:GLU:C    | 33:BI:66:GLU:N     | 2.68                     | 0.49              |
| 34:BN:47:ALA:HB2  | 34:BN:112:LEU:CD1  | 2.41                     | 0.49              |
| 34:BN:111:PRO:HA  | 34:BN:114:ARG:NH1  | 2.27                     | 0.49              |
| 39:BS:17:ARG:CA   | 39:BS:20:ARG:HH12  | 2.22                     | 0.49              |
| 40:BT:53:ARG:HG2  | 40:BT:53:ARG:NH1   | 2.26                     | 0.49              |
| 40:BT:86:ILE:HG12 | 40:BT:87:ASP:N     | 2.27                     | 0.49              |
| 42:BV:31:ALA:O    | 42:BV:61:VAL:N     | 2.45                     | 0.49              |
| 47:B0:5:LYS:NZ    | 47:B0:5:LYS:HB3    | 2.27                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 50:B3:29:ARG:HB2   | 50:B3:30:ARG:HG3   | 1.93                     | 0.49              |
| 55:B8:4:MET:O      | 55:B8:62:LEU:CD1   | 2.60                     | 0.49              |
| 55:B8:60:LEU:HD23  | 55:B8:60:LEU:N     | 2.26                     | 0.49              |
| 1:CA:429:U:O2'     | 1:CA:430:A:H5''    | 2.11                     | 0.49              |
| 1:CA:470:C:OP1     | 1:CA:470:C:O4'     | 2.30                     | 0.49              |
| 1:CA:578:C:O2'     | 1:CA:728:A:N3      | 2.41                     | 0.49              |
| 7:CG:50:ILE:O      | 7:CG:54:THR:HG23   | 2.11                     | 0.49              |
| 12:CL:82:VAL:HG12  | 12:CL:83:VAL:N     | 2.27                     | 0.49              |
| 14:CN:28:GLY:O     | 14:CN:29:ARG:O     | 2.30                     | 0.49              |
| 17:CQ:43:LEU:HD12  | 17:CQ:68:ARG:HG2   | 1.94                     | 0.49              |
| 18:CR:26:LEU:HD21  | 18:CR:42:ARG:NE    | 2.27                     | 0.49              |
| 23:CW:18:G:H1      | 23:CW:55:U:C1'     | 2.23                     | 0.49              |
| 23:CY:28:G:C2      | 23:CY:43:C:C4      | 3.00                     | 0.49              |
| 25:DA:182:A:N3     | 25:DA:433:C:O2'    | 2.42                     | 0.49              |
| 25:DA:271(M):G:H4' | 33:DI:53:ALA:HB2   | 1.94                     | 0.49              |
| 25:DA:748:G:OP1    | 25:DA:2612:C:N4    | 2.45                     | 0.49              |
| 25:DA:1689:A:N6    | 25:DA:1698:A:H2    | 2.06                     | 0.49              |
| 25:DA:2467:C:O2    | 37:DQ:124:LYS:NZ   | 2.38                     | 0.49              |
| 25:DA:2849:U:OP2   | 40:DT:95:ARG:NH1   | 2.40                     | 0.49              |
| 27:DC:154:ARG:C    | 27:DC:156:ILE:H    | 2.20                     | 0.49              |
| 29:DE:8:LYS:O      | 29:DE:193:GLY:N    | 2.43                     | 0.49              |
| 31:DG:97:ASP:H     | 31:DG:100:TRP:HD1  | 1.59                     | 0.49              |
| 31:DG:115:ARG:CG   | 31:DG:115:ARG:HH11 | 2.25                     | 0.49              |
| 33:DI:29:TYR:HD1   | 33:DI:33:ARG:HE    | 1.60                     | 0.49              |
| 33:DI:129:THR:HA   | 33:DI:137:PRO:HA   | 1.94                     | 0.49              |
| 35:DO:18:LYS:HD2   | 35:DO:45:GLU:CD    | 2.37                     | 0.49              |
| 36:DP:92:GLU:HA    | 36:DP:123:LEU:CD1  | 2.43                     | 0.49              |
| 37:DQ:34:LEU:CD1   | 37:DQ:129:THR:HB   | 2.40                     | 0.49              |
| 37:DQ:54:MET:CB    | 37:DQ:64:ILE:HD13  | 2.34                     | 0.49              |
| 38:DR:94:TYR:H     | 38:DR:94:TYR:HD1   | 1.58                     | 0.49              |
| 39:DS:66:ALA:O     | 39:DS:69:VAL:CG1   | 2.60                     | 0.49              |
| 41:DU:74:LEU:C     | 41:DU:74:LEU:HD12  | 2.37                     | 0.49              |
| 47:D0:49:LYS:HB2   | 47:D0:80:HIS:HB3   | 1.92                     | 0.49              |
| 1:AA:366:C:O2'     | 1:AA:367:U:O5'     | 2.30                     | 0.49              |
| 1:AA:1067:A:O2'    | 1:AA:1068:G:OP2    | 2.30                     | 0.49              |
| 2:AB:8:LYS:HZ3     | 2:AB:217:ARG:HH12  | 1.60                     | 0.49              |
| 4:AD:31:CYS:O      | 4:AD:33:MET:N      | 2.45                     | 0.49              |
| 5:AE:139:LEU:C     | 5:AE:141:GLN:N     | 2.70                     | 0.49              |
| 6:AF:69:GLU:N      | 6:AF:69:GLU:OE2    | 2.45                     | 0.49              |
| 9:AI:43:ALA:C      | 9:AI:45:ALA:H      | 2.19                     | 0.49              |
| 10:AJ:50:ILE:N     | 10:AJ:50:ILE:CD1   | 2.61                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:AN:12:ARG:HB3  | 14:AN:14:PRO:CD   | 2.43                     | 0.49              |
| 16:AP:50:LYS:HD3  | 16:AP:51:VAL:N    | 2.27                     | 0.49              |
| 16:AP:53:VAL:O    | 16:AP:57:ARG:HG2  | 2.12                     | 0.49              |
| 18:AR:44:LEU:HD11 | 18:AR:79:LEU:HD13 | 1.94                     | 0.49              |
| 18:AR:70:ILE:HG22 | 18:AR:74:ARG:HD2  | 1.95                     | 0.49              |
| 19:AS:39:THR:CG2  | 19:AS:40:ILE:N    | 2.74                     | 0.49              |
| 20:AT:63:ILE:CD1  | 20:AT:80:ARG:HB2  | 2.42                     | 0.49              |
| 23:AY:30:G:H5'    | 23:AY:31:A:OP2    | 2.11                     | 0.49              |
| 25:BA:1276:A:O2'  | 38:BR:16:HIS:HE1  | 1.95                     | 0.49              |
| 25:BA:1299:G:O4'  | 25:BA:1301:A:C8   | 2.65                     | 0.49              |
| 25:BA:1341:U:O4   | 44:BX:16:LYS:CE   | 2.58                     | 0.49              |
| 25:BA:1693:U:O4   | 25:BA:1976:U:O2'  | 2.27                     | 0.49              |
| 25:BA:2065:C:H1'  | 25:BA:2449:U:O2   | 2.12                     | 0.49              |
| 25:BA:2125:G:N1   | 25:BA:2172:U:OP2  | 2.41                     | 0.49              |
| 25:BA:2468:G:H2'  | 25:BA:2476:A:H8   | 1.78                     | 0.49              |
| 26:BB:104:U:O2'   | 46:BZ:72:ARG:HG3  | 2.11                     | 0.49              |
| 28:BD:108:PRO:HB3 | 28:BD:143:HIS:CE1 | 2.48                     | 0.49              |
| 32:BH:82:GLY:O    | 32:BH:135:GLY:O   | 2.30                     | 0.49              |
| 36:BP:57:THR:O    | 36:BP:60:MET:HG3  | 2.12                     | 0.49              |
| 37:BQ:46:GLN:O    | 37:BQ:48:GLU:N    | 2.46                     | 0.49              |
| 41:BU:88:ILE:C    | 41:BU:90:VAL:H    | 2.21                     | 0.49              |
| 45:BY:19:LYS:HB2  | 45:BY:19:LYS:HZ3  | 1.77                     | 0.49              |
| 48:B1:13:ILE:O    | 48:B1:41:ARG:HA   | 2.11                     | 0.49              |
| 48:B1:64:ALA:O    | 48:B1:67:ILE:CD1  | 2.60                     | 0.49              |
| 1:CA:60:A:O2'     | 1:CA:61:G:O5'     | 2.30                     | 0.49              |
| 1:CA:129:U:O3'    | 1:CA:130:A:OP1    | 2.30                     | 0.49              |
| 1:CA:129(A):G:H4' | 1:CA:130:A:O5'    | 2.12                     | 0.49              |
| 1:CA:664:G:H22    | 1:CA:741:G:H1     | 1.60                     | 0.49              |
| 3:CC:119:ARG:O    | 3:CC:123:GLN:HG3  | 2.12                     | 0.49              |
| 7:CG:37:ASN:O     | 7:CG:41:ARG:HG3   | 2.12                     | 0.49              |
| 7:CG:155:ARG:O    | 7:CG:156:TRP:O    | 2.30                     | 0.49              |
| 8:CH:81:HIS:N     | 8:CH:138:TRP:O    | 2.45                     | 0.49              |
| 9:CI:112:LYS:HA   | 9:CI:119:ALA:HA   | 1.94                     | 0.49              |
| 10:CJ:57:LYS:O    | 10:CJ:58:ASP:OD1  | 2.30                     | 0.49              |
| 20:CT:29:LYS:O    | 20:CT:29:LYS:HG3  | 2.11                     | 0.49              |
| 22:CV:76:C:O5'    | 22:CV:77:A:OP2    | 2.30                     | 0.49              |
| 23:CW:36:A:N1     | 23:CW:37:A:C4     | 2.81                     | 0.49              |
| 25:DA:13:A:N3     | 25:DA:15:G:C6     | 2.80                     | 0.49              |
| 25:DA:583:G:OP2   | 41:DU:10:ARG:NH1  | 2.41                     | 0.49              |
| 25:DA:1565:C:O2'  | 25:DA:1566:A:H8   | 1.95                     | 0.49              |
| 27:DC:77:ILE:HB   | 27:DC:122:ALA:HA  | 1.94                     | 0.49              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 28:DD:11:PRO:C    | 28:DD:13:ARG:N     | 2.61                     | 0.49              |
| 28:DD:17:THR:O    | 28:DD:211:ARG:NH2  | 2.45                     | 0.49              |
| 28:DD:31:LYS:O    | 28:DD:32:SER:C     | 2.55                     | 0.49              |
| 28:DD:270:ILE:C   | 28:DD:271:ILE:HG12 | 2.37                     | 0.49              |
| 31:DG:77:ILE:O    | 31:DG:77:ILE:CG2   | 2.60                     | 0.49              |
| 31:DG:110:ALA:O   | 31:DG:111:LEU:C    | 2.56                     | 0.49              |
| 32:DH:34:GLU:O    | 32:DH:36:PRO:HD3   | 2.12                     | 0.49              |
| 34:DN:59:LYS:O    | 34:DN:60:ILE:C     | 2.55                     | 0.49              |
| 37:DQ:12:GLN:NE2  | 37:DQ:72:LYS:HG3   | 2.28                     | 0.49              |
| 37:DQ:34:LEU:HD12 | 37:DQ:130:LYS:O    | 2.13                     | 0.49              |
| 37:DQ:54:MET:HG2  | 37:DQ:64:ILE:CG2   | 2.42                     | 0.49              |
| 40:DT:130:ALA:O   | 40:DT:131:ALA:C    | 2.55                     | 0.49              |
| 42:DV:99:ILE:HD13 | 42:DV:99:ILE:N     | 2.25                     | 0.49              |
| 49:D2:65:ASN:HB3  | 49:D2:69:ARG:NH2   | 2.27                     | 0.49              |
| 1:AA:375:U:O2'    | 16:AP:28:ARG:HD2   | 2.12                     | 0.49              |
| 1:AA:495:A:O2'    | 1:AA:496:A:O5'     | 2.24                     | 0.49              |
| 1:AA:962:C:H2'    | 1:AA:963:G:C8      | 2.44                     | 0.49              |
| 1:AA:1356:G:H2'   | 1:AA:1357:A:C8     | 2.46                     | 0.49              |
| 1:AA:1423:G:H5'   | 35:BO:49:ARG:NH2   | 2.15                     | 0.49              |
| 4:AD:151:LYS:HG2  | 4:AD:151:LYS:O     | 2.13                     | 0.49              |
| 4:AD:206:PHE:O    | 4:AD:206:PHE:CG    | 2.64                     | 0.49              |
| 5:AE:105:VAL:HG11 | 5:AE:131:ILE:HG22  | 1.94                     | 0.49              |
| 9:AI:35:GLU:O     | 9:AI:38:GLN:HB2    | 2.12                     | 0.49              |
| 10:AJ:5:ARG:HA    | 10:AJ:73:ASP:CG    | 2.37                     | 0.49              |
| 13:AM:90:LEU:O    | 13:AM:91:ARG:HB2   | 2.12                     | 0.49              |
| 25:BA:589:C:H2'   | 25:BA:590:A:C8     | 2.47                     | 0.49              |
| 25:BA:974:G:C2    | 25:BA:989:G:N3     | 2.81                     | 0.49              |
| 25:BA:1453:U:C4'  | 25:BA:1455:G:OP1   | 2.42                     | 0.49              |
| 25:BA:2406:U:N3   | 36:BP:73:GLY:O     | 2.39                     | 0.49              |
| 28:BD:206:LEU:CD2 | 28:BD:211:ARG:HG2  | 2.40                     | 0.49              |
| 29:BE:108:SER:O   | 29:BE:162:ALA:HA   | 2.12                     | 0.49              |
| 39:BS:103:GLU:O   | 39:BS:104:GLY:C    | 2.56                     | 0.49              |
| 49:B2:68:ARG:O    | 49:B2:72:ALA:HB3   | 2.12                     | 0.49              |
| 51:B4:40:ILE:HG13 | 51:B4:57:ILE:CG2   | 2.23                     | 0.49              |
| 5:CE:132:ALA:O    | 5:CE:135:THR:N     | 2.40                     | 0.49              |
| 9:CI:11:LYS:C     | 9:CI:13:ALA:H      | 2.19                     | 0.49              |
| 10:CJ:96:ILE:N    | 10:CJ:96:ILE:HD13  | 2.27                     | 0.49              |
| 20:CT:14:LYS:C    | 20:CT:16:HIS:N     | 2.69                     | 0.49              |
| 25:DA:1963:U:O2   | 25:DA:1963:U:H5'   | 2.12                     | 0.49              |
| 25:DA:2720:U:H3'  | 25:DA:2721:A:H8    | 1.77                     | 0.49              |
| 29:DE:56:PRO:O    | 29:DE:57:LYS:C     | 2.55                     | 0.49              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 29:DE:88:GLY:O     | 29:DE:89:ASP:HB2  | 2.12                     | 0.49              |
| 31:DG:61:ALA:HB2   | 31:DG:68:PRO:HD3  | 1.95                     | 0.49              |
| 31:DG:73:ALA:O     | 31:DG:84:LYS:O    | 2.30                     | 0.49              |
| 33:DI:18:VAL:HG12  | 33:DI:18:VAL:O    | 2.10                     | 0.49              |
| 33:DI:54:GLN:O     | 33:DI:58:LEU:HB2  | 2.12                     | 0.49              |
| 33:DI:57:ARG:O     | 33:DI:61:ARG:HG2  | 2.12                     | 0.49              |
| 34:DN:5:VAL:HG22   | 34:DN:6:PRO:O     | 2.12                     | 0.49              |
| 34:DN:134:ARG:N    | 34:DN:135:PRO:HD3 | 2.27                     | 0.49              |
| 36:DP:91:PHE:CD1   | 36:DP:91:PHE:N    | 2.80                     | 0.49              |
| 41:DU:110:VAL:HG12 | 41:DU:114:LYS:HD2 | 1.94                     | 0.49              |
| 42:DV:35:LEU:C     | 42:DV:37:VAL:H    | 2.20                     | 0.49              |
| 42:DV:35:LEU:CD2   | 42:DV:57:VAL:HG22 | 2.28                     | 0.49              |
| 42:DV:40:LEU:HD23  | 42:DV:47:VAL:HA   | 1.93                     | 0.49              |
| 46:DZ:53:ILE:HG23  | 46:DZ:71:VAL:HG23 | 1.94                     | 0.49              |
| 53:D6:43:CYS:O     | 53:D6:44:ARG:O    | 2.30                     | 0.49              |
| 1:AA:429:U:H4'     | 1:AA:430:A:O5'    | 2.12                     | 0.49              |
| 1:AA:971:G:OP1     | 1:AA:972:C:O5'    | 2.30                     | 0.49              |
| 1:AA:1285:A:H4'    | 1:AA:1286:A:O5'   | 2.13                     | 0.49              |
| 1:AA:1298:C:C4     | 7:AG:114:ARG:HD2  | 2.47                     | 0.49              |
| 1:AA:1298:C:H1'    | 1:AA:1299:A:C6    | 2.47                     | 0.49              |
| 2:AB:17:PHE:HD2    | 2:AB:17:PHE:H     | 1.59                     | 0.49              |
| 3:AC:122:GLU:OE1   | 3:AC:126:ARG:NH2  | 2.46                     | 0.49              |
| 3:AC:147:LYS:HB2   | 3:AC:203:PHE:CD2  | 2.47                     | 0.49              |
| 12:AL:46:LYS:CG    | 12:AL:47:LYS:N    | 2.71                     | 0.49              |
| 25:BA:793:A:OP2    | 25:BA:2071:A:O2'  | 2.25                     | 0.49              |
| 25:BA:2466:C:OP1   | 56:B9:4:ARG:HB2   | 2.12                     | 0.49              |
| 25:BA:2638:G:OP2   | 29:BE:82:ARG:NH2  | 2.46                     | 0.49              |
| 25:BA:2691:C:C6    | 25:BA:2872:G:C6   | 3.01                     | 0.49              |
| 25:BA:2848:G:N7    | 40:BT:97:ALA:HB2  | 2.27                     | 0.49              |
| 25:BA:2875:C:H4'   | 40:BT:5:ALA:HB2   | 1.94                     | 0.49              |
| 30:BF:32:LEU:O     | 30:BF:36:VAL:HG22 | 2.11                     | 0.49              |
| 31:BG:88:ILE:HG13  | 31:BG:89:GLY:N    | 2.27                     | 0.49              |
| 31:BG:101:ILE:HG13 | 51:B4:51:TYR:O    | 2.12                     | 0.49              |
| 34:BN:91:LEU:HD23  | 34:BN:98:VAL:HG21 | 1.94                     | 0.49              |
| 34:BN:123:TYR:CE1  | 34:BN:130:HIS:HE1 | 2.25                     | 0.49              |
| 38:BR:2:ARG:HH22   | 38:BR:5:LYS:HZ3   | 1.60                     | 0.49              |
| 40:BT:57:PHE:O     | 40:BT:58:ASN:C    | 2.55                     | 0.49              |
| 41:BU:18:LEU:O     | 41:BU:19:LYS:C    | 2.55                     | 0.49              |
| 41:BU:45:TYR:O     | 41:BU:46:ALA:C    | 2.53                     | 0.49              |
| 42:BV:62:LEU:HD13  | 42:BV:95:LEU:HB2  | 1.94                     | 0.49              |
| 46:BZ:17:ALA:HA    | 46:BZ:20:ARG:HB2  | 1.94                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 46:BZ:103:ARG:HD3  | 46:BZ:136:PHE:CZ   | 2.47                     | 0.49              |
| 48:B1:90:ILE:CG2   | 48:B1:94:LEU:HD12  | 2.30                     | 0.49              |
| 50:B3:26:LEU:O     | 50:B3:35:ARG:HD3   | 2.12                     | 0.49              |
| 52:B5:42:PRO:O     | 52:B5:43:HIS:HB2   | 2.13                     | 0.49              |
| 1:CA:60:A:O2'      | 1:CA:61:G:OP2      | 2.30                     | 0.49              |
| 1:CA:128:G:H4'     | 17:CQ:3:LYS:HG2    | 1.94                     | 0.49              |
| 1:CA:686:U:O2'     | 1:CA:687:A:OP2     | 2.26                     | 0.49              |
| 1:CA:838:G:H2'     | 1:CA:839:U:H5''    | 1.94                     | 0.49              |
| 1:CA:922:G:H4'     | 5:CE:20:GLN:HA     | 1.94                     | 0.49              |
| 1:CA:1239:A:N6     | 1:CA:1297:C:O4'    | 2.43                     | 0.49              |
| 2:CB:15:VAL:HG21   | 2:CB:209:ARG:NH2   | 2.27                     | 0.49              |
| 5:CE:20:GLN:O      | 5:CE:21:ALA:C      | 2.55                     | 0.49              |
| 7:CG:121:ALA:O     | 7:CG:124:LEU:N     | 2.45                     | 0.49              |
| 9:CI:89:ASN:C      | 9:CI:91:ASP:N      | 2.71                     | 0.49              |
| 10:CJ:6:ILE:HG12   | 10:CJ:72:VAL:O     | 2.12                     | 0.49              |
| 13:CM:8:GLU:OE1    | 13:CM:67:GLU:HB2   | 2.12                     | 0.49              |
| 18:CR:53:ARG:HH21  | 18:CR:60:ALA:N     | 2.10                     | 0.49              |
| 20:CT:29:LYS:CG    | 20:CT:29:LYS:O     | 2.59                     | 0.49              |
| 23:CW:16:U:H3'     | 23:CW:17:C:C5'     | 2.36                     | 0.49              |
| 25:DA:614(C):A:O2' | 25:DA:615:G:O4'    | 2.30                     | 0.49              |
| 25:DA:2046:G:O5'   | 52:D5:19:ARG:HA    | 2.13                     | 0.49              |
| 25:DA:2068:U:N3    | 25:DA:2430:A:H2    | 2.09                     | 0.49              |
| 25:DA:2469:A:H3'   | 25:DA:2470:G:O4'   | 2.11                     | 0.49              |
| 29:DE:111:ARG:NE   | 29:DE:160:TYR:HE1  | 2.10                     | 0.49              |
| 29:DE:111:ARG:NE   | 29:DE:160:TYR:CE1  | 2.80                     | 0.49              |
| 31:DG:4:ASP:O      | 31:DG:5:VAL:HB     | 2.13                     | 0.49              |
| 31:DG:120:LEU:O    | 31:DG:122:PRO:HD3  | 2.12                     | 0.49              |
| 33:DI:76:THR:CG2   | 33:DI:139:GLN:HE22 | 2.24                     | 0.49              |
| 36:DP:31:ALA:C     | 36:DP:32:THR:CG2   | 2.86                     | 0.49              |
| 36:DP:118:GLY:O    | 36:DP:119:GLU:C    | 2.55                     | 0.49              |
| 39:DS:106:ARG:HB3  | 39:DS:110:LEU:HD13 | 1.93                     | 0.49              |
| 40:DT:86:ILE:HG12  | 40:DT:87:ASP:H     | 1.78                     | 0.49              |
| 41:DU:111:GLU:O    | 41:DU:113:ALA:N    | 2.45                     | 0.49              |
| 42:DV:35:LEU:HD22  | 42:DV:57:VAL:O     | 2.12                     | 0.49              |
| 43:DW:73:ALA:O     | 43:DW:106:ILE:HG12 | 2.12                     | 0.49              |
| 45:DY:38:ILE:CG2   | 45:DY:66:PRO:HG3   | 2.43                     | 0.49              |
| 47:D0:51:VAL:HG21  | 47:D0:80:HIS:HA    | 1.95                     | 0.49              |
| 47:D0:72:ARG:CB    | 47:D0:75:LEU:HB3   | 2.41                     | 0.49              |
| 49:D2:13:ALA:HA    | 49:D2:16:LEU:HG    | 1.94                     | 0.49              |
| 52:D5:40:LYS:HD2   | 52:D5:40:LYS:C     | 2.37                     | 0.49              |
| 53:D6:45:LYS:O     | 53:D6:46:HIS:CB    | 2.59                     | 0.49              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 54:D7:24:THR:HG23  | 54:D7:27:GLY:N    | 2.27                     | 0.49              |
| 1:AA:243:A:O2'     | 1:AA:244:U:OP2    | 2.30                     | 0.49              |
| 1:AA:503:C:OP2     | 12:AL:116:SER:HB3 | 2.12                     | 0.49              |
| 1:AA:580:U:H2'     | 1:AA:581:G:O4'    | 2.12                     | 0.49              |
| 2:AB:52:GLU:O      | 2:AB:53:ARG:C     | 2.54                     | 0.49              |
| 3:AC:61:ALA:O      | 3:AC:62:ASP:CB    | 2.61                     | 0.49              |
| 7:AG:57:GLU:O      | 7:AG:58:PRO:C     | 2.55                     | 0.49              |
| 8:AH:103:VAL:HG21  | 8:AH:109:ILE:O    | 2.13                     | 0.49              |
| 10:AJ:90:LEU:N     | 10:AJ:90:LEU:HD12 | 2.28                     | 0.49              |
| 12:AL:26:ALA:O     | 12:AL:27:LEU:CB   | 2.56                     | 0.49              |
| 13:AM:13:LYS:HA    | 13:AM:44:ARG:HH11 | 1.77                     | 0.49              |
| 13:AM:80:ARG:NH1   | 19:AS:69:HIS:NE2  | 2.57                     | 0.49              |
| 13:AM:92:HIS:CE1   | 13:AM:98:VAL:HG21 | 2.48                     | 0.49              |
| 19:AS:43:GLU:HA    | 19:AS:45:VAL:CG1  | 2.42                     | 0.49              |
| 20:AT:13:LEU:C     | 20:AT:13:LEU:HD12 | 2.37                     | 0.49              |
| 22:AV:49:C:O4'     | 22:AV:49:C:O2     | 2.28                     | 0.49              |
| 22:AV:53:G:O2'     | 22:AV:54:G:OP1    | 2.30                     | 0.49              |
| 23:AW:34:G:C5      | 24:AX:14:A:N1     | 2.78                     | 0.49              |
| 25:BA:34:C:HO2'    | 25:BA:35:G:P      | 2.36                     | 0.49              |
| 25:BA:662:G:H4'    | 36:BP:15:ARG:O    | 2.13                     | 0.49              |
| 25:BA:705:A:C8     | 25:BA:727:A:N3    | 2.81                     | 0.49              |
| 25:BA:855:G:H1     | 25:BA:922:U:H3    | 1.61                     | 0.49              |
| 25:BA:1252:G:O2'   | 41:BU:33:ARG:NH1  | 2.46                     | 0.49              |
| 25:BA:1348:G:H2'   | 25:BA:1349:A:H5'' | 1.95                     | 0.49              |
| 25:BA:2126:A:O2'   | 25:BA:2127:G:P    | 2.70                     | 0.49              |
| 25:BA:2181:G:H2'   | 25:BA:2182:G:C8   | 2.46                     | 0.49              |
| 25:BA:2370:G:H21   | 53:B6:45:LYS:HZ1  | 1.59                     | 0.49              |
| 27:BC:21:THR:HG21  | 27:BC:191:ALA:HB2 | 1.95                     | 0.49              |
| 28:BD:142:VAL:HG23 | 28:BD:193:VAL:HA  | 1.94                     | 0.49              |
| 28:BD:264:LYS:HG3  | 28:BD:265:PRO:HD2 | 1.94                     | 0.49              |
| 29:BE:8:LYS:HD3    | 29:BE:191:PRO:O   | 2.12                     | 0.49              |
| 29:BE:31:CYS:HB3   | 29:BE:49:LEU:HD23 | 1.94                     | 0.49              |
| 29:BE:113:PHE:CE2  | 29:BE:158:GLY:HA2 | 2.47                     | 0.49              |
| 30:BF:51:THR:HG22  | 30:BF:92:PRO:HG2  | 1.94                     | 0.49              |
| 31:BG:48:GLU:O     | 31:BG:49:ASP:CB   | 2.60                     | 0.49              |
| 34:BN:57:ALA:O     | 34:BN:58:ASP:C    | 2.56                     | 0.49              |
| 35:BO:2:ILE:CD1    | 35:BO:6:THR:HG21  | 2.41                     | 0.49              |
| 38:BR:97:VAL:HA    | 38:BR:113:LEU:O   | 2.13                     | 0.49              |
| 39:BS:26:LEU:O     | 39:BS:88:ASP:HB3  | 2.12                     | 0.49              |
| 46:BZ:19:ARG:NH1   | 46:BZ:82:ARG:HH21 | 2.11                     | 0.49              |
| 46:BZ:71:VAL:HG22  | 46:BZ:88:PHE:HE2  | 1.77                     | 0.49              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 50:B3:39:ASP:OD2  | 50:B3:39:ASP:O     | 2.30                     | 0.49              |
| 1:CA:64:G:N2      | 1:CA:68:G:O6       | 2.40                     | 0.49              |
| 1:CA:748:C:O2'    | 1:CA:749:C:OP2     | 2.30                     | 0.49              |
| 1:CA:757:U:H2'    | 1:CA:758:G:O4'     | 2.13                     | 0.49              |
| 1:CA:1213:A:C6    | 1:CA:1215:G:H1'    | 2.47                     | 0.49              |
| 2:CB:178:ARG:HH12 | 2:CB:196:LEU:C     | 2.20                     | 0.49              |
| 6:CF:3:ARG:HH11   | 6:CF:3:ARG:HG3     | 1.77                     | 0.49              |
| 8:CH:48:TYR:CD2   | 8:CH:48:TYR:N      | 2.81                     | 0.49              |
| 11:CK:57:THR:CG2  | 11:CK:58:PRO:HD2   | 2.43                     | 0.49              |
| 13:CM:66:LEU:HD12 | 13:CM:66:LEU:N     | 2.26                     | 0.49              |
| 16:CP:21:VAL:O    | 16:CP:33:ILE:HG12  | 2.13                     | 0.49              |
| 18:CR:19:LYS:O    | 18:CR:20:ALA:CB    | 2.60                     | 0.49              |
| 18:CR:33:ASP:OD1  | 18:CR:36:ASN:OD1   | 2.30                     | 0.49              |
| 18:CR:53:ARG:NH2  | 18:CR:60:ALA:N     | 2.61                     | 0.49              |
| 23:CW:55:U:H3'    | 23:CW:55:U:O2      | 2.12                     | 0.49              |
| 24:CX:16:A:C4     | 24:CX:17:U:C5      | 3.00                     | 0.49              |
| 23:CY:28:G:C2     | 23:CY:43:C:N3      | 2.81                     | 0.49              |
| 25:DA:74:A:H4'    | 25:DA:75:G:O5'     | 2.12                     | 0.49              |
| 25:DA:749:C:N3    | 25:DA:1618:A:C2    | 2.81                     | 0.49              |
| 25:DA:1140:C:C4'  | 25:DA:1143:A:C6    | 2.94                     | 0.49              |
| 25:DA:1340:U:C4'  | 25:DA:1341:U:OP2   | 2.58                     | 0.49              |
| 25:DA:2233:U:H2'  | 25:DA:2234:G:C8    | 2.48                     | 0.49              |
| 26:DB:13:A:O2'    | 26:DB:15:A:OP2     | 2.31                     | 0.49              |
| 27:DC:78:ALA:C    | 27:DC:80:GLY:H     | 2.20                     | 0.49              |
| 28:DD:261:LYS:HZ1 | 28:DD:263:ARG:NH1  | 2.11                     | 0.49              |
| 29:DE:65:GLY:HA2  | 29:DE:70:ALA:HB2   | 1.94                     | 0.49              |
| 29:DE:78:LEU:O    | 29:DE:79:ARG:HD2   | 2.12                     | 0.49              |
| 30:DF:39:TRP:CB   | 30:DF:101:LEU:HD22 | 2.43                     | 0.49              |
| 30:DF:42:ALA:O    | 30:DF:45:ARG:HB2   | 2.13                     | 0.49              |
| 30:DF:183:VAL:O   | 30:DF:187:VAL:HG23 | 2.13                     | 0.49              |
| 32:DH:153:LYS:HG2 | 32:DH:162:ILE:CG1  | 2.41                     | 0.49              |
| 34:DN:108:PRO:O   | 34:DN:113:GLY:HA3  | 2.13                     | 0.49              |
| 45:DY:14:LEU:HD23 | 45:DY:14:LEU:O     | 2.12                     | 0.49              |
| 46:DZ:43:GLU:O    | 46:DZ:47:VAL:HG12  | 2.12                     | 0.49              |
| 2:AB:213:LEU:HD23 | 2:AB:213:LEU:C     | 2.38                     | 0.49              |
| 5:AE:76:ILE:HG12  | 5:AE:142:LEU:CD1   | 2.41                     | 0.49              |
| 12:AL:83:VAL:HG22 | 12:AL:100:ILE:CG2  | 2.43                     | 0.49              |
| 12:AL:117:ARG:NH2 | 12:AL:124:LYS:HA   | 2.28                     | 0.49              |
| 19:AS:11:VAL:HA   | 19:AS:38:SER:CB    | 2.38                     | 0.49              |
| 20:AT:63:ILE:CD1  | 20:AT:81:LYS:CG    | 2.91                     | 0.49              |
| 23:AW:49:C:O2'    | 23:AW:50:U:H5'     | 2.12                     | 0.49              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 24:AX:19:U:O5'     | 24:AX:19:U:H6     | 1.96                     | 0.49              |
| 25:BA:601:C:H4'    | 30:BF:104:LYS:HZ3 | 1.77                     | 0.49              |
| 25:BA:614(C):A:O2' | 25:BA:615:G:O4'   | 2.30                     | 0.49              |
| 25:BA:748:G:C8     | 43:BW:89:ALA:HB1  | 2.48                     | 0.49              |
| 25:BA:792:G:H5''   | 25:BA:793:A:H5'   | 1.95                     | 0.49              |
| 25:BA:988:A:H5''   | 50:B3:11:SER:HB2  | 1.95                     | 0.49              |
| 25:BA:1525:G:H2'   | 25:BA:1526:G:H8   | 1.77                     | 0.49              |
| 25:BA:2894:G:N3    | 25:BA:2894:G:H2'  | 2.28                     | 0.49              |
| 29:BE:32:PRO:HA    | 29:BE:90:THR:HA   | 1.95                     | 0.49              |
| 29:BE:37:ARG:C     | 29:BE:38:THR:O    | 2.55                     | 0.49              |
| 33:BI:131:LYS:HE3  | 33:BI:132:PRO:CD  | 2.43                     | 0.49              |
| 36:BP:31:ALA:C     | 36:BP:32:THR:CG2  | 2.86                     | 0.49              |
| 37:BQ:54:MET:HE1   | 37:BQ:104:PHE:CD2 | 2.47                     | 0.49              |
| 38:BR:95:THR:O     | 38:BR:95:THR:HG23 | 2.11                     | 0.49              |
| 39:BS:46:VAL:HG12  | 39:BS:47:THR:N    | 2.26                     | 0.49              |
| 39:BS:85:VAL:HG23  | 39:BS:86:ALA:N    | 2.27                     | 0.49              |
| 39:BS:92:TYR:N     | 39:BS:92:TYR:CD1  | 2.80                     | 0.49              |
| 41:BU:79:PHE:CE2   | 41:BU:83:LEU:HD22 | 2.47                     | 0.49              |
| 42:BV:62:LEU:CD1   | 42:BV:95:LEU:HB2  | 2.42                     | 0.49              |
| 43:BW:8:ARG:HH11   | 43:BW:8:ARG:CB    | 2.25                     | 0.49              |
| 47:B0:54:GLY:O     | 47:B0:56:ASP:N    | 2.46                     | 0.49              |
| 49:B2:19:VAL:HA    | 49:B2:22:GLU:HG3  | 1.94                     | 0.49              |
| 50:B3:7:LYS:CB     | 50:B3:34:GLU:HG2  | 2.42                     | 0.49              |
| 1:CA:1064:G:C4'    | 1:CA:1065:U:H5'   | 2.39                     | 0.49              |
| 5:CE:84:PHE:O      | 5:CE:86:ALA:N     | 2.39                     | 0.49              |
| 9:CI:53:VAL:HG23   | 9:CI:55:ALA:H     | 1.78                     | 0.49              |
| 10:CJ:78:ASN:ND2   | 10:CJ:80:LYS:N    | 2.48                     | 0.49              |
| 12:CL:113:ARG:HH21 | 12:CL:116:SER:H   | 1.59                     | 0.49              |
| 19:CS:67:VAL:HG12  | 19:CS:68:GLY:N    | 2.27                     | 0.49              |
| 20:CT:89:ARG:HB2   | 20:CT:104:LEU:CD1 | 2.43                     | 0.49              |
| 22:CV:35:C:H2'     | 22:CV:36:A:C8     | 2.47                     | 0.49              |
| 25:DA:1636:C:H2'   | 25:DA:1637:A:C8   | 2.47                     | 0.49              |
| 25:DA:2182:G:H2'   | 25:DA:2183:C:C6   | 2.48                     | 0.49              |
| 25:DA:2311:A:C1'   | 31:DG:82:LEU:HD11 | 2.41                     | 0.49              |
| 25:DA:2572:A:N7    | 29:DE:144:ARG:NE  | 2.58                     | 0.49              |
| 28:DD:43:ARG:NH1   | 28:DD:44:ASN:HD21 | 2.07                     | 0.49              |
| 28:DD:209:ALA:C    | 28:DD:210:GLY:O   | 2.54                     | 0.49              |
| 28:DD:270:ILE:HD12 | 28:DD:270:ILE:O   | 2.13                     | 0.49              |
| 29:DE:61:ARG:CB    | 29:DE:62:PRO:HD3  | 2.43                     | 0.49              |
| 29:DE:111:ARG:HB3  | 38:DR:1:MET:CE    | 2.42                     | 0.49              |
| 30:DF:123:LEU:HD13 | 30:DF:192:LEU:HB3 | 1.92                     | 0.49              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 31:DG:137:GLU:CB  | 31:DG:152:LEU:HD22 | 2.43                     | 0.49              |
| 32:DH:89:ILE:HA   | 32:DH:162:ILE:HA   | 1.94                     | 0.49              |
| 32:DH:127:GLU:HB2 | 32:DH:130:ARG:HD2  | 1.94                     | 0.49              |
| 33:DI:127:VAL:HA  | 33:DI:139:GLN:HA   | 1.95                     | 0.49              |
| 34:DN:38:HIS:NE2  | 34:DN:50:ASP:OD2   | 2.45                     | 0.49              |
| 36:DP:27:HIS:N    | 36:DP:27:HIS:ND1   | 2.59                     | 0.49              |
| 36:DP:109:GLY:O   | 36:DP:110:TYR:O    | 2.31                     | 0.49              |
| 38:DR:80:PHE:O    | 38:DR:85:PRO:HD3   | 2.12                     | 0.49              |
| 40:DT:6:LEU:O     | 40:DT:6:LEU:HD23   | 2.13                     | 0.49              |
| 43:DW:34:ASN:O    | 43:DW:37:ARG:HB3   | 2.13                     | 0.49              |
| 48:D1:53:VAL:HG22 | 48:D1:74:VAL:HG13  | 1.95                     | 0.49              |
| 49:D2:16:LEU:O    | 49:D2:17:SER:CB    | 2.61                     | 0.49              |
| 49:D2:67:LYS:C    | 49:D2:69:ARG:H     | 2.21                     | 0.49              |
| 53:D6:11:LEU:HD13 | 53:D6:12:GLU:N     | 2.28                     | 0.49              |
| 1:AA:689:C:H2'    | 1:AA:690:G:O4'     | 2.12                     | 0.49              |
| 1:AA:1186:G:H21   | 14:AN:61:TRP:C     | 2.21                     | 0.49              |
| 2:AB:114:ARG:NH1  | 2:AB:118:LEU:HD21  | 2.28                     | 0.49              |
| 7:AG:5:ARG:C      | 7:AG:7:ALA:H       | 2.20                     | 0.49              |
| 7:AG:15:ASP:N     | 7:AG:24:THR:HG21   | 2.28                     | 0.49              |
| 7:AG:135:VAL:O    | 7:AG:139:GLU:HG3   | 2.12                     | 0.49              |
| 18:AR:19:LYS:O    | 18:AR:20:ALA:CB    | 2.60                     | 0.49              |
| 20:AT:73:HIS:HB3  | 20:AT:74:LYS:HG2   | 1.93                     | 0.49              |
| 25:BA:300:A:H2'   | 25:BA:334:C:H1'    | 1.94                     | 0.49              |
| 25:BA:434:U:C4'   | 25:BA:435:C:OP1    | 2.32                     | 0.49              |
| 25:BA:726:G:H5'   | 25:BA:1432:C:O2'   | 2.13                     | 0.49              |
| 25:BA:1045:A:H2'  | 25:BA:1045:A:N3    | 2.28                     | 0.49              |
| 25:BA:1286:A:N1   | 25:BA:1289:C:C2    | 2.81                     | 0.49              |
| 25:BA:1495:A:H3'  | 25:BA:1496:A:C2    | 2.47                     | 0.49              |
| 25:BA:1803:A:O2'  | 28:BD:259:THR:HG21 | 2.13                     | 0.49              |
| 25:BA:2249:U:H1'  | 25:BA:2275:C:N4    | 2.27                     | 0.49              |
| 25:BA:2418:A:H2'  | 25:BA:2419:U:C6    | 2.48                     | 0.49              |
| 25:BA:2468:G:H22  | 25:BA:2481:G:H2'   | 1.78                     | 0.49              |
| 25:BA:2638:G:O2'  | 25:BA:2639:A:C8    | 2.66                     | 0.49              |
| 29:BE:195:LEU:O   | 29:BE:195:LEU:HG   | 2.11                     | 0.49              |
| 31:BG:9:ARG:O     | 31:BG:11:TYR:N     | 2.45                     | 0.49              |
| 31:BG:72:ARG:CD   | 31:BG:86:MET:CB    | 2.86                     | 0.49              |
| 31:BG:102:PHE:CE2 | 31:BG:141:PHE:HE1  | 2.29                     | 0.49              |
| 32:BH:132:ARG:O   | 32:BH:133:VAL:HG23 | 2.13                     | 0.49              |
| 32:BH:146:ALA:HB2 | 32:BH:164:TYR:OH   | 2.12                     | 0.49              |
| 33:BI:30:LEU:HD22 | 33:BI:35:LEU:HD12  | 1.94                     | 0.49              |
| 34:BN:82:LEU:CD2  | 34:BN:84:LYS:HE2   | 2.42                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 34:BN:94:HIS:N    | 34:BN:95:PRO:CD   | 2.75                     | 0.49              |
| 35:BO:104:ARG:CZ  | 35:BO:104:ARG:CB  | 2.90                     | 0.49              |
| 36:BP:15:ARG:HG3  | 36:BP:16:ARG:N    | 2.28                     | 0.49              |
| 37:BQ:132:VAL:HB  | 37:BQ:137:TYR:OH  | 2.13                     | 0.49              |
| 40:BT:92:GLY:O    | 40:BT:93:ARG:HB3  | 2.12                     | 0.49              |
| 45:BY:31:LEU:CD2  | 45:BY:36:ALA:O    | 2.58                     | 0.49              |
| 48:B1:29:GLY:O    | 48:B1:30:VAL:HG23 | 2.12                     | 0.49              |
| 51:B4:53:THR:O    | 51:B4:54:LYS:HG3  | 2.13                     | 0.49              |
| 55:B8:4:MET:O     | 55:B8:62:LEU:HD11 | 2.13                     | 0.49              |
| 55:B8:58:ILE:O    | 55:B8:61:LEU:HD23 | 2.13                     | 0.49              |
| 1:CA:325:A:OP2    | 20:CT:70:SER:OG   | 2.20                     | 0.49              |
| 1:CA:496:A:H5''   | 1:CA:498:U:OP2    | 2.12                     | 0.49              |
| 1:CA:950:U:OP2    | 13:CM:102:ARG:HD2 | 2.12                     | 0.49              |
| 1:CA:1201:A:O2'   | 1:CA:1202:G:OP2   | 2.30                     | 0.49              |
| 3:CC:73:PRO:C     | 3:CC:75:VAL:H     | 2.20                     | 0.49              |
| 7:CG:14:PRO:CG    | 7:CG:21:VAL:HG13  | 2.40                     | 0.49              |
| 7:CG:71:PRO:O     | 7:CG:96:GLN:HG3   | 2.12                     | 0.49              |
| 8:CH:103:VAL:CG1  | 8:CH:108:GLY:HA3  | 2.41                     | 0.49              |
| 8:CH:114:THR:HG22 | 8:CH:130:GLY:C    | 2.38                     | 0.49              |
| 13:CM:19:LEU:HB3  | 13:CM:25:ILE:HG21 | 1.94                     | 0.49              |
| 13:CM:120:LYS:O   | 13:CM:121:LYS:HB2 | 2.13                     | 0.49              |
| 20:CT:63:ILE:CG2  | 20:CT:77:ALA:HB1  | 2.43                     | 0.49              |
| 22:CV:75:C:H2'    | 22:CV:76:C:H5'    | 1.93                     | 0.49              |
| 23:CY:29:G:H21    | 23:CY:30:G:H1'    | 1.78                     | 0.49              |
| 25:DA:644:A:O3'   | 25:DA:645:C:C6    | 2.65                     | 0.49              |
| 25:DA:1694:C:C4'  | 25:DA:1695:G:C4   | 2.95                     | 0.49              |
| 25:DA:2645:G:H8   | 25:DA:2645:G:OP2  | 1.95                     | 0.49              |
| 26:DB:117:G:H4'   | 39:DS:54:LEU:CD1  | 2.42                     | 0.49              |
| 27:DC:45:ALA:O    | 27:DC:46:LYS:HB2  | 2.12                     | 0.49              |
| 27:DC:168:THR:HA  | 27:DC:173:ALA:HB1 | 1.94                     | 0.49              |
| 28:DD:11:PRO:O    | 28:DD:13:ARG:N    | 2.46                     | 0.49              |
| 30:DF:125:LEU:HA  | 30:DF:194:MET:O   | 2.12                     | 0.49              |
| 33:DI:111:PRO:O   | 33:DI:114:LEU:HB2 | 2.13                     | 0.49              |
| 34:DN:91:LEU:CD2  | 34:DN:98:VAL:HG21 | 2.43                     | 0.49              |
| 36:DP:46:LYS:HG2  | 36:DP:51:PHE:CZ   | 2.48                     | 0.49              |
| 36:DP:48:PRO:O    | 36:DP:50:ARG:N    | 2.45                     | 0.49              |
| 39:DS:5:THR:HG1   | 39:DS:8:GLU:HG3   | 1.74                     | 0.49              |
| 39:DS:94:TYR:CE2  | 39:DS:99:LYS:HG3  | 2.48                     | 0.49              |
| 42:DV:18:LEU:HD23 | 42:DV:19:LYS:N    | 2.28                     | 0.49              |
| 44:DX:29:TRP:CZ3  | 44:DX:78:LYS:HB3  | 2.47                     | 0.49              |
| 45:DY:38:ILE:HG22 | 45:DY:66:PRO:HA   | 1.94                     | 0.49              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 46:DZ:14:LYS:C    | 46:DZ:16:SER:N     | 2.71                     | 0.49              |
| 46:DZ:66:SER:C    | 46:DZ:67:LEU:HD12  | 2.38                     | 0.49              |
| 46:DZ:114:GLY:HA3 | 46:DZ:177:PRO:CB   | 2.42                     | 0.49              |
| 53:D6:13:CYS:O    | 53:D6:21:TYR:HA    | 2.13                     | 0.49              |
| 1:AA:250:A:O2'    | 1:AA:251:G:OP2     | 2.30                     | 0.49              |
| 1:AA:1065:U:O2'   | 1:AA:1066:C:OP2    | 2.30                     | 0.49              |
| 6:AF:67:MET:HB2   | 6:AF:68:PRO:CD     | 2.42                     | 0.49              |
| 9:AI:8:GLY:O      | 9:AI:76:ALA:HB1    | 2.12                     | 0.49              |
| 9:AI:16:ARG:NH2   | 9:AI:64:THR:HG21   | 2.28                     | 0.49              |
| 18:AR:59:SER:O    | 18:AR:60:ALA:C     | 2.56                     | 0.49              |
| 19:AS:15:LEU:O    | 19:AS:16:LEU:C     | 2.54                     | 0.49              |
| 20:AT:94:ALA:O    | 20:AT:95:ALA:HB3   | 2.12                     | 0.49              |
| 23:AW:23:A:C6     | 23:AW:24:G:C6      | 3.01                     | 0.49              |
| 25:BA:395:U:O2'   | 25:BA:396:G:C8     | 2.66                     | 0.49              |
| 25:BA:958:U:C5    | 37:BQ:41:TRP:CE3   | 3.01                     | 0.49              |
| 25:BA:1396:U:O2   | 25:BA:1396:U:H2'   | 2.11                     | 0.49              |
| 25:BA:1826:G:C4'  | 28:BD:242:ARG:HH21 | 2.21                     | 0.49              |
| 25:BA:2282:G:O2'  | 25:BA:2283:C:OP2   | 2.28                     | 0.49              |
| 25:BA:2716:U:H2'  | 25:BA:2717:G:H8    | 1.78                     | 0.49              |
| 27:BC:20:TYR:CG   | 27:BC:21:THR:N     | 2.81                     | 0.49              |
| 27:BC:37:PHE:C    | 27:BC:39:GLU:H     | 2.20                     | 0.49              |
| 32:BH:17:VAL:O    | 32:BH:45:VAL:HG22  | 2.12                     | 0.49              |
| 32:BH:20:ALA:HB1  | 32:BH:21:PRO:CD    | 2.42                     | 0.49              |
| 33:BI:6:LEU:O     | 33:BI:15:VAL:HG12  | 2.12                     | 0.49              |
| 37:BQ:2:LEU:O     | 37:BQ:70:PRO:HG2   | 2.13                     | 0.49              |
| 43:BW:48:ALA:O    | 43:BW:50:VAL:N     | 2.46                     | 0.49              |
| 44:BX:10:ALA:HB1  | 44:BX:11:PRO:HD2   | 1.94                     | 0.49              |
| 49:B2:21:LEU:O    | 49:B2:22:GLU:C     | 2.55                     | 0.49              |
| 49:B2:48:HIS:CG   | 49:B2:49:LYS:N     | 2.81                     | 0.49              |
| 55:B8:33:ASN:OD1  | 55:B8:33:ASN:N     | 2.46                     | 0.49              |
| 1:CA:346:G:OP2    | 40:DT:35:LYS:HD2   | 2.12                     | 0.49              |
| 7:CG:60:LYS:HA    | 7:CG:60:LYS:HZ2    | 1.78                     | 0.49              |
| 9:CI:4:TYR:CD2    | 9:CI:59:PHE:HE2    | 2.31                     | 0.49              |
| 9:CI:79:LEU:HD22  | 9:CI:79:LEU:O      | 2.13                     | 0.49              |
| 10:CJ:40:LEU:HG   | 10:CJ:69:ASN:CB    | 2.41                     | 0.49              |
| 22:CV:75:C:C2'    | 22:CV:76:C:H5'     | 2.43                     | 0.49              |
| 25:DA:300:A:H1'   | 25:DA:319:C:H1'    | 1.95                     | 0.49              |
| 25:DA:639:U:H2'   | 25:DA:640:C:C6     | 2.48                     | 0.49              |
| 25:DA:1342:A:O4'  | 25:DA:1397:U:H4'   | 2.13                     | 0.49              |
| 25:DA:1668:A:OP1  | 35:DO:5:GLN:HG3    | 2.12                     | 0.49              |
| 25:DA:1799:G:O2'  | 25:DA:1800:C:OP2   | 2.30                     | 0.49              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 27:DC:49:ILE:HD12  | 27:DC:49:ILE:N    | 2.22                     | 0.49              |
| 29:DE:93:VAL:HG21  | 29:DE:180:ASN:C   | 2.38                     | 0.49              |
| 31:DG:133:LEU:CD2  | 31:DG:157:ILE:HB  | 2.42                     | 0.49              |
| 37:DQ:141:GLN:HE22 | 46:DZ:72:ARG:CA   | 2.21                     | 0.49              |
| 40:DT:15:VAL:HA    | 40:DT:79:HIS:HD2  | 1.77                     | 0.49              |
| 40:DT:33:LYS:HE3   | 40:DT:43:GLN:HE22 | 1.67                     | 0.49              |
| 40:DT:89:VAL:HG12  | 40:DT:91:ARG:HG3  | 1.94                     | 0.49              |
| 41:DU:42:ALA:O     | 41:DU:43:GLY:C    | 2.56                     | 0.49              |
| 41:DU:61:TRP:O     | 41:DU:62:ILE:C    | 2.55                     | 0.49              |
| 42:DV:8:GLY:O      | 42:DV:10:LYS:HE2  | 2.13                     | 0.49              |
| 46:DZ:96:VAL:HG22  | 46:DZ:97:GLU:H    | 1.77                     | 0.49              |
| 55:D8:46:ARG:O     | 55:D8:47:LYS:HB3  | 2.11                     | 0.49              |
| 1:AA:407:G:OP1     | 4:AD:115:ARG:NH2  | 2.46                     | 0.49              |
| 1:AA:453:A:C6      | 1:AA:454:C:C4     | 3.01                     | 0.49              |
| 1:AA:673:G:H2'     | 1:AA:674:G:C8     | 2.47                     | 0.49              |
| 1:AA:992:U:O2'     | 1:AA:993:G:OP2    | 2.30                     | 0.49              |
| 1:AA:1077:G:N2     | 1:AA:1080:A:OP2   | 2.42                     | 0.49              |
| 1:AA:1203:C:OP1    | 14:AN:3:ARG:HD3   | 2.13                     | 0.49              |
| 2:AB:31:TYR:N      | 2:AB:31:TYR:CD2   | 2.79                     | 0.49              |
| 12:AL:70:ILE:HD13  | 12:AL:77:LEU:HD12 | 1.95                     | 0.49              |
| 12:AL:71:PRO:O     | 12:AL:102:ARG:NH1 | 2.45                     | 0.49              |
| 13:AM:15:VAL:HG13  | 13:AM:43:THR:O    | 2.13                     | 0.49              |
| 22:AV:52:C:C2      | 22:AV:53:G:C8     | 3.00                     | 0.49              |
| 25:BA:34:C:O2'     | 25:BA:35:G:OP1    | 2.30                     | 0.49              |
| 25:BA:587:C:C4'    | 25:BA:588:U:OP2   | 2.55                     | 0.49              |
| 25:BA:614(C):A:O2' | 25:BA:615:G:O5'   | 2.30                     | 0.49              |
| 25:BA:1397:U:O4    | 25:BA:1602:U:O2   | 2.31                     | 0.49              |
| 25:BA:1917:U:H2'   | 25:BA:1918:A:H5'  | 1.95                     | 0.49              |
| 25:BA:2145:C:O2'   | 25:BA:2146:C:OP1  | 2.29                     | 0.49              |
| 25:BA:2250:G:O2'   | 25:BA:2497:A:OP2  | 2.26                     | 0.49              |
| 25:BA:2517:C:C4    | 25:BA:2542:A:C6   | 3.01                     | 0.49              |
| 29:BE:60:ASN:CG    | 29:BE:62:PRO:HD2  | 2.37                     | 0.49              |
| 31:BG:63:ILE:HD12  | 31:BG:141:PHE:CE1 | 2.48                     | 0.49              |
| 31:BG:83:ARG:O     | 31:BG:84:LYS:HB2  | 2.13                     | 0.49              |
| 34:BN:62:VAL:O     | 34:BN:63:THR:O    | 2.30                     | 0.49              |
| 35:BO:115:VAL:HG12 | 35:BO:116:SER:H   | 1.78                     | 0.49              |
| 36:BP:115:LEU:HD23 | 36:BP:131:SER:HB2 | 1.94                     | 0.49              |
| 37:BQ:16:ARG:HG2   | 37:BQ:18:LYS:HD2  | 1.94                     | 0.49              |
| 40:BT:30:VAL:HG21  | 40:BT:84:GLN:H    | 1.78                     | 0.49              |
| 40:BT:31:SER:HB3   | 40:BT:43:GLN:CA   | 2.43                     | 0.49              |
| 40:BT:100:TYR:O    | 40:BT:103:ARG:N   | 2.44                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 41:BU:95:LEU:HB3   | 42:BV:4:ILE:HD13   | 1.94                     | 0.49              |
| 42:BV:39:LEU:HA    | 42:BV:47:VAL:CG1   | 2.43                     | 0.49              |
| 47:B0:68:GLU:HG3   | 47:B0:80:HIS:HB2   | 1.94                     | 0.49              |
| 1:CA:48:C:O2'      | 1:CA:49:U:OP1      | 2.30                     | 0.49              |
| 1:CA:173:U:O5'     | 1:CA:174:C:OP2     | 2.30                     | 0.49              |
| 1:CA:486:U:H2'     | 1:CA:487:A:C8      | 2.47                     | 0.49              |
| 1:CA:652:U:O2'     | 1:CA:653:A:O5'     | 2.29                     | 0.49              |
| 1:CA:1456:G:N2     | 1:CA:1457:G:C4     | 2.80                     | 0.49              |
| 3:CC:14:ILE:CG1    | 3:CC:15:THR:N      | 2.72                     | 0.49              |
| 6:CF:7:ASN:O       | 6:CF:88:VAL:HA     | 2.12                     | 0.49              |
| 11:CK:95:ILE:O     | 11:CK:98:LEU:HB2   | 2.13                     | 0.49              |
| 13:CM:125:ARG:O    | 13:CM:126:LYS:C    | 2.54                     | 0.49              |
| 16:CP:1:MET:O      | 16:CP:3:LYS:HG3    | 2.13                     | 0.49              |
| 20:CT:14:LYS:HB2   | 20:CT:17:ARG:HH21  | 1.78                     | 0.49              |
| 20:CT:49:ALA:O     | 20:CT:50:GLU:O     | 2.30                     | 0.49              |
| 22:CV:54:G:O2'     | 22:CV:55:U:OP2     | 2.30                     | 0.49              |
| 25:DA:528:A:C2     | 25:DA:2042:A:H2'   | 2.48                     | 0.49              |
| 25:DA:572:A:C4     | 25:DA:573:G:H1'    | 2.48                     | 0.49              |
| 25:DA:910:A:N3     | 25:DA:2264:C:O2'   | 2.35                     | 0.49              |
| 25:DA:2494:G:O2'   | 37:DQ:80:GLU:HA    | 2.12                     | 0.49              |
| 25:DA:2581:G:H2'   | 25:DA:2610:C:H41   | 1.77                     | 0.49              |
| 25:DA:2751:G:OP2   | 32:DH:4:ILE:HG22   | 2.13                     | 0.49              |
| 27:DC:56:GLN:NE2   | 27:DC:173:ALA:HB1  | 2.28                     | 0.49              |
| 30:DF:123:LEU:HD13 | 30:DF:192:LEU:HD13 | 1.95                     | 0.49              |
| 31:DG:106:LEU:HA   | 31:DG:110:ALA:CB   | 2.43                     | 0.49              |
| 40:DT:23:ARG:CG    | 40:DT:120:ARG:CZ   | 2.87                     | 0.49              |
| 41:DU:12:ARG:C     | 41:DU:14:HIS:H     | 2.19                     | 0.49              |
| 42:DV:62:LEU:CD1   | 42:DV:95:LEU:HB2   | 2.42                     | 0.49              |
| 45:DY:44:ILE:HD12  | 45:DY:45:VAL:H     | 1.78                     | 0.49              |
| 45:DY:84:ARG:O     | 45:DY:95:LYS:HD3   | 2.13                     | 0.49              |
| 45:DY:97:ARG:N     | 45:DY:97:ARG:CD    | 2.75                     | 0.49              |
| 1:AA:256:U:H2'     | 1:AA:257:G:C8      | 2.48                     | 0.48              |
| 1:AA:421:U:O4'     | 1:AA:421:U:O2      | 2.30                     | 0.48              |
| 1:AA:1392:G:N2     | 1:AA:1502:A:H8     | 2.04                     | 0.48              |
| 3:AC:79:ARG:NH2    | 11:CK:100:ALA:HB2  | 2.28                     | 0.48              |
| 4:AD:59:ARG:HE     | 4:AD:59:ARG:HA     | 1.78                     | 0.48              |
| 4:AD:150:GLU:CD    | 4:AD:150:GLU:N     | 2.71                     | 0.48              |
| 6:AF:67:MET:HB2    | 6:AF:68:PRO:HD2    | 1.95                     | 0.48              |
| 7:AG:91:VAL:HG11   | 7:AG:96:GLN:HG3    | 1.95                     | 0.48              |
| 8:AH:25:ASP:C      | 8:AH:26:VAL:HG12   | 2.37                     | 0.48              |
| 14:AN:9:LYS:HG3    | 14:AN:12:ARG:HH22  | 1.77                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:AW:67:C:C4     | 23:AW:68:C:N4     | 2.80                     | 0.48              |
| 25:BA:309:G:H4'   | 45:BY:18:GLY:HA3  | 1.95                     | 0.48              |
| 25:BA:383:U:H2'   | 25:BA:385:C:H5    | 1.78                     | 0.48              |
| 25:BA:1658:C:OP1  | 29:BE:132:HIS:CE1 | 2.66                     | 0.48              |
| 28:BD:236:GLY:O   | 28:BD:238:GLY:N   | 2.42                     | 0.48              |
| 28:BD:270:ILE:H   | 28:BD:270:ILE:CD1 | 2.17                     | 0.48              |
| 29:BE:152:LYS:HG2 | 34:BN:78:TYR:CD1  | 2.47                     | 0.48              |
| 33:BI:126:TYR:O   | 33:BI:139:GLN:HA  | 2.13                     | 0.48              |
| 42:BV:40:LEU:HA   | 42:BV:45:THR:HB   | 1.94                     | 0.48              |
| 47:B0:50:ASN:C    | 47:B0:62:LEU:HB2  | 2.38                     | 0.48              |
| 1:CA:484:G:O2'    | 1:CA:485:G:O5'    | 2.30                     | 0.48              |
| 1:CA:1067:A:O2'   | 1:CA:1068:G:OP2   | 2.30                     | 0.48              |
| 1:CA:1171:G:H2'   | 1:CA:1172:C:C6    | 2.48                     | 0.48              |
| 1:CA:1439:C:OP1   | 20:CT:38:LYS:HD2  | 2.13                     | 0.48              |
| 2:CB:154:LEU:O    | 2:CB:156:LYS:HG2  | 2.13                     | 0.48              |
| 2:CB:158:LEU:HD12 | 2:CB:158:LEU:H    | 1.77                     | 0.48              |
| 10:CJ:54:PHE:CD1  | 10:CJ:55:LYS:HE3  | 2.48                     | 0.48              |
| 13:CM:93:ARG:CZ   | 25:DA:888:C:OP1   | 2.61                     | 0.48              |
| 16:CP:11:SER:H    | 16:CP:14:ASN:HB3  | 1.78                     | 0.48              |
| 16:CP:32:TYR:HD2  | 16:CP:32:TYR:O    | 1.96                     | 0.48              |
| 19:CS:6:LYS:C     | 19:CS:7:LYS:HD3   | 2.38                     | 0.48              |
| 20:CT:38:LYS:C    | 20:CT:40:ALA:N    | 2.69                     | 0.48              |
| 22:CV:30:G:C5     | 22:CV:43:G:N1     | 2.81                     | 0.48              |
| 25:DA:442:G:H4'   | 25:DA:443:A:OP1   | 2.13                     | 0.48              |
| 25:DA:686:G:N2    | 25:DA:788:A:H61   | 2.10                     | 0.48              |
| 25:DA:1012:U:C4   | 34:DN:28:THR:HG21 | 2.48                     | 0.48              |
| 25:DA:1203:G:O6   | 25:DA:1204:A:N6   | 2.46                     | 0.48              |
| 25:DA:1453:U:O2'  | 25:DA:1455:G:O5'  | 2.30                     | 0.48              |
| 25:DA:2330:G:H2'  | 25:DA:2331:G:O4'  | 2.13                     | 0.48              |
| 26:DB:51:G:H5'    | 26:DB:52:A:OP2    | 2.13                     | 0.48              |
| 32:DH:152:ARG:HE  | 32:DH:153:LYS:CE  | 2.26                     | 0.48              |
| 33:DI:62:LYS:O    | 33:DI:66:GLU:HG2  | 2.13                     | 0.48              |
| 34:DN:89:LYS:NZ   | 34:DN:89:LYS:HB3  | 2.27                     | 0.48              |
| 36:DP:15:ARG:HG3  | 36:DP:16:ARG:N    | 2.28                     | 0.48              |
| 38:DR:63:ARG:HA   | 38:DR:80:PHE:CE2  | 2.47                     | 0.48              |
| 40:DT:100:TYR:HD2 | 40:DT:103:ARG:NH2 | 2.10                     | 0.48              |
| 42:DV:44:LYS:C    | 42:DV:46:VAL:N    | 2.68                     | 0.48              |
| 43:DW:14:PRO:O    | 43:DW:15:ARG:C    | 2.56                     | 0.48              |
| 45:DY:47:LYS:C    | 45:DY:49:VAL:N    | 2.69                     | 0.48              |
| 46:DZ:13:GLU:HB3  | 46:DZ:14:LYS:HZ1  | 1.78                     | 0.48              |
| 46:DZ:18:LEU:HD12 | 46:DZ:25:PRO:HG3  | 1.95                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 52:D5:4:HIS:CB     | 52:D5:5:PRO:CD     | 2.90                     | 0.48              |
| 1:AA:204:U:H4'     | 1:AA:216:G:C8      | 2.48                     | 0.48              |
| 1:AA:674:G:H2'     | 1:AA:675:A:C8      | 2.48                     | 0.48              |
| 1:AA:1126:U:H6     | 1:AA:1126:U:P      | 2.37                     | 0.48              |
| 1:AA:1343:G:O3'    | 9:AI:122:ALA:HB3   | 2.13                     | 0.48              |
| 1:AA:1363(A):A:H1' | 1:AA:1365:G:C8     | 2.48                     | 0.48              |
| 3:AC:71:ALA:HB1    | 3:AC:109:PRO:HG3   | 1.95                     | 0.48              |
| 3:AC:113:ALA:O     | 3:AC:116:VAL:N     | 2.45                     | 0.48              |
| 3:AC:148:GLY:HA3   | 3:AC:172:ARG:O     | 2.12                     | 0.48              |
| 4:AD:10:ARG:CG     | 4:AD:10:ARG:NH1    | 2.72                     | 0.48              |
| 4:AD:106:TYR:CD2   | 4:AD:106:TYR:C     | 2.91                     | 0.48              |
| 7:AG:75:VAL:HA     | 7:AG:87:VAL:O      | 2.13                     | 0.48              |
| 9:AI:16:ARG:O      | 9:AI:63:ILE:HG23   | 2.12                     | 0.48              |
| 25:BA:141:A:H8     | 25:BA:1408:C:HO2'  | 1.60                     | 0.48              |
| 25:BA:270:A:OP2    | 25:BA:271(X):G:N1  | 2.42                     | 0.48              |
| 25:BA:272:G:HO2'   | 25:BA:272(A):U:C5' | 2.25                     | 0.48              |
| 25:BA:1719:G:HO2'  | 25:BA:1720:U:H5'   | 1.78                     | 0.48              |
| 29:BE:4:ILE:CG2    | 29:BE:198:VAL:HB   | 2.43                     | 0.48              |
| 29:BE:31:CYS:CB    | 29:BE:49:LEU:HD23  | 2.43                     | 0.48              |
| 31:BG:51:ARG:NH1   | 31:BG:53:LEU:HD21  | 2.28                     | 0.48              |
| 32:BH:150:ALA:C    | 32:BH:152:ARG:H    | 2.20                     | 0.48              |
| 34:BN:126:PRO:O    | 34:BN:127:ASP:CB   | 2.61                     | 0.48              |
| 36:BP:46:LYS:HG2   | 36:BP:51:PHE:CG    | 2.48                     | 0.48              |
| 38:BR:103:ARG:CA   | 38:BR:109:ALA:O    | 2.61                     | 0.48              |
| 40:BT:29:ARG:NE    | 40:BT:86:ILE:O     | 2.46                     | 0.48              |
| 46:BZ:46:LYS:O     | 46:BZ:50:GLN:HG3   | 2.13                     | 0.48              |
| 49:B2:40:SER:C     | 49:B2:42:GLY:H     | 2.19                     | 0.48              |
| 1:CA:250:A:H8      | 1:CA:250:A:O5'     | 1.95                     | 0.48              |
| 1:CA:277:C:P       | 17:CQ:68:ARG:HH12  | 2.36                     | 0.48              |
| 1:CA:691:G:N7      | 11:CK:26:ASN:HB3   | 2.28                     | 0.48              |
| 1:CA:1308:U:OP1    | 13:CM:98:VAL:N     | 2.46                     | 0.48              |
| 1:CA:1380:U:H5''   | 1:CA:1381:U:OP1    | 2.13                     | 0.48              |
| 2:CB:107:THR:O     | 2:CB:110:GLN:HB2   | 2.12                     | 0.48              |
| 4:CD:70:ILE:HG23   | 4:CD:75:PHE:HB2    | 1.95                     | 0.48              |
| 4:CD:138:TYR:CE2   | 4:CD:139:ARG:O     | 2.66                     | 0.48              |
| 9:CI:46:ALA:HB1    | 9:CI:77:ILE:HG22   | 1.95                     | 0.48              |
| 9:CI:111:ARG:HG2   | 9:CI:112:LYS:N     | 2.28                     | 0.48              |
| 10:CJ:45:ARG:HB3   | 10:CJ:65:LEU:HB3   | 1.95                     | 0.48              |
| 12:CL:60:LEU:HD23  | 12:CL:64:TYR:HB3   | 1.95                     | 0.48              |
| 15:CO:34:LEU:HD12  | 15:CO:34:LEU:O     | 2.13                     | 0.48              |
| 20:CT:22:ARG:O     | 20:CT:26:ASN:OD1   | 2.30                     | 0.48              |

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| Atom-1              | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|-------------------|--------------------------|-------------------|
| 23:CW:28:G:N2       | 23:CW:43:C:C2     | 2.81                     | 0.48              |
| 25:DA:392:C:H5''    | 25:DA:409:C:H5''  | 1.95                     | 0.48              |
| 25:DA:749:C:H5'     | 25:DA:1271:G:H1'  | 1.95                     | 0.48              |
| 25:DA:1747(A):G:H2' | 25:DA:1748:G:H5'' | 1.95                     | 0.48              |
| 25:DA:2790:A:O2'    | 25:DA:2893:G:N3   | 2.43                     | 0.48              |
| 28:DD:31:LYS:NZ     | 28:DD:102:LYS:NZ  | 2.60                     | 0.48              |
| 33:DI:37:VAL:CG1    | 33:DI:38:LEU:HD12 | 2.43                     | 0.48              |
| 33:DI:69:LYS:HG3    | 33:DI:136:VAL:CG2 | 2.43                     | 0.48              |
| 33:DI:124:GLY:H     | 33:DI:142:VAL:CG2 | 2.26                     | 0.48              |
| 34:DN:3:THR:C       | 34:DN:5:VAL:H     | 2.21                     | 0.48              |
| 37:DQ:133:ARG:HH11  | 37:DQ:133:ARG:HG3 | 1.78                     | 0.48              |
| 40:DT:65:LYS:O      | 40:DT:72:VAL:N    | 2.37                     | 0.48              |
| 45:DY:54:LYS:O      | 45:DY:55:TYR:CB   | 2.60                     | 0.48              |
| 53:D6:20:ASN:ND2    | 53:D6:21:TYR:N    | 2.60                     | 0.48              |
| 1:AA:1317:C:C2      | 14:AN:16:PHE:CE1  | 3.02                     | 0.48              |
| 3:AC:113:ALA:O      | 3:AC:115:LEU:N    | 2.46                     | 0.48              |
| 5:AE:121:LYS:C      | 5:AE:122:GLU:HG3  | 2.38                     | 0.48              |
| 7:AG:152:ALA:C      | 7:AG:154:TYR:H    | 2.21                     | 0.48              |
| 10:AJ:61:GLU:HG3    | 14:AN:58:LYS:NZ   | 2.28                     | 0.48              |
| 11:AK:41:THR:CG2    | 11:AK:42:TRP:N    | 2.75                     | 0.48              |
| 11:AK:98:LEU:HD23   | 11:AK:98:LEU:HA   | 1.59                     | 0.48              |
| 12:AL:18:VAL:HG23   | 12:AL:19:ARG:N    | 2.24                     | 0.48              |
| 14:AN:23:ARG:O      | 14:AN:24:CYS:O    | 2.30                     | 0.48              |
| 15:AO:53:HIS:O      | 15:AO:56:LEU:HB3  | 2.13                     | 0.48              |
| 16:AP:82:GLN:CG     | 16:AP:83:GLU:N    | 2.70                     | 0.48              |
| 17:AQ:77:VAL:O      | 17:AQ:78:GLU:HB3  | 2.13                     | 0.48              |
| 19:AS:28:LYS:HB3    | 19:AS:29:ARG:NH1  | 2.28                     | 0.48              |
| 23:AW:16:U:C5       | 23:AW:18:G:O5'    | 2.66                     | 0.48              |
| 23:AW:50:U:C2       | 23:AW:65:G:N2     | 2.81                     | 0.48              |
| 25:BA:50:U:C4'      | 25:BA:51:G:OP2    | 2.60                     | 0.48              |
| 25:BA:307:G:H21     | 25:BA:330:A:H62   | 1.61                     | 0.48              |
| 25:BA:813:U:OP2     | 36:BP:23:PRO:O    | 2.31                     | 0.48              |
| 25:BA:920:G:H2'     | 25:BA:921:G:H8    | 1.78                     | 0.48              |
| 25:BA:2745:C:H4'    | 32:BH:142:GLY:O   | 2.14                     | 0.48              |
| 25:BA:2848:G:O2'    | 25:BA:2867:G:N2   | 2.46                     | 0.48              |
| 26:BB:66:A:C6       | 26:BB:108:U:C4    | 3.02                     | 0.48              |
| 32:BH:13:LYS:O      | 32:BH:15:VAL:N    | 2.45                     | 0.48              |
| 37:BQ:2:LEU:H       | 37:BQ:3:MET:HE3   | 1.77                     | 0.48              |
| 42:BV:15:GLU:CB     | 42:BV:16:PRO:CD   | 2.87                     | 0.48              |
| 45:BY:95:LYS:HE2    | 45:BY:99:CYS:O    | 2.13                     | 0.48              |
| 46:BZ:91:LEU:HD12   | 46:BZ:91:LEU:H    | 1.77                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 46:BZ:121:HIS:ND1 | 46:BZ:169:GLU:HG2 | 2.28                     | 0.48              |
| 47:B0:10:THR:CG2  | 47:B0:12:ASN:HB2  | 2.43                     | 0.48              |
| 1:CA:67:C:H2'     | 1:CA:68:G:H8      | 1.79                     | 0.48              |
| 1:CA:100:C:H2'    | 1:CA:101:A:O4'    | 2.13                     | 0.48              |
| 1:CA:1004:A:H5''  | 1:CA:1025:U:H3    | 1.78                     | 0.48              |
| 1:CA:1152:A:H2'   | 1:CA:1153:C:C6    | 2.48                     | 0.48              |
| 1:CA:1244:C:H2'   | 1:CA:1245:A:C8    | 2.48                     | 0.48              |
| 2:CB:12:GLU:O     | 2:CB:16:HIS:ND1   | 2.31                     | 0.48              |
| 3:CC:19:GLU:O     | 3:CC:19:GLU:HG2   | 2.14                     | 0.48              |
| 3:CC:186:PHE:CG   | 3:CC:187:ALA:N    | 2.80                     | 0.48              |
| 6:CF:39:LYS:CG    | 6:CF:40:VAL:H     | 2.26                     | 0.48              |
| 6:CF:63:TYR:N     | 6:CF:63:TYR:CD2   | 2.78                     | 0.48              |
| 7:CG:146:GLU:O    | 7:CG:149:ARG:HB3  | 2.12                     | 0.48              |
| 9:CI:83:ARG:NE    | 9:CI:102:LEU:HD11 | 2.26                     | 0.48              |
| 9:CI:99:LEU:HD12  | 9:CI:101:PHE:CD1  | 2.48                     | 0.48              |
| 13:CM:67:GLU:CD   | 13:CM:68:GLY:N    | 2.71                     | 0.48              |
| 18:CR:59:SER:HB3  | 18:CR:62:GLU:HB2  | 1.95                     | 0.48              |
| 25:DA:581:C:H2'   | 25:DA:582:G:H8    | 1.78                     | 0.48              |
| 25:DA:1230:C:H2'  | 25:DA:1231:G:C8   | 2.49                     | 0.48              |
| 25:DA:1449:A:H2   | 25:DA:1529:G:H1'  | 1.78                     | 0.48              |
| 25:DA:1567:A:OP2  | 28:DD:84:TYR:OH   | 2.25                     | 0.48              |
| 25:DA:1889:A:N1   | 25:DA:2234:G:H1'  | 2.28                     | 0.48              |
| 26:DB:14:U:H4'    | 26:DB:15:A:OP2    | 2.10                     | 0.48              |
| 28:DD:79:VAL:HG12 | 28:DD:113:VAL:HA  | 1.96                     | 0.48              |
| 28:DD:267:SER:HA  | 28:DD:270:ILE:CG1 | 2.43                     | 0.48              |
| 30:DF:179:GLU:CD  | 30:DF:179:GLU:N   | 2.72                     | 0.48              |
| 33:DI:61:ARG:NH2  | 33:DI:64:GLU:OE2  | 2.46                     | 0.48              |
| 33:DI:77:LEU:CD1  | 33:DI:78:THR:H    | 2.25                     | 0.48              |
| 34:DN:48:MET:H    | 34:DN:48:MET:CE   | 2.26                     | 0.48              |
| 35:DO:50:GLY:C    | 35:DO:52:VAL:N    | 2.70                     | 0.48              |
| 35:DO:60:ALA:HB2  | 35:DO:86:ILE:HA   | 1.96                     | 0.48              |
| 41:DU:92:ARG:C    | 41:DU:94:ASN:N    | 2.70                     | 0.48              |
| 42:DV:61:VAL:C    | 42:DV:62:LEU:HD12 | 2.37                     | 0.48              |
| 44:DX:11:PRO:HB2  | 44:DX:13:LEU:HD21 | 1.96                     | 0.48              |
| 45:DY:42:VAL:HB   | 45:DY:67:LEU:CD1  | 2.41                     | 0.48              |
| 45:DY:50:ARG:CB   | 45:DY:53:PRO:HD2  | 2.43                     | 0.48              |
| 46:DZ:22:GLY:O    | 46:DZ:23:LYS:HG2  | 2.13                     | 0.48              |
| 46:DZ:77:ASP:O    | 46:DZ:78:LYS:C    | 2.56                     | 0.48              |
| 1:AA:119:A:H4'    | 1:AA:120:A:O5'    | 2.13                     | 0.48              |
| 1:AA:625:G:O4'    | 16:AP:16:HIS:HD2  | 1.97                     | 0.48              |
| 1:AA:1053:G:N7    | 1:AA:1199:U:H3'   | 2.28                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:1064:G:H4'    | 1:AA:1065:U:O5'    | 2.13                     | 0.48              |
| 1:AA:1301:U:O4     | 1:AA:1303:C:C1'    | 2.61                     | 0.48              |
| 1:AA:1530:G:H2'    | 1:AA:1531:A:O5'    | 2.14                     | 0.48              |
| 2:AB:57:PHE:HD2    | 2:AB:185:ILE:HD11  | 1.77                     | 0.48              |
| 3:AC:83:ARG:HG3    | 3:AC:87:LEU:HD11   | 1.95                     | 0.48              |
| 4:AD:4:TYR:CE2     | 4:AD:6:GLY:O       | 2.65                     | 0.48              |
| 4:AD:120:LEU:O     | 4:AD:121:VAL:C     | 2.54                     | 0.48              |
| 4:AD:175:SER:OG    | 4:AD:186:LEU:HD21  | 2.13                     | 0.48              |
| 5:AE:51:VAL:O      | 5:AE:52:PRO:C      | 2.55                     | 0.48              |
| 5:AE:121:LYS:O     | 5:AE:122:GLU:CG    | 2.62                     | 0.48              |
| 7:AG:95:ARG:O      | 7:AG:96:GLN:C      | 2.56                     | 0.48              |
| 10:AJ:47:PHE:CZ    | 14:AN:37:PHE:CE2   | 3.02                     | 0.48              |
| 11:AK:99:GLN:HA    | 11:AK:105:VAL:CG2  | 2.43                     | 0.48              |
| 13:AM:3:ARG:HH12   | 31:BG:113:ARG:HE   | 1.60                     | 0.48              |
| 13:AM:66:LEU:O     | 13:AM:67:GLU:C     | 2.56                     | 0.48              |
| 13:AM:79:LYS:O     | 13:AM:82:MET:SD    | 2.72                     | 0.48              |
| 20:AT:43:LEU:HB2   | 20:AT:52:ALA:CB    | 2.41                     | 0.48              |
| 23:AW:5:G:N2       | 23:AW:6:G:H1'      | 2.28                     | 0.48              |
| 23:AW:11:C:H2'     | 23:AW:12:U:H6      | 1.76                     | 0.48              |
| 25:BA:272:G:O2'    | 25:BA:272(A):U:O5' | 2.25                     | 0.48              |
| 25:BA:1689:A:H62   | 25:BA:1698:A:H2    | 1.61                     | 0.48              |
| 25:BA:2050:C:H1'   | 29:BE:156:MET:HE2  | 1.95                     | 0.48              |
| 25:BA:2848:G:O2'   | 25:BA:2849:U:O5'   | 2.27                     | 0.48              |
| 26:BB:3:C:N4       | 26:BB:118:G:H1     | 2.11                     | 0.48              |
| 28:BD:142:VAL:HG22 | 28:BD:143:HIS:N    | 2.28                     | 0.48              |
| 29:BE:1:MET:O      | 29:BE:2:LYS:C      | 2.57                     | 0.48              |
| 30:BF:3:GLU:HG3    | 30:BF:19:GLU:CB    | 2.39                     | 0.48              |
| 30:BF:199:TRP:CZ3  | 30:BF:203:GLN:CG   | 2.96                     | 0.48              |
| 31:BG:20:ILE:O     | 31:BG:24:GLY:CA    | 2.62                     | 0.48              |
| 31:BG:81:LYS:O     | 31:BG:82:LEU:O     | 2.31                     | 0.48              |
| 32:BH:152:ARG:HB3  | 32:BH:161:GLY:HA2  | 1.95                     | 0.48              |
| 33:BI:118:LYS:HD2  | 33:BI:119:PRO:CD   | 2.31                     | 0.48              |
| 34:BN:68:GLU:HA    | 34:BN:68:GLU:OE1   | 2.13                     | 0.48              |
| 36:BP:146:VAL:CG2  | 36:BP:147:LEU:H    | 2.15                     | 0.48              |
| 37:BQ:10:ARG:CG    | 37:BQ:10:ARG:NH1   | 2.64                     | 0.48              |
| 37:BQ:141:GLN:OE1  | 46:BZ:72:ARG:HD3   | 2.12                     | 0.48              |
| 38:BR:47:PHE:CD2   | 38:BR:47:PHE:C     | 2.91                     | 0.48              |
| 40:BT:36:GLU:C     | 40:BT:38:ASN:N     | 2.70                     | 0.48              |
| 42:BV:65:GLY:O     | 42:BV:91:TYR:CD1   | 2.66                     | 0.48              |
| 44:BX:5:TYR:CZ     | 49:B2:30:ARG:HB2   | 2.48                     | 0.48              |
| 45:BY:46:LYS:CD    | 45:BY:47:LYS:HZ2   | 2.25                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 45:BY:46:LYS:CG    | 45:BY:47:LYS:HZ2   | 2.26                     | 0.48              |
| 48:B1:7:ILE:HB     | 48:B1:62:VAL:CG2   | 2.42                     | 0.48              |
| 1:CA:274:A:O2'     | 1:CA:275:G:O5'     | 2.30                     | 0.48              |
| 1:CA:518:C:O2'     | 12:CL:50:SER:HB3   | 2.12                     | 0.48              |
| 1:CA:1442(B):A:O2' | 1:CA:1443:G:O5'    | 2.32                     | 0.48              |
| 5:CE:51:VAL:O      | 5:CE:55:VAL:HG23   | 2.14                     | 0.48              |
| 5:CE:90:VAL:HG23   | 5:CE:121:LYS:H     | 1.78                     | 0.48              |
| 7:CG:145:ALA:C     | 7:CG:147:ALA:N     | 2.71                     | 0.48              |
| 9:CI:48:GLU:N      | 9:CI:49:PRO:CD     | 2.76                     | 0.48              |
| 11:CK:32:ILE:HD12  | 11:CK:72:ALA:CB    | 2.44                     | 0.48              |
| 12:CL:28:LYS:O     | 12:CL:29:GLY:C     | 2.57                     | 0.48              |
| 13:CM:44:ARG:C     | 13:CM:46:LYS:H     | 2.21                     | 0.48              |
| 14:CN:27:CYS:HG    | 59:CN:101:ZN:ZN    | 1.25                     | 0.48              |
| 15:CO:26:GLU:HB3   | 15:CO:81:LEU:HD22  | 1.95                     | 0.48              |
| 18:CR:56:THR:HB    | 18:CR:58:LEU:HD11  | 1.95                     | 0.48              |
| 19:CS:35:SER:C     | 19:CS:37:ARG:N     | 2.71                     | 0.48              |
| 23:CW:57:G:H2'     | 23:CW:57:G:N3      | 2.28                     | 0.48              |
| 25:DA:483:A:H3'    | 25:DA:484:C:C6     | 2.49                     | 0.48              |
| 25:DA:2712:U:O2'   | 25:DA:2713:A:H5'   | 2.14                     | 0.48              |
| 25:DA:2723:C:H5''  | 38:DR:1:MET:HG2    | 1.96                     | 0.48              |
| 32:DH:96:ALA:HB2   | 32:DH:105:LEU:HB3  | 1.95                     | 0.48              |
| 33:DI:76:THR:CG2   | 33:DI:77:LEU:H     | 2.25                     | 0.48              |
| 34:DN:63:THR:HG22  | 34:DN:64:GLY:H     | 1.78                     | 0.48              |
| 40:DT:16:ARG:NH2   | 40:DT:82:LEU:O     | 2.46                     | 0.48              |
| 40:DT:51:ARG:HG3   | 40:DT:98:LYS:HG3   | 1.96                     | 0.48              |
| 41:DU:25:TRP:CG    | 41:DU:26:GLY:N     | 2.78                     | 0.48              |
| 42:DV:22:VAL:CG1   | 42:DV:23:GLU:N     | 2.76                     | 0.48              |
| 46:DZ:124:ILE:HG23 | 46:DZ:165:VAL:HG23 | 1.95                     | 0.48              |
| 47:D0:25:ARG:HA    | 47:D0:29:GLN:HE22  | 1.78                     | 0.48              |
| 1:AA:329:A:C2      | 1:AA:332:G:C8      | 3.01                     | 0.48              |
| 1:AA:651:C:N4      | 1:AA:753:A:OP2     | 2.46                     | 0.48              |
| 1:AA:983:A:N1      | 1:AA:1222:G:N2     | 2.61                     | 0.48              |
| 1:AA:1240:U:H5     | 7:AG:109:ASN:OD1   | 1.95                     | 0.48              |
| 1:AA:1279:A:C1'    | 1:AA:1282:C:N4     | 2.76                     | 0.48              |
| 1:AA:1491:G:N7     | 58:AA:7111:PAR:O53 | 2.37                     | 0.48              |
| 3:AC:182:ILE:HG12  | 3:AC:203:PHE:HA    | 1.94                     | 0.48              |
| 7:AG:44:TYR:C      | 7:AG:46:ALA:N      | 2.70                     | 0.48              |
| 7:AG:47:CYS:HB3    | 7:AG:58:PRO:HG3    | 1.95                     | 0.48              |
| 11:AK:34:ASP:HB2   | 11:AK:35:PRO:CD    | 2.44                     | 0.48              |
| 12:AL:45:PRO:HG3   | 12:AL:51:ALA:N     | 2.27                     | 0.48              |
| 12:AL:53:ARG:HH12  | 12:AL:92:ASP:HB3   | 1.76                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 15:AO:36:ILE:O     | 15:AO:37:ASN:C     | 2.57                     | 0.48              |
| 16:AP:58:TYR:C     | 16:AP:61:SER:HB3   | 2.39                     | 0.48              |
| 18:AR:75:ILE:C     | 18:AR:77:GLY:N     | 2.71                     | 0.48              |
| 25:BA:272(J):C:H2' | 25:BA:363:G:H22    | 1.77                     | 0.48              |
| 25:BA:912:C:OP1    | 37:BQ:9:TYR:OH     | 2.29                     | 0.48              |
| 25:BA:1456:G:H2'   | 25:BA:1457:A:C8    | 2.46                     | 0.48              |
| 25:BA:2345:G:O2'   | 25:BA:2382:G:C5'   | 2.61                     | 0.48              |
| 28:BD:13:ARG:O     | 28:BD:13:ARG:CG    | 2.61                     | 0.48              |
| 28:BD:24:ILE:O     | 28:BD:25:THR:O     | 2.31                     | 0.48              |
| 29:BE:28:ALA:HB3   | 29:BE:93:VAL:HG23  | 1.96                     | 0.48              |
| 29:BE:61:ARG:HB3   | 29:BE:62:PRO:CD    | 2.44                     | 0.48              |
| 30:BF:139:PHE:CB   | 30:BF:166:ALA:HB1  | 2.43                     | 0.48              |
| 30:BF:195:ASP:HB2  | 30:BF:198:ALA:H    | 1.78                     | 0.48              |
| 31:BG:116:ASP:O    | 31:BG:117:PHE:HB3  | 2.14                     | 0.48              |
| 34:BN:41:ASP:O     | 34:BN:42:TRP:C     | 2.56                     | 0.48              |
| 38:BR:79:LEU:HD13  | 38:BR:80:PHE:HD1   | 1.78                     | 0.48              |
| 42:BV:34:GLU:O     | 42:BV:36:PRO:CD    | 2.57                     | 0.48              |
| 44:BX:3:THR:O      | 44:BX:4:ALA:HB3    | 2.14                     | 0.48              |
| 45:BY:28:LYS:N     | 45:BY:28:LYS:CE    | 2.70                     | 0.48              |
| 1:CA:130:A:O2'     | 1:CA:131:C:O5'     | 2.30                     | 0.48              |
| 1:CA:633:G:H5'     | 1:CA:634:C:OP2     | 2.13                     | 0.48              |
| 1:CA:820:U:O2'     | 1:CA:821:G:OP1     | 2.30                     | 0.48              |
| 1:CA:1148:U:H5''   | 9:CI:7:THR:HG21    | 1.96                     | 0.48              |
| 1:CA:1429:C:H2'    | 1:CA:1430:C:C6     | 2.48                     | 0.48              |
| 4:CD:14:ARG:HB2    | 4:CD:40:PRO:HD2    | 1.95                     | 0.48              |
| 13:CM:3:ARG:NH2    | 13:CM:7:VAL:HG13   | 2.28                     | 0.48              |
| 18:CR:22:VAL:O     | 18:CR:23:LYS:C     | 2.56                     | 0.48              |
| 23:CY:30:G:C6      | 23:CY:31:A:N7      | 2.81                     | 0.48              |
| 25:DA:642:G:H21    | 25:DA:646:A:H2     | 1.60                     | 0.48              |
| 25:DA:1131:G:H4'   | 34:DN:82:LEU:HB2   | 1.96                     | 0.48              |
| 25:DA:1266:G:OP2   | 52:D5:19:ARG:NH1   | 2.46                     | 0.48              |
| 25:DA:1275:A:H4'   | 25:DA:1276:A:O5'   | 2.13                     | 0.48              |
| 25:DA:1786:A:O3'   | 25:DA:1787:A:H8    | 1.96                     | 0.48              |
| 25:DA:2126:A:N1    | 25:DA:2162:G:O2'   | 2.43                     | 0.48              |
| 25:DA:2520:C:N4    | 25:DA:2567:G:C5    | 2.82                     | 0.48              |
| 26:DB:114:C:O2'    | 39:DS:46:VAL:HG13  | 2.13                     | 0.48              |
| 27:DC:68:LEU:CD1   | 27:DC:179:SER:HA   | 2.37                     | 0.48              |
| 28:DD:182:LEU:HB2  | 28:DD:271:ILE:O    | 2.11                     | 0.48              |
| 31:DG:20:ILE:O     | 31:DG:24:GLY:HA2   | 2.12                     | 0.48              |
| 31:DG:139:LEU:HA   | 31:DG:144:ILE:HG21 | 1.96                     | 0.48              |
| 33:DI:79:ILE:HG22  | 33:DI:79:ILE:O     | 2.12                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 34:DN:2:LYS:NZ    | 41:DU:95:LEU:HD21 | 2.27                     | 0.48              |
| 34:DN:26:LEU:CD2  | 34:DN:30:ILE:HD11 | 2.43                     | 0.48              |
| 34:DN:58:ASP:C    | 34:DN:60:ILE:N    | 2.54                     | 0.48              |
| 35:DO:63:VAL:HG22 | 35:DO:83:ALA:O    | 2.13                     | 0.48              |
| 39:DS:5:THR:HG1   | 39:DS:7:TYR:HB3   | 1.76                     | 0.48              |
| 39:DS:48:LEU:CD2  | 39:DS:82:ILE:HD11 | 2.44                     | 0.48              |
| 40:DT:32:TYR:CD2  | 40:DT:81:PRO:HB2  | 2.49                     | 0.48              |
| 45:DY:5:MET:HG2   | 45:DY:35:TYR:CE2  | 2.49                     | 0.48              |
| 45:DY:56:PRO:O    | 45:DY:57:GLN:NE2  | 2.47                     | 0.48              |
| 45:DY:61:ILE:HG23 | 45:DY:62:GLU:N    | 2.28                     | 0.48              |
| 46:DZ:48:PHE:CE2  | 46:DZ:71:VAL:HG11 | 2.47                     | 0.48              |
| 49:D2:16:LEU:HD12 | 49:D2:21:LEU:HD21 | 1.95                     | 0.48              |
| 49:D2:35:LEU:HB3  | 49:D2:50:ILE:HD13 | 1.94                     | 0.48              |
| 1:AA:828:A:N3     | 2:AB:26:PRO:HG3   | 2.29                     | 0.48              |
| 1:AA:1201:A:HO2'  | 1:AA:1202:G:P     | 2.37                     | 0.48              |
| 3:AC:59:ARG:HA    | 3:AC:63:ASN:O     | 2.14                     | 0.48              |
| 3:AC:134:ILE:N    | 3:AC:134:ILE:HD13 | 2.28                     | 0.48              |
| 7:AG:85:TYR:CD1   | 7:AG:154:TYR:HE1  | 2.32                     | 0.48              |
| 12:AL:24:VAL:HG13 | 12:AL:98:TYR:CE2  | 2.49                     | 0.48              |
| 12:AL:32:PHE:CE1  | 12:AL:86:ARG:HG3  | 2.49                     | 0.48              |
| 13:AM:90:LEU:HA   | 13:AM:93:ARG:CB   | 2.43                     | 0.48              |
| 17:AQ:45:HIS:HB2  | 17:AQ:65:ILE:HD13 | 1.94                     | 0.48              |
| 20:AT:69:GLY:C    | 20:AT:71:THR:H    | 2.22                     | 0.48              |
| 25:BA:668:G:C4    | 25:BA:670:A:N7    | 2.82                     | 0.48              |
| 25:BA:1427:A:O2'  | 25:BA:1428:C:OP2  | 2.27                     | 0.48              |
| 25:BA:1542:A:H1'  | 25:BA:1544:A:O4'  | 2.13                     | 0.48              |
| 25:BA:2009:G:H1'  | 38:BR:107:ASP:O   | 2.14                     | 0.48              |
| 25:BA:2079:U:O3'  | 48:B1:35:THR:OG1  | 2.32                     | 0.48              |
| 25:BA:2296:U:H4'  | 25:BA:2297:C:OP1  | 2.13                     | 0.48              |
| 25:BA:2781:A:H8   | 25:BA:2781:A:O5'  | 1.97                     | 0.48              |
| 25:BA:2867:G:O2'  | 25:BA:2868:A:OP2  | 2.30                     | 0.48              |
| 28:BD:159:ALA:HB1 | 28:BD:198:ASN:O   | 2.13                     | 0.48              |
| 29:BE:137:HIS:HB3 | 29:BE:138:PRO:CD  | 2.42                     | 0.48              |
| 31:BG:122:PRO:HG2 | 31:BG:123:ASN:OD1 | 2.14                     | 0.48              |
| 32:BH:126:PRO:O   | 32:BH:130:ARG:HB3 | 2.14                     | 0.48              |
| 33:BI:29:TYR:O    | 33:BI:32:PRO:HG2  | 2.14                     | 0.48              |
| 37:BQ:3:MET:HB3   | 37:BQ:3:MET:HE2   | 1.68                     | 0.48              |
| 40:BT:56:GLY:C    | 40:BT:59:THR:HG22 | 2.38                     | 0.48              |
| 41:BU:95:LEU:CD1  | 42:BV:4:ILE:HG21  | 2.40                     | 0.48              |
| 47:B0:43:THR:O    | 47:B0:43:THR:CG2  | 2.58                     | 0.48              |
| 47:B0:78:TYR:HB3  | 47:B0:80:HIS:CE1  | 2.48                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CA:278:G:O3'    | 1:CA:281:G:H5'    | 2.14                     | 0.48              |
| 1:CA:405:U:OP2    | 4:CD:3:ARG:HD2    | 2.12                     | 0.48              |
| 1:CA:436:C:H2'    | 1:CA:437:U:H6     | 1.79                     | 0.48              |
| 1:CA:824:C:H2'    | 1:CA:825:G:C8     | 2.49                     | 0.48              |
| 1:CA:1212:U:OP1   | 1:CA:1212:U:H4'   | 2.14                     | 0.48              |
| 1:CA:1300:G:O2'   | 1:CA:1301:U:O5'   | 2.30                     | 0.48              |
| 2:CB:239:VAL:O    | 2:CB:239:VAL:HG12 | 2.14                     | 0.48              |
| 3:CC:69:HIS:ND1   | 3:CC:69:HIS:N     | 2.60                     | 0.48              |
| 3:CC:109:PRO:HB3  | 3:CC:115:LEU:HD12 | 1.96                     | 0.48              |
| 11:CK:69:ALA:O    | 11:CK:72:ALA:N    | 2.43                     | 0.48              |
| 13:CM:90:LEU:HD12 | 13:CM:91:ARG:N    | 2.28                     | 0.48              |
| 16:CP:57:ARG:O    | 16:CP:58:TYR:C    | 2.56                     | 0.48              |
| 20:CT:83:ARG:C    | 20:CT:85:MET:N    | 2.66                     | 0.48              |
| 22:CV:35:C:HO2'   | 22:CV:36:A:P      | 2.37                     | 0.48              |
| 25:DA:90:U:O2'    | 25:DA:92:A:H5''   | 2.13                     | 0.48              |
| 25:DA:1419:A:N6   | 25:DA:1494:A:H61  | 2.12                     | 0.48              |
| 25:DA:2103:C:H3'  | 25:DA:2104:G:H5'' | 1.95                     | 0.48              |
| 25:DA:2393:A:C4'  | 36:DP:60:MET:O    | 2.62                     | 0.48              |
| 25:DA:2713:A:C5'  | 25:DA:2714:G:OP2  | 2.60                     | 0.48              |
| 25:DA:2831:G:H1'  | 25:DA:2883:A:H2'  | 1.94                     | 0.48              |
| 25:DA:2849:U:C4   | 40:DT:23:ARG:NH2  | 2.77                     | 0.48              |
| 29:DE:1:MET:O     | 29:DE:2:LYS:C     | 2.57                     | 0.48              |
| 32:DH:149:ARG:HG3 | 32:DH:162:ILE:O   | 2.12                     | 0.48              |
| 38:DR:17:ARG:CG   | 38:DR:17:ARG:NH1  | 2.75                     | 0.48              |
| 39:DS:26:LEU:HD22 | 39:DS:87:PHE:HD1  | 1.78                     | 0.48              |
| 39:DS:88:ASP:CG   | 39:DS:89:ARG:N    | 2.71                     | 0.48              |
| 39:DS:89:ARG:O    | 39:DS:90:GLY:C    | 2.57                     | 0.48              |
| 40:DT:32:TYR:CG   | 40:DT:81:PRO:HB2  | 2.48                     | 0.48              |
| 40:DT:83:ILE:HG13 | 40:DT:84:GLN:N    | 2.29                     | 0.48              |
| 45:DY:50:ARG:C    | 45:DY:53:PRO:HD2  | 2.38                     | 0.48              |
| 48:D1:29:GLY:C    | 48:D1:31:GLY:H    | 2.22                     | 0.48              |
| 48:D1:73:LEU:HB3  | 48:D1:94:LEU:HD23 | 1.95                     | 0.48              |
| 50:D3:6:VAL:HB    | 50:D3:54:VAL:HG11 | 1.96                     | 0.48              |
| 1:AA:103:C:OP2    | 20:AT:14:LYS:HD2  | 2.14                     | 0.48              |
| 1:AA:376:G:P      | 16:AP:67:THR:HG21 | 2.54                     | 0.48              |
| 1:AA:831:U:OP1    | 2:AB:22:LYS:HG3   | 2.13                     | 0.48              |
| 4:AD:72:GLU:O     | 4:AD:73:ARG:C     | 2.56                     | 0.48              |
| 4:AD:171:GLY:HA3  | 4:AD:173:TRP:CZ3  | 2.49                     | 0.48              |
| 6:AF:97:PHE:CD2   | 18:AR:31:LEU:HD21 | 2.49                     | 0.48              |
| 13:AM:84:ILE:O    | 13:AM:84:ILE:HG22 | 2.13                     | 0.48              |
| 17:AQ:97:SER:O    | 17:AQ:98:LEU:HD23 | 2.14                     | 0.48              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 19:AS:51:VAL:HG23 | 19:AS:60:VAL:HG11  | 1.96                     | 0.48              |
| 23:AW:9:A:H5'     | 23:AW:46:G:H21     | 1.78                     | 0.48              |
| 24:AX:14:A:O2'    | 24:AX:15:A:O4'     | 2.27                     | 0.48              |
| 25:BA:332:A:O2'   | 25:BA:333:G:OP1    | 2.30                     | 0.48              |
| 25:BA:945:A:C4    | 25:BA:2448:A:C2    | 3.02                     | 0.48              |
| 25:BA:1363:C:O2'  | 25:BA:1809:A:N3    | 2.42                     | 0.48              |
| 25:BA:1548:C:H2'  | 25:BA:1549:C:C6    | 2.48                     | 0.48              |
| 25:BA:2318:G:O2'  | 25:BA:2319:G:OP1   | 2.30                     | 0.48              |
| 25:BA:2602:A:H62  | 47:B0:2:ALA:CB     | 2.27                     | 0.48              |
| 25:BA:2689:U:H4'  | 25:BA:2690:C:OP2   | 2.12                     | 0.48              |
| 28:BD:24:ILE:HG23 | 28:BD:25:THR:N     | 2.24                     | 0.48              |
| 29:BE:175:VAL:C   | 29:BE:176:ILE:HD12 | 2.38                     | 0.48              |
| 30:BF:20:LEU:HG   | 30:BF:21:ALA:H     | 1.78                     | 0.48              |
| 34:BN:18:ALA:HB3  | 34:BN:21:LYS:HB3   | 1.95                     | 0.48              |
| 36:BP:46:LYS:HG2  | 36:BP:51:PHE:CZ    | 2.48                     | 0.48              |
| 36:BP:83:VAL:HG12 | 36:BP:112:LEU:CD2  | 2.41                     | 0.48              |
| 36:BP:147:LEU:C   | 36:BP:148:LEU:HD23 | 2.39                     | 0.48              |
| 37:BQ:57:HIS:CE1  | 37:BQ:116:GLU:HB3  | 2.48                     | 0.48              |
| 40:BT:12:SER:C    | 40:BT:13:ARG:CZ    | 2.86                     | 0.48              |
| 40:BT:15:VAL:HG23 | 40:BT:79:HIS:NE2   | 2.29                     | 0.48              |
| 42:BV:59:ALA:CB   | 42:BV:94:LEU:HD13  | 2.43                     | 0.48              |
| 44:BX:64:LYS:NZ   | 44:BX:73:ARG:HH21  | 2.12                     | 0.48              |
| 46:BZ:158:PRO:CB  | 46:BZ:159:PRO:CD   | 2.91                     | 0.48              |
| 49:B2:42:GLY:O    | 49:B2:43:GLN:C     | 2.57                     | 0.48              |
| 52:B5:3:LYS:HD2   | 52:B5:3:LYS:HA     | 1.59                     | 0.48              |
| 52:B5:46:CYS:SG   | 52:B5:47:PRO:HD2   | 2.54                     | 0.48              |
| 54:B7:28:ARG:NH1  | 54:B7:28:ARG:HG3   | 2.28                     | 0.48              |
| 1:CA:375:U:OP1    | 16:CP:69:THR:HG21  | 2.13                     | 0.48              |
| 1:CA:508:C:H5''   | 1:CA:509:A:OP1     | 2.12                     | 0.48              |
| 1:CA:673:G:H2'    | 1:CA:674:G:C8      | 2.48                     | 0.48              |
| 1:CA:675:A:H1'    | 11:CK:116:HIS:CD2  | 2.49                     | 0.48              |
| 1:CA:748:C:O2'    | 1:CA:749:C:O5'     | 2.30                     | 0.48              |
| 1:CA:1507:A:H2'   | 1:CA:1508:G:C8     | 2.49                     | 0.48              |
| 3:CC:51:GLY:O     | 3:CC:70:VAL:HG13   | 2.14                     | 0.48              |
| 3:CC:157:ILE:HB   | 3:CC:164:ARG:NH2   | 2.29                     | 0.48              |
| 6:CF:1:MET:N      | 6:CF:68:PRO:HA     | 2.29                     | 0.48              |
| 9:CI:16:ARG:N     | 9:CI:64:THR:O      | 2.42                     | 0.48              |
| 12:CL:34:ARG:HA   | 12:CL:84:LEU:HD23  | 1.96                     | 0.48              |
| 16:CP:74:LEU:HB3  | 16:CP:79:VAL:HG21  | 1.95                     | 0.48              |
| 18:CR:29:PHE:HD2  | 18:CR:29:PHE:H     | 1.62                     | 0.48              |
| 19:CS:10:PHE:CE2  | 19:CS:37:ARG:O     | 2.67                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:DA:205:G:HO2'   | 25:DA:206:U:P      | 2.35                     | 0.48              |
| 25:DA:625:G:O6     | 36:DP:107:LYS:HD3  | 2.14                     | 0.48              |
| 25:DA:1739:U:O2    | 25:DA:1739:U:C4'   | 2.62                     | 0.48              |
| 25:DA:1914:C:H2'   | 25:DA:1915:U:O4'   | 2.14                     | 0.48              |
| 25:DA:2199:A:O2'   | 33:DI:28:ASN:ND2   | 2.45                     | 0.48              |
| 25:DA:2702:U:O2'   | 25:DA:2703:C:OP2   | 2.21                     | 0.48              |
| 25:DA:2791:C:H1'   | 25:DA:2792:G:N7    | 2.27                     | 0.48              |
| 26:DB:34:U:H5''    | 26:DB:35:U:OP1     | 2.14                     | 0.48              |
| 28:DD:159:ALA:HB1  | 28:DD:198:ASN:O    | 2.14                     | 0.48              |
| 29:DE:199:ARG:HB2  | 29:DE:199:ARG:NH1  | 2.26                     | 0.48              |
| 33:DI:114:LEU:O    | 33:DI:115:ALA:CB   | 2.60                     | 0.48              |
| 34:DN:91:LEU:HD23  | 34:DN:98:VAL:HG21  | 1.95                     | 0.48              |
| 36:DP:46:LYS:HG2   | 36:DP:51:PHE:CG    | 2.48                     | 0.48              |
| 39:DS:20:ARG:HE    | 39:DS:21:THR:HA    | 1.78                     | 0.48              |
| 39:DS:95:HIS:O     | 39:DS:96:GLY:C     | 2.56                     | 0.48              |
| 42:DV:8:GLY:O      | 42:DV:10:LYS:HE3   | 2.13                     | 0.48              |
| 46:DZ:28:MET:CE    | 46:DZ:59:LEU:HD12  | 2.43                     | 0.48              |
| 53:D6:32:ASN:HD22  | 53:D6:33:LYS:HE3   | 1.77                     | 0.48              |
| 53:D6:41:PRO:HD2   | 53:D6:46:HIS:HA    | 1.92                     | 0.48              |
| 1:AA:59:A:H5'      | 1:AA:60:A:O5'      | 2.13                     | 0.48              |
| 1:AA:509:A:O2'     | 1:AA:510:A:OP1     | 2.31                     | 0.48              |
| 2:AB:15:VAL:H      | 2:AB:16:HIS:HD1    | 1.58                     | 0.48              |
| 2:AB:37:ASN:C      | 2:AB:39:ILE:H      | 2.21                     | 0.48              |
| 2:AB:171:ALA:HA    | 2:AB:174:VAL:CG2   | 2.44                     | 0.48              |
| 3:AC:27:LYS:HB3    | 3:AC:27:LYS:NZ     | 2.29                     | 0.48              |
| 3:AC:154:SER:OG    | 3:AC:196:LEU:HD13  | 2.13                     | 0.48              |
| 5:AE:110:LEU:O     | 5:AE:111:GLU:C     | 2.53                     | 0.48              |
| 5:AE:131:ILE:HD13  | 5:AE:131:ILE:HA    | 1.75                     | 0.48              |
| 10:AJ:63:PHE:CD2   | 10:AJ:63:PHE:N     | 2.81                     | 0.48              |
| 13:AM:39:ILE:HD13  | 13:AM:52:GLU:HB3   | 1.96                     | 0.48              |
| 22:AV:20:G:H5''    | 22:AV:21:U:H3      | 1.79                     | 0.48              |
| 25:BA:271(C):C:H2' | 25:BA:271(D):G:C8  | 2.48                     | 0.48              |
| 25:BA:329:G:OP2    | 45:BY:71:LYS:NZ    | 2.41                     | 0.48              |
| 25:BA:628:G:N2     | 25:BA:636:G:H1'    | 2.28                     | 0.48              |
| 25:BA:848:G:H2'    | 25:BA:849:A:C8     | 2.48                     | 0.48              |
| 25:BA:1329:U:H5''  | 25:BA:1330:C:H5    | 1.79                     | 0.48              |
| 25:BA:1952:A:C5    | 35:BO:22:ILE:HD11  | 2.49                     | 0.48              |
| 25:BA:2056:G:H2'   | 25:BA:2056:G:N3    | 2.28                     | 0.48              |
| 25:BA:2126:A:O2'   | 25:BA:2127:G:O4'   | 2.30                     | 0.48              |
| 25:BA:2453:A:O2'   | 25:BA:2572:A:H1'   | 2.13                     | 0.48              |
| 28:BD:176:ARG:HA   | 28:BD:182:LEU:HD23 | 1.94                     | 0.48              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 28:BD:197:GLY:O    | 28:BD:198:ASN:HB3 | 2.14                     | 0.48              |
| 28:BD:268:ARG:CZ   | 28:BD:268:ARG:HB2 | 2.42                     | 0.48              |
| 30:BF:63:LYS:HE3   | 30:BF:65:TRP:O    | 2.12                     | 0.48              |
| 30:BF:152:GLU:HA   | 30:BF:190:GLU:OE2 | 2.14                     | 0.48              |
| 31:BG:106:LEU:O    | 31:BG:110:ALA:HB3 | 2.14                     | 0.48              |
| 31:BG:152:LEU:O    | 31:BG:153:ARG:HD3 | 2.14                     | 0.48              |
| 32:BH:159:GLU:HG3  | 32:BH:160:LYS:CG  | 2.43                     | 0.48              |
| 40:BT:31:SER:CB    | 40:BT:43:GLN:O    | 2.58                     | 0.48              |
| 45:BY:20:TYR:CE1   | 45:BY:42:VAL:N    | 2.81                     | 0.48              |
| 55:B8:9:GLY:O      | 55:B8:13:ARG:HG2  | 2.13                     | 0.48              |
| 1:CA:429:U:O2'     | 1:CA:430:A:OP2    | 2.30                     | 0.48              |
| 1:CA:1346:A:N6     | 1:CA:1375:A:OP2   | 2.44                     | 0.48              |
| 2:CB:37:ASN:O      | 2:CB:37:ASN:ND2   | 2.39                     | 0.48              |
| 2:CB:215:LEU:O     | 2:CB:219:VAL:HG23 | 2.14                     | 0.48              |
| 3:CC:16:ARG:NH1    | 3:CC:16:ARG:HB2   | 2.28                     | 0.48              |
| 5:CE:76:ILE:HG12   | 5:CE:142:LEU:HD22 | 1.94                     | 0.48              |
| 5:CE:80:ILE:HG23   | 5:CE:91:LEU:HB2   | 1.95                     | 0.48              |
| 5:CE:147:ASP:O     | 5:CE:151:LEU:HG   | 2.14                     | 0.48              |
| 11:CK:33:THR:HB    | 11:CK:38:ASN:O    | 2.13                     | 0.48              |
| 11:CK:119:CYS:O    | 11:CK:121:PRO:HD3 | 2.14                     | 0.48              |
| 14:CN:36:PHE:CD1   | 14:CN:37:PHE:CD2  | 3.00                     | 0.48              |
| 15:CO:26:GLU:HA    | 15:CO:81:LEU:CD2  | 2.44                     | 0.48              |
| 19:CS:24:ALA:O     | 19:CS:25:LYS:HB2  | 2.13                     | 0.48              |
| 23:CY:40:C:O2'     | 23:CY:41:C:H5'    | 2.13                     | 0.48              |
| 25:DA:94:C:H5'     | 25:DA:94(A):G:OP2 | 2.13                     | 0.48              |
| 25:DA:141:A:H8     | 25:DA:1408:C:O2'  | 1.97                     | 0.48              |
| 25:DA:558:G:OP1    | 34:DN:111:PRO:HD2 | 2.14                     | 0.48              |
| 25:DA:1568:G:OP2   | 28:DD:63:ARG:NH2  | 2.40                     | 0.48              |
| 25:DA:2238:G:H5'   | 25:DA:2239:G:OP1  | 2.14                     | 0.48              |
| 25:DA:2776:A:O2'   | 25:DA:2781:A:H4'  | 2.13                     | 0.48              |
| 26:DB:66:A:H61     | 26:DB:108:U:C2'   | 2.25                     | 0.48              |
| 29:DE:4:ILE:O      | 29:DE:4:ILE:HG23  | 2.13                     | 0.48              |
| 29:DE:78:LEU:C     | 29:DE:79:ARG:HD2  | 2.38                     | 0.48              |
| 32:DH:153:LYS:HE2  | 32:DH:153:LYS:CA  | 2.43                     | 0.48              |
| 35:DO:104:ARG:HH22 | 40:DT:35:LYS:HE3  | 1.77                     | 0.48              |
| 37:DQ:27:VAL:HG12  | 37:DQ:29:PHE:H    | 1.78                     | 0.48              |
| 38:DR:104:ARG:HH11 | 38:DR:104:ARG:CB  | 2.26                     | 0.48              |
| 41:DU:88:ILE:C     | 41:DU:90:VAL:H    | 2.21                     | 0.48              |
| 41:DU:88:ILE:O     | 41:DU:88:ILE:HG13 | 2.13                     | 0.48              |
| 48:D1:52:ARG:O     | 48:D1:56:GLN:O    | 2.31                     | 0.48              |
| 51:D4:18:CYS:SG    | 51:D4:38:LYS:HB2  | 2.53                     | 0.48              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AA:457:C:H2'    | 1:AA:458:C:C6      | 2.49                     | 0.48              |
| 1:AA:1328:C:O2'   | 13:AM:29:ARG:NH2   | 2.45                     | 0.48              |
| 6:AF:21:LEU:C     | 6:AF:23:LYS:H      | 2.22                     | 0.48              |
| 8:AH:20:TYR:CE1   | 8:AH:76:PRO:O      | 2.67                     | 0.48              |
| 8:AH:21:LYS:O     | 8:AH:22:GLU:C      | 2.56                     | 0.48              |
| 11:AK:99:GLN:HA   | 11:AK:105:VAL:HG21 | 1.95                     | 0.48              |
| 13:AM:65:LYS:HD2  | 13:AM:69:GLU:CB    | 2.44                     | 0.48              |
| 15:AO:82:ILE:CG1  | 15:AO:87:ILE:HB    | 2.40                     | 0.48              |
| 23:AW:6:G:O2'     | 23:AW:7:A:H5'      | 2.13                     | 0.48              |
| 25:BA:242:G:H1'   | 25:BA:243:U:H5     | 1.79                     | 0.48              |
| 25:BA:521:G:H2'   | 25:BA:522:G:H8     | 1.78                     | 0.48              |
| 25:BA:1385:G:O6   | 25:BA:1403:C:C4    | 2.67                     | 0.48              |
| 27:BC:47:LEU:HD23 | 27:BC:47:LEU:N     | 2.28                     | 0.48              |
| 28:BD:24:ILE:O    | 28:BD:26:LYS:HD3   | 2.14                     | 0.48              |
| 28:BD:248:SER:O   | 28:BD:250:TRP:N    | 2.47                     | 0.48              |
| 31:BG:131:TYR:HE2 | 31:BG:133:LEU:CD2  | 2.27                     | 0.48              |
| 33:BI:121:LYS:O   | 33:BI:122:GLU:CB   | 2.49                     | 0.48              |
| 34:BN:38:HIS:ND1  | 34:BN:39:ARG:HG3   | 2.29                     | 0.48              |
| 34:BN:57:ALA:C    | 34:BN:58:ASP:OD1   | 2.57                     | 0.48              |
| 36:BP:47:ASP:CG   | 36:BP:49:ARG:HB2   | 2.39                     | 0.48              |
| 36:BP:109:GLY:O   | 36:BP:110:TYR:O    | 2.31                     | 0.48              |
| 39:BS:71:ARG:HA   | 39:BS:74:ALA:HB3   | 1.95                     | 0.48              |
| 40:BT:91:ARG:HB3  | 40:BT:116:ALA:HA   | 1.95                     | 0.48              |
| 43:BW:5:ALA:HB2   | 43:BW:54:ALA:CB    | 2.40                     | 0.48              |
| 51:B4:38:ALA:O    | 51:B4:50:THR:O     | 2.32                     | 0.48              |
| 51:B4:39:ARG:HG2  | 51:B4:49:GLU:HG3   | 1.94                     | 0.48              |
| 54:B7:43:THR:HG22 | 54:B7:44:PRO:O     | 2.12                     | 0.48              |
| 1:CA:445:G:H2'    | 1:CA:446:G:C8      | 2.49                     | 0.48              |
| 1:CA:674:G:H2'    | 1:CA:675:A:H8      | 1.79                     | 0.48              |
| 1:CA:1067:A:C1'   | 1:CA:1068:G:O4'    | 2.62                     | 0.48              |
| 1:CA:1456:G:H2'   | 1:CA:1457:G:H5'    | 1.95                     | 0.48              |
| 6:CF:101:ALA:OXT  | 18:CR:28:GLU:HG3   | 2.14                     | 0.48              |
| 8:CH:67:PRO:O     | 8:CH:76:PRO:HB3    | 2.14                     | 0.48              |
| 8:CH:121:ASP:OD1  | 8:CH:121:ASP:N     | 2.46                     | 0.48              |
| 23:CW:36:A:C2'    | 23:CW:37:A:C5'     | 2.89                     | 0.48              |
| 25:DA:27:G:N2     | 25:DA:513:A:OP2    | 2.47                     | 0.48              |
| 25:DA:360:G:H2'   | 25:DA:361:G:H8     | 1.79                     | 0.48              |
| 25:DA:1609:A:H4'  | 25:DA:1617:C:OP1   | 2.14                     | 0.48              |
| 25:DA:2564:A:C2   | 25:DA:2647:U:H4'   | 2.49                     | 0.48              |
| 25:DA:2787:C:O2'  | 29:DE:61:ARG:HG3   | 2.14                     | 0.48              |
| 25:DA:2814:C:O2'  | 52:D5:29:THR:HG21  | 2.14                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 28:DD:24:ILE:O     | 28:DD:25:THR:O     | 2.31                     | 0.48              |
| 29:DE:47:VAL:O     | 29:DE:80:GLU:HA    | 2.13                     | 0.48              |
| 29:DE:101:ARG:HH21 | 29:DE:171:GLU:CB   | 2.26                     | 0.48              |
| 29:DE:119:ARG:HG2  | 29:DE:160:TYR:HB2  | 1.95                     | 0.48              |
| 30:DF:88:VAL:HG11  | 30:DF:91:GLY:HA3   | 1.95                     | 0.48              |
| 34:DN:26:LEU:HD21  | 34:DN:30:ILE:HD11  | 1.94                     | 0.48              |
| 40:DT:23:ARG:HD3   | 40:DT:120:ARG:HD3  | 1.94                     | 0.48              |
| 46:DZ:117:LEU:CA   | 46:DZ:174:VAL:HG22 | 2.42                     | 0.48              |
| 49:D2:46:GLN:OE1   | 49:D2:46:GLN:HA    | 2.13                     | 0.48              |
| 1:AA:109:A:C6      | 1:AA:326:G:C6      | 3.02                     | 0.48              |
| 1:AA:301:G:H2'     | 1:AA:302:G:C8      | 2.49                     | 0.48              |
| 1:AA:366:C:HO2'    | 1:AA:367:U:P       | 2.37                     | 0.48              |
| 3:AC:73:PRO:O      | 3:AC:76:VAL:HG13   | 2.13                     | 0.48              |
| 4:AD:89:THR:O      | 4:AD:90:GLY:C      | 2.56                     | 0.48              |
| 6:AF:45:LEU:HD12   | 6:AF:46:ARG:N      | 2.26                     | 0.48              |
| 7:AG:22:LEU:HD23   | 7:AG:62:PHE:CE2    | 2.40                     | 0.48              |
| 12:AL:11:VAL:HG12  | 12:AL:12:ARG:HG2   | 1.96                     | 0.48              |
| 12:AL:17:LYS:HZ3   | 12:AL:18:VAL:HG22  | 1.78                     | 0.48              |
| 12:AL:45:PRO:HD3   | 12:AL:51:ALA:O     | 2.14                     | 0.48              |
| 14:AN:21:TYR:C     | 14:AN:22:THR:O     | 2.57                     | 0.48              |
| 19:AS:15:LEU:H     | 19:AS:15:LEU:HD22  | 1.79                     | 0.48              |
| 20:AT:49:ALA:O     | 20:AT:100:ILE:HD13 | 2.13                     | 0.48              |
| 25:BA:659:C:H4'    | 30:BF:100:THR:O    | 2.14                     | 0.48              |
| 25:BA:811:U:O2     | 25:BA:1250:G:O5'   | 2.32                     | 0.48              |
| 25:BA:856:C:H1'    | 47:B0:27:GLU:HB3   | 1.95                     | 0.48              |
| 25:BA:1819:A:O4'   | 25:BA:1821:A:C5    | 2.67                     | 0.48              |
| 30:BF:66:PRO:O     | 30:BF:67:GLN:CB    | 2.61                     | 0.48              |
| 30:BF:83:PHE:O     | 30:BF:86:GLY:N     | 2.47                     | 0.48              |
| 40:BT:9:LEU:HD23   | 40:BT:9:LEU:HA     | 1.74                     | 0.48              |
| 40:BT:18:ASP:OD1   | 40:BT:18:ASP:N     | 2.34                     | 0.48              |
| 40:BT:23:ARG:O     | 40:BT:24:PRO:C     | 2.56                     | 0.48              |
| 41:BU:25:TRP:HD1   | 41:BU:26:GLY:HA2   | 1.79                     | 0.48              |
| 41:BU:68:ALA:O     | 41:BU:71:GLN:HB2   | 2.14                     | 0.48              |
| 44:BX:12:VAL:CG1   | 44:BX:17:ALA:HB1   | 2.43                     | 0.48              |
| 49:B2:18:PRO:O     | 49:B2:21:LEU:HB2   | 2.13                     | 0.48              |
| 1:CA:284:G:H2'     | 1:CA:285:G:H8      | 1.78                     | 0.48              |
| 1:CA:975:A:H62     | 10:CJ:60:ARG:NH1   | 2.12                     | 0.48              |
| 1:CA:1002:G:N2     | 1:CA:1039:C:O2     | 2.47                     | 0.48              |
| 3:CC:83:ARG:C      | 3:CC:85:ARG:H      | 2.22                     | 0.48              |
| 3:CC:189:ALA:HB3   | 3:CC:196:LEU:HB2   | 1.95                     | 0.48              |
| 5:CE:37:ARG:C      | 5:CE:38:GLN:HG2    | 2.39                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:CK:11:LYS:HB2   | 11:CK:12:ARG:H     | 1.55                     | 0.48              |
| 11:CK:44:SER:OG    | 11:CK:47:VAL:HG23  | 2.13                     | 0.48              |
| 11:CK:54:ARG:HH12  | 23:CW:40:C:C5'     | 2.23                     | 0.48              |
| 12:CL:71:PRO:O     | 12:CL:102:ARG:HD3  | 2.13                     | 0.48              |
| 12:CL:119:LYS:O    | 12:CL:121:GLY:N    | 2.46                     | 0.48              |
| 13:CM:74:VAL:O     | 13:CM:78:ILE:HG13  | 2.14                     | 0.48              |
| 14:CN:4:LYS:O      | 14:CN:5:ALA:C      | 2.56                     | 0.48              |
| 17:CQ:22:LEU:HD22  | 17:CQ:88:TYR:CD1   | 2.49                     | 0.48              |
| 22:CV:35:C:H42     | 24:CX:18:G:H1      | 1.60                     | 0.48              |
| 22:CV:35:C:O2'     | 22:CV:36:A:P       | 2.72                     | 0.48              |
| 25:DA:328:U:O2'    | 45:DY:71:LYS:HD3   | 2.14                     | 0.48              |
| 25:DA:481:G:H1'    | 25:DA:506:G:N2     | 2.28                     | 0.48              |
| 25:DA:636:G:C4     | 36:DP:115:LEU:HD11 | 2.49                     | 0.48              |
| 25:DA:1542:A:O2'   | 25:DA:1543:C:P     | 2.72                     | 0.48              |
| 25:DA:1799:G:O2'   | 25:DA:1800:C:H5''  | 2.13                     | 0.48              |
| 27:DC:83:ILE:HG23  | 27:DC:94:VAL:HG23  | 1.96                     | 0.48              |
| 29:DE:118:LYS:HE3  | 38:DR:1:MET:HE1    | 1.95                     | 0.48              |
| 31:DG:151:ALA:HB3  | 31:DG:153:ARG:HH12 | 1.79                     | 0.48              |
| 36:DP:114:ILE:HG21 | 36:DP:125:VAL:HG21 | 1.95                     | 0.48              |
| 37:DQ:32:TYR:OH    | 37:DQ:111:GLU:HB2  | 2.14                     | 0.48              |
| 37:DQ:116:GLU:HA   | 37:DQ:116:GLU:OE1  | 2.14                     | 0.48              |
| 38:DR:1:MET:HG3    | 38:DR:3:HIS:CE1    | 2.49                     | 0.48              |
| 40:DT:78:LEU:O     | 40:DT:79:HIS:ND1   | 2.47                     | 0.48              |
| 42:DV:91:TYR:C     | 42:DV:91:TYR:HD1   | 2.21                     | 0.48              |
| 45:DY:19:LYS:O     | 45:DY:19:LYS:HD2   | 2.13                     | 0.48              |
| 45:DY:44:ILE:HD12  | 45:DY:45:VAL:HG23  | 1.95                     | 0.48              |
| 45:DY:75:ILE:HD13  | 45:DY:76:CYS:N     | 2.28                     | 0.48              |
| 46:DZ:81:ARG:O     | 46:DZ:82:ARG:HB2   | 2.14                     | 0.48              |
| 1:AA:130:A:H1'     | 1:AA:264:U:H5'     | 1.96                     | 0.47              |
| 1:AA:232:G:O2'     | 1:AA:263:A:N1      | 2.39                     | 0.47              |
| 1:AA:284:G:H2'     | 1:AA:285:G:H8      | 1.78                     | 0.47              |
| 1:AA:337:C:H2'     | 1:AA:338:A:C8      | 2.49                     | 0.47              |
| 1:AA:757:U:H2'     | 1:AA:758:G:O4'     | 2.13                     | 0.47              |
| 1:AA:985:C:H2'     | 1:AA:986:A:C8      | 2.47                     | 0.47              |
| 1:AA:1473:A:H2'    | 1:AA:1474:G:C8     | 2.48                     | 0.47              |
| 1:AA:1503:A:O2'    | 1:AA:1504:G:OP2    | 2.31                     | 0.47              |
| 3:AC:42:LEU:HD12   | 3:AC:45:LYS:HZ3    | 1.79                     | 0.47              |
| 3:AC:73:PRO:HA     | 3:AC:76:VAL:CG1    | 2.44                     | 0.47              |
| 4:AD:55:ALA:O      | 4:AD:59:ARG:HG2    | 2.14                     | 0.47              |
| 7:AG:92:SER:HB3    | 7:AG:95:ARG:CB     | 2.44                     | 0.47              |
| 8:AH:44:PHE:HD1    | 8:AH:79:VAL:HG12   | 1.79                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:AI:76:ALA:O     | 9:AI:79:LEU:HB3   | 2.14                     | 0.47              |
| 16:AP:8:ARG:C     | 16:AP:9:PHE:HD2   | 2.22                     | 0.47              |
| 25:BA:51:G:N3     | 25:BA:119:A:C2    | 2.82                     | 0.47              |
| 25:BA:340:A:C5    | 25:BA:341:G:C5    | 3.02                     | 0.47              |
| 25:BA:704:G:O2'   | 25:BA:705:A:OP2   | 2.30                     | 0.47              |
| 25:BA:1695:G:H1'  | 28:BD:8:PRO:O     | 2.14                     | 0.47              |
| 25:BA:1966:A:O2'  | 25:BA:2592:G:O3'  | 2.30                     | 0.47              |
| 25:BA:2015:A:C1'  | 52:B5:2:ALA:HA    | 2.40                     | 0.47              |
| 25:BA:2067:G:H5'' | 25:BA:2068:U:OP2  | 2.14                     | 0.47              |
| 25:BA:2689:U:O2'  | 25:BA:2690:C:P    | 2.72                     | 0.47              |
| 27:BC:59:ARG:NH2  | 27:BC:199:HIS:H   | 2.12                     | 0.47              |
| 30:BF:22:ALA:CA   | 30:BF:26:ALA:HB2  | 2.45                     | 0.47              |
| 31:BG:38:VAL:HG22 | 31:BG:93:THR:HA   | 1.96                     | 0.47              |
| 32:BH:19:VAL:HG21 | 32:BH:44:VAL:HA   | 1.95                     | 0.47              |
| 32:BH:85:LYS:O    | 32:BH:132:ARG:CA  | 2.59                     | 0.47              |
| 32:BH:98:LEU:HD12 | 32:BH:102:ALA:O   | 2.14                     | 0.47              |
| 41:BU:31:SER:O    | 41:BU:35:ALA:N    | 2.38                     | 0.47              |
| 44:BX:65:ARG:HD3  | 44:BX:70:LEU:HD12 | 1.95                     | 0.47              |
| 46:BZ:126:VAL:HA  | 46:BZ:164:ALA:HB2 | 1.96                     | 0.47              |
| 1:CA:49:U:O2      | 1:CA:362:G:H1'    | 2.13                     | 0.47              |
| 1:CA:1080:A:H5'   | 5:CE:16:THR:HG21  | 1.96                     | 0.47              |
| 1:CA:1441:G:H4'   | 1:CA:1442:G:C5    | 2.49                     | 0.47              |
| 7:CG:108:ALA:CB   | 7:CG:120:ILE:HD13 | 2.44                     | 0.47              |
| 11:CK:20:TYR:CB   | 11:CK:31:THR:HG22 | 2.43                     | 0.47              |
| 11:CK:21:ILE:HB   | 11:CK:84:VAL:HG12 | 1.96                     | 0.47              |
| 12:CL:100:ILE:CG2 | 12:CL:101:VAL:N   | 2.77                     | 0.47              |
| 17:CQ:59:ILE:HG22 | 17:CQ:71:PHE:CB   | 2.32                     | 0.47              |
| 22:CV:19:G:C2     | 22:CV:59:A:C5     | 3.02                     | 0.47              |
| 22:CV:48:U:H6     | 22:CV:51:U:OP1    | 1.96                     | 0.47              |
| 23:CW:12:U:C4     | 23:CW:13:C:C5     | 3.02                     | 0.47              |
| 25:DA:121:G:H4'   | 25:DA:149:A:H5'   | 1.96                     | 0.47              |
| 25:DA:332:A:O2'   | 25:DA:333:G:OP1   | 2.32                     | 0.47              |
| 25:DA:396:G:O3'   | 48:D1:44:PRO:HA   | 2.13                     | 0.47              |
| 25:DA:746:A:C5    | 25:DA:2611:U:H5'' | 2.49                     | 0.47              |
| 25:DA:813:U:H2'   | 25:DA:814:C:C6    | 2.49                     | 0.47              |
| 25:DA:1578:U:C2'  | 25:DA:1579:A:H5'  | 2.44                     | 0.47              |
| 28:DD:70:TRP:CH2  | 28:DD:150:LYS:HA  | 2.49                     | 0.47              |
| 30:DF:62:ARG:NH1  | 30:DF:62:ARG:CG   | 2.55                     | 0.47              |
| 30:DF:178:PRO:HB3 | 30:DF:198:ALA:CB  | 2.44                     | 0.47              |
| 34:DN:89:LYS:O    | 34:DN:93:THR:HG22 | 2.13                     | 0.47              |
| 35:DO:49:ARG:NH1  | 35:DO:49:ARG:CG   | 2.76                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:DO:104:ARG:HH21 | 40:DT:33:LYS:HE3   | 1.78                     | 0.47              |
| 43:DW:60:ASN:N     | 43:DW:60:ASN:ND2   | 2.61                     | 0.47              |
| 44:DX:44:GLU:C     | 44:DX:46:ALA:H     | 2.22                     | 0.47              |
| 46:DZ:22:GLY:HA2   | 46:DZ:41:LEU:HD11  | 1.96                     | 0.47              |
| 48:D1:64:ALA:C     | 48:D1:66:HIS:N     | 2.71                     | 0.47              |
| 53:D6:42:TRP:CE3   | 53:D6:42:TRP:HA    | 2.49                     | 0.47              |
| 56:D9:9:ARG:HH11   | 56:D9:9:ARG:CB     | 2.26                     | 0.47              |
| 1:AA:1120:G:H2'    | 1:AA:1121:U:C6     | 2.50                     | 0.47              |
| 1:AA:1201:A:O2'    | 1:AA:1202:G:OP2    | 2.30                     | 0.47              |
| 1:AA:1530:G:C2'    | 1:AA:1531:A:O5'    | 2.62                     | 0.47              |
| 2:AB:221:LEU:O     | 2:AB:222:ILE:C     | 2.56                     | 0.47              |
| 3:AC:113:ALA:C     | 3:AC:115:LEU:H     | 2.22                     | 0.47              |
| 4:AD:149:ALA:HB3   | 4:AD:152:SER:OG    | 2.14                     | 0.47              |
| 5:AE:105:VAL:HG12  | 5:AE:106:PRO:CD    | 2.44                     | 0.47              |
| 6:AF:62:TRP:CD1    | 18:AR:35:ARG:CZ    | 2.97                     | 0.47              |
| 7:AG:72:ARG:HG3    | 7:AG:73:MET:HE2    | 1.96                     | 0.47              |
| 7:AG:137:LYS:HE2   | 7:AG:137:LYS:HB3   | 1.74                     | 0.47              |
| 12:AL:7:ILE:HA     | 12:AL:10:LEU:CD1   | 2.40                     | 0.47              |
| 13:AM:3:ARG:CD     | 31:BG:113:ARG:HH21 | 2.28                     | 0.47              |
| 17:AQ:59:ILE:CG2   | 17:AQ:71:PHE:HB3   | 2.44                     | 0.47              |
| 18:AR:25:THR:HG22  | 18:AR:42:ARG:NH1   | 2.29                     | 0.47              |
| 22:AV:48:U:C6      | 22:AV:51:U:OP1     | 2.67                     | 0.47              |
| 23:AW:66:U:H2'     | 23:AW:67:C:H6      | 1.74                     | 0.47              |
| 23:AY:37:A:H2'     | 23:AY:38:A:O4'     | 2.14                     | 0.47              |
| 25:BA:204:A:O2'    | 25:BA:205:G:H4'    | 2.14                     | 0.47              |
| 25:BA:271(J):C:H5' | 25:BA:271(K):U:OP2 | 2.15                     | 0.47              |
| 25:BA:703:U:N3     | 25:BA:727:A:N6     | 2.62                     | 0.47              |
| 25:BA:773:U:H4'    | 28:BD:47:GLY:HA2   | 1.96                     | 0.47              |
| 25:BA:1301:A:H5''  | 25:BA:1301:A:C2    | 2.47                     | 0.47              |
| 25:BA:1412:A:H2'   | 25:BA:1413:G:C8    | 2.49                     | 0.47              |
| 25:BA:1966:A:H1'   | 25:BA:2593:U:C4'   | 2.43                     | 0.47              |
| 25:BA:2127:G:C6    | 25:BA:2162:G:N1    | 2.82                     | 0.47              |
| 25:BA:2810:A:H2'   | 29:BE:61:ARG:NH2   | 2.29                     | 0.47              |
| 32:BH:12:PRO:HG3   | 32:BH:50:VAL:HG23  | 1.94                     | 0.47              |
| 34:BN:35:ARG:C     | 34:BN:37:LYS:H     | 2.21                     | 0.47              |
| 37:BQ:114:ALA:C    | 37:BQ:116:GLU:N    | 2.73                     | 0.47              |
| 38:BR:39:PRO:C     | 38:BR:41:ALA:N     | 2.71                     | 0.47              |
| 38:BR:63:ARG:O     | 38:BR:67:LEU:HB2   | 2.14                     | 0.47              |
| 42:BV:4:ILE:O      | 42:BV:39:LEU:HD22  | 2.14                     | 0.47              |
| 45:BY:36:ALA:HA    | 45:BY:69:ALA:N     | 2.29                     | 0.47              |
| 54:B7:1:MET:HE2    | 54:B7:1:MET:HB2    | 1.73                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:173:U:H1'     | 1:CA:197:A:C6      | 2.49                     | 0.47              |
| 1:CA:609:A:H5'     | 16:CP:18:ARG:HH22  | 1.80                     | 0.47              |
| 1:CA:1300:G:O4'    | 1:CA:1300:G:OP2    | 2.32                     | 0.47              |
| 1:CA:1346:A:H1'    | 1:CA:1348:U:C6     | 2.49                     | 0.47              |
| 3:CC:61:ALA:N      | 3:CC:63:ASN:OD1    | 2.35                     | 0.47              |
| 8:CH:103:VAL:CG1   | 8:CH:138:TRP:HD1   | 2.27                     | 0.47              |
| 13:CM:124:PRO:HB3  | 13:CM:125:ARG:CA   | 2.41                     | 0.47              |
| 18:CR:36:ASN:HB2   | 18:CR:39:VAL:CG2   | 2.44                     | 0.47              |
| 22:CV:44:A:H2'     | 22:CV:45:A:C8      | 2.49                     | 0.47              |
| 22:CV:48:U:C5      | 22:CV:51:U:OP1     | 2.67                     | 0.47              |
| 23:CW:2:C:C2       | 23:CW:3:C:C5       | 3.02                     | 0.47              |
| 23:CW:16:U:C5      | 23:CW:18:G:H3'     | 2.49                     | 0.47              |
| 24:CX:17:U:O2'     | 24:CX:18:G:H5'     | 2.14                     | 0.47              |
| 25:DA:271(E):U:H2' | 25:DA:271(F):C:C6  | 2.49                     | 0.47              |
| 25:DA:994:C:H3'    | 41:DU:54:LYS:HE3   | 1.96                     | 0.47              |
| 25:DA:1340:U:O2'   | 25:DA:1341:U:OP1   | 2.30                     | 0.47              |
| 25:DA:1385:G:H4'   | 25:DA:1386:C:OP1   | 2.14                     | 0.47              |
| 25:DA:1434:A:H61   | 25:DA:1558:A:N6    | 2.09                     | 0.47              |
| 25:DA:1790:C:H2'   | 25:DA:1791:A:C5    | 2.49                     | 0.47              |
| 25:DA:1964:G:H4'   | 25:DA:1965:C:OP2   | 2.14                     | 0.47              |
| 29:DE:117:MET:HE3  | 29:DE:124:GLY:HA3  | 1.95                     | 0.47              |
| 29:DE:188:VAL:HG22 | 29:DE:189:PRO:HD2  | 1.95                     | 0.47              |
| 30:DF:170:LEU:HD23 | 30:DF:172:TRP:CZ2  | 2.49                     | 0.47              |
| 31:DG:99:MET:HE2   | 31:DG:103:LEU:HD12 | 1.96                     | 0.47              |
| 32:DH:151:ILE:O    | 32:DH:152:ARG:HG2  | 2.14                     | 0.47              |
| 33:DI:64:GLU:HA    | 33:DI:64:GLU:OE1   | 2.14                     | 0.47              |
| 36:DP:112:LEU:C    | 36:DP:112:LEU:HD13 | 2.39                     | 0.47              |
| 36:DP:114:ILE:HG12 | 36:DP:130:PHE:CD1  | 2.49                     | 0.47              |
| 37:DQ:25:ASP:CG    | 46:DZ:78:LYS:HD2   | 2.39                     | 0.47              |
| 37:DQ:66:ILE:HG22  | 37:DQ:104:PHE:HE2  | 1.78                     | 0.47              |
| 37:DQ:115:MET:HE2  | 37:DQ:115:MET:HA   | 1.96                     | 0.47              |
| 39:DS:88:ASP:CG    | 39:DS:89:ARG:H     | 2.22                     | 0.47              |
| 40:DT:39:ARG:C     | 40:DT:40:THR:CG2   | 2.87                     | 0.47              |
| 41:DU:91:ASP:N     | 41:DU:92:ARG:HD3   | 2.29                     | 0.47              |
| 41:DU:114:LYS:O    | 41:DU:117:GLN:HB2  | 2.13                     | 0.47              |
| 45:DY:94:LYS:CD    | 45:DY:101:LYS:HZ3  | 2.27                     | 0.47              |
| 47:D0:10:THR:HG22  | 47:D0:12:ASN:H     | 1.78                     | 0.47              |
| 52:D5:6:VAL:CG2    | 52:D5:7:PRO:HD2    | 2.44                     | 0.47              |
| 53:D6:15:GLU:HG3   | 53:D6:47:THR:CB    | 2.43                     | 0.47              |
| 1:AA:8:A:N6        | 4:AD:208:SER:HB2   | 2.29                     | 0.47              |
| 1:AA:552:U:H2'     | 1:AA:553:A:H8      | 1.80                     | 0.47              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AA:1275:A:C4    | 1:AA:1276:G:C8     | 3.03                     | 0.47              |
| 2:AB:47:THR:O     | 2:AB:51:LEU:HG     | 2.14                     | 0.47              |
| 2:AB:76:GLN:H     | 2:AB:76:GLN:HG3    | 1.37                     | 0.47              |
| 2:AB:92:TYR:CD2   | 2:AB:151:GLY:HA3   | 2.49                     | 0.47              |
| 3:AC:29:TYR:C     | 3:AC:29:TYR:HD2    | 2.21                     | 0.47              |
| 3:AC:116:VAL:CG2  | 3:AC:202:ILE:HD11  | 2.43                     | 0.47              |
| 4:AD:80:GLU:O     | 4:AD:84:LYS:HG2    | 2.13                     | 0.47              |
| 4:AD:96:LEU:HD12  | 4:AD:96:LEU:N      | 2.28                     | 0.47              |
| 5:AE:53:LEU:HD12  | 5:AE:53:LEU:N      | 2.30                     | 0.47              |
| 6:AF:8:ILE:HG12   | 6:AF:88:VAL:HG22   | 1.97                     | 0.47              |
| 6:AF:100:ASN:ND2  | 18:AR:23:LYS:HE3   | 2.29                     | 0.47              |
| 7:AG:51:GLN:O     | 7:AG:54:THR:O      | 2.31                     | 0.47              |
| 9:AI:125:TYR:HD2  | 9:AI:126:SER:N     | 2.11                     | 0.47              |
| 10:AJ:50:ILE:O    | 10:AJ:51:ARG:C     | 2.58                     | 0.47              |
| 10:AJ:94:VAL:HG12 | 10:AJ:95:GLU:N     | 2.29                     | 0.47              |
| 12:AL:41:ARG:HG2  | 12:AL:42:THR:N     | 2.29                     | 0.47              |
| 16:AP:57:ARG:CZ   | 16:AP:79:VAL:O     | 2.63                     | 0.47              |
| 17:AQ:20:THR:HA   | 17:AQ:43:LEU:HD23  | 1.95                     | 0.47              |
| 18:AR:26:LEU:HD21 | 18:AR:42:ARG:HD2   | 1.96                     | 0.47              |
| 23:AW:59:U:C5     | 23:AW:60:U:N3      | 2.82                     | 0.47              |
| 25:BA:565:C:H4'   | 25:BA:1253:A:C6    | 2.49                     | 0.47              |
| 25:BA:1550:C:H6   | 25:BA:1550:C:O5'   | 1.98                     | 0.47              |
| 25:BA:2198:A:C5'  | 25:BA:2199:A:OP1   | 2.61                     | 0.47              |
| 25:BA:2231:C:H2'  | 25:BA:2232:U:O4'   | 2.14                     | 0.47              |
| 25:BA:2691:C:C6   | 25:BA:2872:G:N1    | 2.83                     | 0.47              |
| 25:BA:2844:G:H3'  | 25:BA:2845:G:C8    | 2.49                     | 0.47              |
| 30:BF:65:TRP:CZ3  | 30:BF:72:ARG:CB    | 2.97                     | 0.47              |
| 30:BF:158:THR:OG1 | 30:BF:160:ASN:N    | 2.40                     | 0.47              |
| 31:BG:91:ARG:HG3  | 31:BG:91:ARG:HH11  | 1.78                     | 0.47              |
| 33:BI:15:VAL:C    | 33:BI:17:GLN:H     | 2.22                     | 0.47              |
| 33:BI:98:ALA:HA   | 33:BI:101:LEU:HB2  | 1.97                     | 0.47              |
| 36:BP:11:GLY:O    | 36:BP:12:ALA:HB3   | 2.15                     | 0.47              |
| 38:BR:103:ARG:O   | 38:BR:104:ARG:C    | 2.56                     | 0.47              |
| 40:BT:28:VAL:CG1  | 40:BT:29:ARG:HH21  | 2.27                     | 0.47              |
| 41:BU:80:ILE:HD11 | 41:BU:93:LYS:HE3   | 1.95                     | 0.47              |
| 41:BU:96:ALA:O    | 41:BU:98:LEU:N     | 2.47                     | 0.47              |
| 41:BU:108:GLU:HG3 | 42:BV:44:LYS:HZ2   | 1.79                     | 0.47              |
| 43:BW:55:ALA:O    | 43:BW:58:ALA:N     | 2.46                     | 0.47              |
| 46:BZ:105:VAL:O   | 46:BZ:105:VAL:HG13 | 2.14                     | 0.47              |
| 49:B2:63:VAL:O    | 49:B2:64:LEU:C     | 2.58                     | 0.47              |
| 55:B8:2:PRO:O     | 55:B8:3:LYS:C      | 2.57                     | 0.47              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:CA:120:A:O2'    | 1:CA:121:C:H5'     | 2.13                     | 0.47              |
| 1:CA:324:G:N2     | 1:CA:327:A:OP2     | 2.47                     | 0.47              |
| 1:CA:792:A:C4     | 1:CA:794:A:N6      | 2.82                     | 0.47              |
| 1:CA:1054:C:C4    | 23:CY:34:G:H1'     | 2.45                     | 0.47              |
| 1:CA:1190:G:P     | 3:CC:5:ILE:HG13    | 2.54                     | 0.47              |
| 1:CA:1501:C:OP2   | 1:CA:1504:G:H2'    | 2.15                     | 0.47              |
| 8:CH:44:PHE:CZ    | 8:CH:137:VAL:HG12  | 2.49                     | 0.47              |
| 11:CK:61:ALA:O    | 11:CK:64:ALA:HB3   | 2.13                     | 0.47              |
| 12:CL:53:ARG:HB3  | 12:CL:93:LEU:HD11  | 1.97                     | 0.47              |
| 23:CW:35:A:H8     | 23:CW:35:A:O5'     | 1.97                     | 0.47              |
| 25:DA:97:C:H5''   | 49:D2:2:LYS:HB2    | 1.96                     | 0.47              |
| 25:DA:910:A:C6    | 25:DA:911:A:C6     | 3.02                     | 0.47              |
| 25:DA:911:A:H2'   | 37:DQ:9:TYR:OH     | 2.14                     | 0.47              |
| 25:DA:1455:G:H21  | 25:DA:1456:G:C1'   | 2.27                     | 0.47              |
| 25:DA:1693:U:H2'  | 28:DD:14:ARG:HH22  | 1.66                     | 0.47              |
| 25:DA:1693:U:OP2  | 25:DA:1694:C:N4    | 2.47                     | 0.47              |
| 25:DA:2126:A:O2'  | 25:DA:2127:G:OP2   | 2.31                     | 0.47              |
| 25:DA:2712:U:H1'  | 25:DA:2712(A):A:C8 | 2.49                     | 0.47              |
| 25:DA:2750:A:O2'  | 25:DA:2751:G:OP1   | 2.30                     | 0.47              |
| 29:DE:203:LYS:O   | 29:DE:203:LYS:HE3  | 2.15                     | 0.47              |
| 30:DF:54:ARG:HG2  | 30:DF:81:PRO:HD3   | 1.96                     | 0.47              |
| 31:DG:37:VAL:HG23 | 31:DG:99:MET:HE1   | 1.96                     | 0.47              |
| 31:DG:88:ILE:O    | 31:DG:88:ILE:CG2   | 2.62                     | 0.47              |
| 40:DT:33:LYS:CG   | 40:DT:43:GLN:CB    | 2.82                     | 0.47              |
| 41:DU:98:LEU:O    | 41:DU:101:ARG:O    | 2.32                     | 0.47              |
| 42:DV:59:ALA:HA   | 42:DV:95:LEU:O     | 2.14                     | 0.47              |
| 43:DW:64:MET:HE2  | 43:DW:109:GLU:HG2  | 1.94                     | 0.47              |
| 45:DY:45:VAL:HG12 | 45:DY:60:PHE:HB3   | 1.95                     | 0.47              |
| 46:DZ:61:LEU:HG   | 46:DZ:67:LEU:HD11  | 1.94                     | 0.47              |
| 48:D1:80:LEU:HB3  | 48:D1:82:LEU:HD22  | 1.95                     | 0.47              |
| 54:D7:19:ARG:HH11 | 54:D7:19:ARG:HG2   | 1.79                     | 0.47              |
| 1:AA:224:C:H2'    | 1:AA:225:C:C6      | 2.50                     | 0.47              |
| 1:AA:819:A:H4'    | 1:AA:820:U:OP2     | 2.14                     | 0.47              |
| 2:AB:212:GLN:C    | 2:AB:212:GLN:OE1   | 2.58                     | 0.47              |
| 3:AC:86:VAL:HG23  | 3:AC:87:LEU:HD23   | 1.96                     | 0.47              |
| 3:AC:132:ARG:O    | 3:AC:133:ALA:C     | 2.57                     | 0.47              |
| 4:AD:162:LEU:HD13 | 4:AD:181:MET:HG2   | 1.96                     | 0.47              |
| 9:AI:40:LEU:C     | 9:AI:42:ARG:N      | 2.71                     | 0.47              |
| 23:AW:63:G:HO2'   | 27:BC:53:ARG:HG2   | 1.76                     | 0.47              |
| 25:BA:126:A:O5'   | 54:B7:19:ARG:HG3   | 2.14                     | 0.47              |
| 25:BA:236:C:H2'   | 25:BA:237:C:C6     | 2.49                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:BA:520:G:H2'    | 25:BA:521:G:C8     | 2.48                     | 0.47              |
| 25:BA:748:G:OP1    | 25:BA:2612:C:N4    | 2.47                     | 0.47              |
| 26:BB:65:C:H3'     | 26:BB:109:C:H42    | 1.79                     | 0.47              |
| 28:BD:143:HIS:HB3  | 28:BD:194:GLY:O    | 2.14                     | 0.47              |
| 28:BD:201:HIS:O    | 28:BD:204:ILE:HG12 | 2.15                     | 0.47              |
| 30:BF:122:LYS:HB3  | 30:BF:191:ARG:HG2  | 1.97                     | 0.47              |
| 33:BI:131:LYS:HD2  | 33:BI:131:LYS:HA   | 1.61                     | 0.47              |
| 35:BO:87:ILE:HG22  | 35:BO:88:ASN:O     | 2.13                     | 0.47              |
| 36:BP:112:LEU:HD13 | 36:BP:112:LEU:C    | 2.39                     | 0.47              |
| 40:BT:53:ARG:HH11  | 40:BT:53:ARG:CG    | 2.27                     | 0.47              |
| 41:BU:61:TRP:O     | 41:BU:62:ILE:C     | 2.56                     | 0.47              |
| 42:BV:98:GLU:CD    | 42:BV:100:ARG:HD3  | 2.38                     | 0.47              |
| 43:BW:51:LEU:HD13  | 43:BW:51:LEU:O     | 2.10                     | 0.47              |
| 47:B0:25:ARG:HA    | 47:B0:29:GLN:NE2   | 2.29                     | 0.47              |
| 55:B8:32:LEU:C     | 55:B8:33:ASN:CG    | 2.80                     | 0.47              |
| 1:CA:142:G:H2'     | 1:CA:143:A:H8      | 1.79                     | 0.47              |
| 1:CA:563:A:H2'     | 1:CA:567:G:C8      | 2.49                     | 0.47              |
| 2:CB:119:GLU:O     | 2:CB:122:PHE:HB3   | 2.14                     | 0.47              |
| 2:CB:132:LYS:HG3   | 2:CB:135:GLN:OE1   | 2.15                     | 0.47              |
| 4:CD:9:CYS:SG      | 4:CD:22:LYS:HD3    | 2.55                     | 0.47              |
| 4:CD:92:VAL:HG12   | 4:CD:96:LEU:CD1    | 2.45                     | 0.47              |
| 8:CH:123:GLU:O     | 8:CH:127:LEU:HB2   | 2.15                     | 0.47              |
| 9:CI:118:LYS:NZ    | 9:CI:118:LYS:HB3   | 2.30                     | 0.47              |
| 13:CM:48:LEU:N     | 13:CM:48:LEU:HD23  | 2.28                     | 0.47              |
| 14:CN:43:CYS:O     | 14:CN:46:GLU:N     | 2.47                     | 0.47              |
| 17:CQ:93:GLN:O     | 17:CQ:95:TYR:N     | 2.47                     | 0.47              |
| 18:CR:75:ILE:HG22  | 18:CR:76:LEU:CD2   | 2.44                     | 0.47              |
| 21:CU:5:ASP:O      | 21:CU:8:THR:HG23   | 2.15                     | 0.47              |
| 25:DA:889:C:O2'    | 25:DA:890:A:OP2    | 2.30                     | 0.47              |
| 25:DA:1653:G:O6    | 38:DR:9:LYS:O      | 2.33                     | 0.47              |
| 25:DA:1902:C:H2'   | 25:DA:1903:G:O4'   | 2.14                     | 0.47              |
| 25:DA:2011:U:OP1   | 43:DW:42:ARG:NH1   | 2.48                     | 0.47              |
| 25:DA:2073:C:H4'   | 28:DD:228:PRO:HB2  | 1.95                     | 0.47              |
| 25:DA:2328:A:H2'   | 25:DA:2329:G:C8    | 2.48                     | 0.47              |
| 26:DB:12:C:O2'     | 26:DB:13:A:H5''    | 2.13                     | 0.47              |
| 28:DD:73:VAL:HG13  | 28:DD:120:GLY:HA2  | 1.96                     | 0.47              |
| 28:DD:213:ARG:HD2  | 28:DD:213:ARG:HA   | 1.55                     | 0.47              |
| 29:DE:45:THR:CG2   | 29:DE:83:ASP:HA    | 2.44                     | 0.47              |
| 31:DG:173:LEU:O    | 31:DG:178:PHE:HB2  | 2.14                     | 0.47              |
| 32:DH:19:VAL:O     | 32:DH:20:ALA:HB2   | 2.14                     | 0.47              |
| 32:DH:80:SER:C     | 32:DH:81:GLU:OE1   | 2.57                     | 0.47              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 32:DH:92:ILE:CD1   | 32:DH:160:LYS:HD3 | 2.44                     | 0.47              |
| 33:DI:12:LEU:O     | 33:DI:13:GLY:O    | 2.33                     | 0.47              |
| 33:DI:128:LEU:HD13 | 33:DI:128:LEU:C   | 2.39                     | 0.47              |
| 34:DN:126:PRO:O    | 34:DN:127:ASP:CB  | 2.63                     | 0.47              |
| 35:DO:24:VAL:HB    | 35:DO:33:ALA:HB2  | 1.96                     | 0.47              |
| 36:DP:47:ASP:CG    | 36:DP:49:ARG:HB2  | 2.39                     | 0.47              |
| 38:DR:84:ALA:HB3   | 38:DR:85:PRO:HD3  | 1.96                     | 0.47              |
| 46:DZ:137:ILE:HD11 | 46:DZ:158:PRO:HG3 | 1.96                     | 0.47              |
| 1:AA:1049:U:O2'    | 1:AA:1050:G:OP2   | 2.30                     | 0.47              |
| 1:AA:1277:C:O2'    | 1:AA:1278:U:H5'   | 2.13                     | 0.47              |
| 3:AC:47:LEU:HD23   | 3:AC:52:LEU:HD13  | 1.97                     | 0.47              |
| 3:AC:114:PRO:HD3   | 3:AC:183:ASP:OD2  | 2.13                     | 0.47              |
| 6:AF:72:VAL:O      | 6:AF:73:ASN:C     | 2.57                     | 0.47              |
| 7:AG:121:ALA:O     | 7:AG:125:MET:HG3  | 2.14                     | 0.47              |
| 11:AK:61:ALA:HB1   | 11:AK:94:ALA:HB2  | 1.97                     | 0.47              |
| 17:AQ:75:ARG:NH1   | 17:AQ:75:ARG:HG3  | 2.30                     | 0.47              |
| 19:AS:6:LYS:CD     | 19:AS:7:LYS:CE    | 2.92                     | 0.47              |
| 19:AS:53:ASN:OD1   | 19:AS:54:GLY:N    | 2.47                     | 0.47              |
| 23:AW:18:G:N1      | 23:AW:55:U:O2'    | 2.41                     | 0.47              |
| 25:BA:560:C:C5'    | 41:BU:52:ARG:HH22 | 2.26                     | 0.47              |
| 25:BA:704:G:C2     | 25:BA:726:G:C5    | 3.03                     | 0.47              |
| 25:BA:1209:G:O2'   | 25:BA:1237:A:N1   | 2.44                     | 0.47              |
| 27:BC:168:THR:HA   | 27:BC:173:ALA:HB1 | 1.96                     | 0.47              |
| 27:BC:194:ARG:C    | 27:BC:196:LEU:H   | 2.23                     | 0.47              |
| 28:BD:149:PRO:O    | 28:BD:150:LYS:HB2 | 2.13                     | 0.47              |
| 29:BE:182:LEU:HD12 | 29:BE:183:LEU:N   | 2.30                     | 0.47              |
| 35:BO:47:ILE:HG13  | 35:BO:48:PRO:CD   | 2.44                     | 0.47              |
| 36:BP:84:ASN:N     | 36:BP:84:ASN:HD22 | 2.12                     | 0.47              |
| 36:BP:114:ILE:HG12 | 36:BP:130:PHE:CD1 | 2.49                     | 0.47              |
| 37:BQ:69:PHE:CG    | 37:BQ:70:PRO:HD2  | 2.48                     | 0.47              |
| 40:BT:28:VAL:HG13  | 40:BT:46:GLU:N    | 2.29                     | 0.47              |
| 40:BT:29:ARG:CD    | 40:BT:85:LYS:C    | 2.88                     | 0.47              |
| 42:BV:35:LEU:C     | 42:BV:37:VAL:N    | 2.72                     | 0.47              |
| 45:BY:12:THR:CG2   | 45:BY:13:VAL:N    | 2.77                     | 0.47              |
| 45:BY:81:LYS:O     | 45:BY:82:PRO:O    | 2.32                     | 0.47              |
| 46:BZ:133:ILE:HG22 | 46:BZ:133:ILE:O   | 2.13                     | 0.47              |
| 48:B1:64:ALA:C     | 48:B1:66:HIS:N    | 2.72                     | 0.47              |
| 49:B2:10:LEU:HD22  | 49:B2:14:ARG:CZ   | 2.44                     | 0.47              |
| 49:B2:53:LEU:O     | 49:B2:54:LYS:C    | 2.57                     | 0.47              |
| 54:B7:28:ARG:HG3   | 54:B7:28:ARG:HH11 | 1.79                     | 0.47              |
| 1:CA:278:G:C6      | 17:CQ:95:TYR:HD2  | 2.33                     | 0.47              |

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| Atom-1               | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|--------------------|--------------------------|-------------------|
| 1:CA:444:C:H42       | 1:CA:490:G:H1      | 1.62                     | 0.47              |
| 2:CB:100:GLY:O       | 2:CB:104:ASN:N     | 2.47                     | 0.47              |
| 3:CC:83:ARG:O        | 3:CC:86:VAL:HG22   | 2.14                     | 0.47              |
| 4:CD:189:PRO:HB2     | 4:CD:194:LEU:HD21  | 1.95                     | 0.47              |
| 5:CE:102:ALA:CB      | 5:CE:106:PRO:CG    | 2.93                     | 0.47              |
| 9:CI:9:ARG:HE        | 9:CI:14:VAL:HG22   | 1.79                     | 0.47              |
| 9:CI:19:LEU:HD23     | 9:CI:61:ALA:CA     | 2.44                     | 0.47              |
| 10:CJ:84:GLN:O       | 10:CJ:85:LEU:HD23  | 2.14                     | 0.47              |
| 11:CK:44:SER:O       | 11:CK:47:VAL:HG23  | 2.14                     | 0.47              |
| 13:CM:16:ASP:OD2     | 13:CM:16:ASP:N     | 2.46                     | 0.47              |
| 15:CO:87:ILE:HG22    | 15:CO:88:ARG:H     | 1.79                     | 0.47              |
| 16:CP:9:PHE:CE1      | 16:CP:18:ARG:NH2   | 2.76                     | 0.47              |
| 17:CQ:59:ILE:CG2     | 17:CQ:71:PHE:HB3   | 2.34                     | 0.47              |
| 22:CV:54:G:C2        | 22:CV:55:U:C5      | 3.02                     | 0.47              |
| 25:DA:324:A:N6       | 25:DA:338:G:O2'    | 2.46                     | 0.47              |
| 25:DA:340:A:H2'      | 25:DA:341:G:C8     | 2.47                     | 0.47              |
| 25:DA:637:A:H4'      | 25:DA:638:G:O5'    | 2.14                     | 0.47              |
| 25:DA:776:G:N1       | 25:DA:2072:G:OP1   | 2.44                     | 0.47              |
| 25:DA:779:U:OP1      | 28:DD:49:ILE:HG22  | 2.13                     | 0.47              |
| 25:DA:993:G:OP1      | 41:DU:50:ARG:NH2   | 2.47                     | 0.47              |
| 25:DA:2125:G:N2      | 25:DA:2172:U:OP2   | 2.44                     | 0.47              |
| 25:DA:2287:A:H2      | 25:DA:2346:A:N1    | 2.12                     | 0.47              |
| 25:DA:2801(A):A:H5'' | 25:DA:2802:G:OP1   | 2.15                     | 0.47              |
| 26:DB:109:C:H5'      | 26:DB:110:G:OP1    | 2.15                     | 0.47              |
| 27:DC:42:GLU:H       | 27:DC:213:TYR:H    | 1.62                     | 0.47              |
| 28:DD:59:LYS:HG3     | 28:DD:60:ARG:N     | 2.30                     | 0.47              |
| 29:DE:33:VAL:O       | 29:DE:69:LYS:HE2   | 2.14                     | 0.47              |
| 29:DE:73:GLU:HG3     | 29:DE:74:PRO:CD    | 2.34                     | 0.47              |
| 29:DE:120:TRP:CD2    | 29:DE:155:LYS:HD3  | 2.49                     | 0.47              |
| 32:DH:56:SER:OG      | 32:DH:58:GLU:HG3   | 2.13                     | 0.47              |
| 32:DH:59:ARG:HG3     | 32:DH:59:ARG:NH1   | 2.27                     | 0.47              |
| 33:DI:37:VAL:HG12    | 33:DI:38:LEU:N     | 2.28                     | 0.47              |
| 34:DN:128:HIS:C      | 34:DN:130:HIS:H    | 2.23                     | 0.47              |
| 35:DO:88:ASN:O       | 35:DO:91:LEU:N     | 2.48                     | 0.47              |
| 36:DP:83:VAL:CG2     | 36:DP:105:LEU:HD22 | 2.45                     | 0.47              |
| 39:DS:58:LEU:N       | 39:DS:58:LEU:CD2   | 2.78                     | 0.47              |
| 53:D6:11:LEU:HG      | 53:D6:26:ASN:ND2   | 2.29                     | 0.47              |
| 53:D6:15:GLU:OE1     | 53:D6:18:ARG:HG3   | 2.14                     | 0.47              |
| 1:AA:992:U:H1'       | 1:AA:993:G:C2      | 2.50                     | 0.47              |
| 1:AA:1049:U:H5''     | 1:AA:1050:G:O5'    | 2.14                     | 0.47              |
| 1:AA:1251:A:HO2'     | 1:AA:1369:C:HO2'   | 1.60                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AA:1276:G:H2'   | 1:AA:1277:C:H5'   | 1.96                     | 0.47              |
| 2:AB:47:THR:HA    | 2:AB:202:PRO:HG2  | 1.97                     | 0.47              |
| 2:AB:91:PRO:HG3   | 2:AB:154:LEU:CB   | 2.37                     | 0.47              |
| 2:AB:124:SER:C    | 2:AB:126:GLU:H    | 2.22                     | 0.47              |
| 2:AB:127:ILE:HG23 | 2:AB:135:GLN:HE21 | 1.80                     | 0.47              |
| 3:AC:60:ALA:O     | 3:AC:61:ALA:HB2   | 2.15                     | 0.47              |
| 4:AD:10:ARG:HA    | 4:AD:13:ARG:HD2   | 1.96                     | 0.47              |
| 4:AD:108:LEU:CB   | 4:AD:110:PHE:HE1  | 2.26                     | 0.47              |
| 4:AD:187:ARG:HG3  | 4:AD:188:LEU:N    | 2.29                     | 0.47              |
| 5:AE:76:ILE:CG1   | 5:AE:142:LEU:CD1  | 2.92                     | 0.47              |
| 9:AI:48:GLU:O     | 9:AI:51:ARG:HB2   | 2.14                     | 0.47              |
| 9:AI:58:HIS:CB    | 9:AI:59:PHE:HE1   | 2.22                     | 0.47              |
| 19:AS:62:ILE:O    | 19:AS:62:ILE:HG23 | 2.14                     | 0.47              |
| 20:AT:44:ALA:C    | 20:AT:91:LEU:HB3  | 2.39                     | 0.47              |
| 20:AT:50:GLU:HA   | 20:AT:100:ILE:CG1 | 2.43                     | 0.47              |
| 20:AT:67:ALA:O    | 20:AT:73:HIS:CE1  | 2.68                     | 0.47              |
| 21:AU:2:GLY:C     | 21:AU:4:GLY:N     | 2.62                     | 0.47              |
| 25:BA:247:G:H4'   | 25:BA:386:G:C5    | 2.49                     | 0.47              |
| 25:BA:311:A:N7    | 25:BA:332:A:N6    | 2.63                     | 0.47              |
| 25:BA:1237:A:O2'  | 25:BA:1238:G:O4'  | 2.26                     | 0.47              |
| 25:BA:1422:G:H4'  | 25:BA:1493:C:OP1  | 2.14                     | 0.47              |
| 25:BA:1944:U:H5'' | 25:BA:1945:G:OP2  | 2.14                     | 0.47              |
| 25:BA:2544:G:H1'  | 25:BA:2646:C:H5'  | 1.95                     | 0.47              |
| 28:BD:177:LEU:HB3 | 28:BD:178:PRO:CD  | 2.45                     | 0.47              |
| 28:BD:181:GLU:HG2 | 28:BD:182:LEU:H   | 1.79                     | 0.47              |
| 29:BE:47:VAL:CG2  | 29:BE:84:PHE:O    | 2.62                     | 0.47              |
| 29:BE:200:GLU:O   | 29:BE:201:THR:O   | 2.31                     | 0.47              |
| 31:BG:72:ARG:CB   | 31:BG:86:MET:O    | 2.62                     | 0.47              |
| 31:BG:86:MET:N    | 31:BG:87:PRO:HD2  | 2.23                     | 0.47              |
| 32:BH:62:LYS:C    | 32:BH:64:LEU:H    | 2.21                     | 0.47              |
| 32:BH:72:ILE:H    | 32:BH:72:ILE:HD12 | 1.79                     | 0.47              |
| 33:BI:133:HIS:O   | 33:BI:134:PRO:C   | 2.57                     | 0.47              |
| 34:BN:12:ARG:O    | 34:BN:13:TRP:C    | 2.58                     | 0.47              |
| 39:BS:42:ASP:C    | 39:BS:44:LYS:N    | 2.73                     | 0.47              |
| 43:BW:10:VAL:O    | 43:BW:11:ARG:CB   | 2.60                     | 0.47              |
| 47:B0:49:LYS:O    | 47:B0:50:ASN:CB   | 2.62                     | 0.47              |
| 48:B1:89:GLU:O    | 48:B1:93:GLU:HB2  | 2.13                     | 0.47              |
| 1:CA:173:U:O2'    | 1:CA:174:C:OP1    | 2.30                     | 0.47              |
| 1:CA:262:A:H5''   | 20:CT:76:ALA:HB2  | 1.95                     | 0.47              |
| 1:CA:265:G:H2'    | 1:CA:266:G:H5''   | 1.97                     | 0.47              |
| 1:CA:279:A:O5'    | 1:CA:281:G:H5'    | 2.15                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CA:819:A:H4'    | 1:CA:820:U:OP2    | 2.13                     | 0.47              |
| 1:CA:871:U:O2'    | 1:CA:872:A:OP1    | 2.26                     | 0.47              |
| 1:CA:1402:C:H2'   | 1:CA:1403:C:O4'   | 2.15                     | 0.47              |
| 2:CB:79:ASP:O     | 2:CB:82:ARG:HB3   | 2.15                     | 0.47              |
| 2:CB:122:PHE:HA   | 2:CB:139:LYS:NZ   | 2.30                     | 0.47              |
| 3:CC:76:VAL:HG21  | 3:CC:103:VAL:HG11 | 1.96                     | 0.47              |
| 6:CF:8:ILE:HG22   | 6:CF:10:LEU:CD1   | 2.44                     | 0.47              |
| 7:CG:75:VAL:HA    | 7:CG:87:VAL:O     | 2.14                     | 0.47              |
| 9:CI:16:ARG:HE    | 9:CI:64:THR:HG23  | 1.79                     | 0.47              |
| 12:CL:28:LYS:C    | 12:CL:30:ALA:N    | 2.72                     | 0.47              |
| 22:CV:5:G:O2'     | 22:CV:6:G:H5'     | 2.15                     | 0.47              |
| 25:DA:531:C:H4'   | 25:DA:532:A:N3    | 2.29                     | 0.47              |
| 25:DA:545:C:H3'   | 25:DA:547:A:C8    | 2.50                     | 0.47              |
| 25:DA:1491:G:O2'  | 28:DD:101:GLU:HB2 | 2.14                     | 0.47              |
| 25:DA:1827:C:H2'  | 25:DA:1828:G:O4'  | 2.15                     | 0.47              |
| 25:DA:2150:U:H2'  | 25:DA:2151:G:C8   | 2.49                     | 0.47              |
| 25:DA:2296:U:HO2' | 25:DA:2333:A:H2   | 1.62                     | 0.47              |
| 27:DC:41:VAL:CA   | 27:DC:213:TYR:HA  | 2.43                     | 0.47              |
| 28:DD:27:THR:O    | 28:DD:27:THR:HG23 | 2.15                     | 0.47              |
| 30:DF:57:VAL:HG13 | 30:DF:58:ALA:H    | 1.78                     | 0.47              |
| 31:DG:2:PRO:C     | 31:DG:4:ASP:N     | 2.73                     | 0.47              |
| 31:DG:75:LYS:HD2  | 31:DG:77:ILE:HD11 | 1.96                     | 0.47              |
| 31:DG:96:ARG:O    | 31:DG:98:ARG:N    | 2.48                     | 0.47              |
| 32:DH:126:PRO:CG  | 32:DH:130:ARG:NH1 | 2.78                     | 0.47              |
| 33:DI:96:ASP:C    | 33:DI:98:ALA:N    | 2.71                     | 0.47              |
| 36:DP:55:ARG:HG2  | 36:DP:56:SER:N    | 2.25                     | 0.47              |
| 37:DQ:111:GLU:O   | 37:DQ:115:MET:HG2 | 2.14                     | 0.47              |
| 39:DS:18:ILE:HD13 | 39:DS:87:PHE:O    | 2.15                     | 0.47              |
| 40:DT:65:LYS:NZ   | 40:DT:66:VAL:HB   | 2.29                     | 0.47              |
| 43:DW:24:ILE:HG21 | 43:DW:36:LEU:HD21 | 1.96                     | 0.47              |
| 43:DW:68:ARG:HD2  | 43:DW:110:LYS:HB2 | 1.96                     | 0.47              |
| 46:DZ:53:ILE:H    | 46:DZ:71:VAL:HG23 | 1.77                     | 0.47              |
| 55:D8:61:LEU:H    | 55:D8:61:LEU:HG   | 1.26                     | 0.47              |
| 1:AA:189(H):G:H2' | 1:AA:189(I):G:C8  | 2.49                     | 0.47              |
| 1:AA:328:C:H4'    | 1:AA:329:A:C5'    | 2.44                     | 0.47              |
| 1:AA:707:C:H2'    | 1:AA:708:C:C6     | 2.50                     | 0.47              |
| 1:AA:792:A:H1'    | 1:AA:794:A:N7     | 2.30                     | 0.47              |
| 1:AA:1191:A:P     | 3:AC:3:ASN:HD21   | 2.38                     | 0.47              |
| 2:AB:19:HIS:ND1   | 2:AB:189:ASP:OD2  | 2.48                     | 0.47              |
| 2:AB:30:ARG:HH21  | 2:AB:194:PRO:CB   | 2.27                     | 0.47              |
| 2:AB:181:PHE:CD1  | 8:AH:70:GLN:HB3   | 2.47                     | 0.47              |

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| Atom-1            | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 3:AC:101:LEU:HD23 | 3:AC:101:LEU:C      | 2.39                     | 0.47              |
| 3:AC:174:PRO:C    | 3:AC:176:HIS:H      | 2.23                     | 0.47              |
| 4:AD:4:TYR:CD2    | 4:AD:5:ILE:O        | 2.68                     | 0.47              |
| 4:AD:113:SER:O    | 4:AD:114:ARG:C      | 2.56                     | 0.47              |
| 6:AF:33:TYR:C     | 6:AF:71:ARG:HH21    | 2.23                     | 0.47              |
| 8:AH:122:ARG:HB2  | 8:AH:122:ARG:HH11   | 1.80                     | 0.47              |
| 10:AJ:6:ILE:CG2   | 10:AJ:98:ILE:HG13   | 2.44                     | 0.47              |
| 10:AJ:35:SER:O    | 10:AJ:36:GLY:C      | 2.57                     | 0.47              |
| 10:AJ:63:PHE:HB3  | 14:AN:59:ALA:H      | 1.79                     | 0.47              |
| 12:AL:46:LYS:CD   | 12:AL:47:LYS:HG3    | 2.45                     | 0.47              |
| 12:AL:53:ARG:HH12 | 12:AL:92:ASP:HB2    | 1.80                     | 0.47              |
| 14:AN:24:CYS:H    | 14:AN:33:VAL:CG1    | 2.27                     | 0.47              |
| 16:AP:28:ARG:HG2  | 16:AP:28:ARG:NH1    | 2.23                     | 0.47              |
| 17:AQ:84:LEU:HD23 | 17:AQ:84:LEU:HA     | 1.66                     | 0.47              |
| 20:AT:22:ARG:O    | 20:AT:26:ASN:OD1    | 2.33                     | 0.47              |
| 20:AT:81:LYS:C    | 20:AT:85:MET:HG3    | 2.39                     | 0.47              |
| 21:AU:3:LYS:HB3   | 21:AU:14:TRP:CD1    | 2.50                     | 0.47              |
| 22:AV:53:G:H2'    | 22:AV:54:G:C5'      | 2.43                     | 0.47              |
| 23:AY:27:G:H2'    | 23:AY:28:G:C8       | 2.50                     | 0.47              |
| 25:BA:459:U:H2'   | 25:BA:460:A:C8      | 2.50                     | 0.47              |
| 25:BA:795:C:H2'   | 25:BA:796:C:C6      | 2.50                     | 0.47              |
| 25:BA:811:U:C4'   | 25:BA:1251:C:O4'    | 2.63                     | 0.47              |
| 25:BA:887:A:C4    | 25:BA:889:C:C5      | 3.03                     | 0.47              |
| 25:BA:1008:C:H5'' | 25:BA:1009:A:OP1    | 2.14                     | 0.47              |
| 25:BA:1019:U:H3   | 25:BA:1142(A):A:H62 | 1.62                     | 0.47              |
| 25:BA:1022:G:O2'  | 25:BA:1023:U:P      | 2.73                     | 0.47              |
| 25:BA:1032:A:N3   | 56:B9:18:ARG:NH2    | 2.62                     | 0.47              |
| 25:BA:1126:A:OP1  | 25:BA:1126:A:H8     | 1.96                     | 0.47              |
| 25:BA:1210:A:H4'  | 25:BA:1211:U:O5'    | 2.14                     | 0.47              |
| 25:BA:1468:C:H2'  | 25:BA:1469:A:C8     | 2.49                     | 0.47              |
| 25:BA:1722:A:O2'  | 25:BA:1739:U:O2     | 2.32                     | 0.47              |
| 25:BA:1824:G:OP1  | 28:BD:52:ARG:HD3    | 2.14                     | 0.47              |
| 25:BA:1993:U:H4'  | 29:BE:128:SER:OG    | 2.15                     | 0.47              |
| 25:BA:2171:A:HO2' | 25:BA:2172:U:H5'    | 1.77                     | 0.47              |
| 25:BA:2227:A:H5'  | 28:BD:263:ARG:HH11  | 1.80                     | 0.47              |
| 25:BA:2364:C:H2'  | 25:BA:2365:G:O4'    | 2.15                     | 0.47              |
| 25:BA:2429:G:N7   | 36:BP:56:SER:OG     | 2.48                     | 0.47              |
| 25:BA:2579:C:H4'  | 29:BE:134:ILE:HD12  | 1.95                     | 0.47              |
| 25:BA:2788:C:O2'  | 25:BA:2809:A:N3     | 2.41                     | 0.47              |
| 26:BB:91:C:OP1    | 37:BQ:16:ARG:HG3    | 2.14                     | 0.47              |
| 28:BD:49:ILE:HD11 | 28:BD:52:ARG:CA     | 2.43                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 29:BE:29:GLY:HA3   | 29:BE:51:PHE:CE2   | 2.41                     | 0.47              |
| 29:BE:119:ARG:O    | 29:BE:120:TRP:CG   | 2.68                     | 0.47              |
| 29:BE:152:LYS:HB3  | 34:BN:78:TYR:CE2   | 2.49                     | 0.47              |
| 30:BF:66:PRO:O     | 30:BF:67:GLN:CG    | 2.62                     | 0.47              |
| 30:BF:194:MET:HE3  | 30:BF:199:TRP:CD1  | 2.49                     | 0.47              |
| 30:BF:195:ASP:HB3  | 30:BF:197:ASP:OD1  | 2.14                     | 0.47              |
| 31:BG:11:TYR:OH    | 31:BG:33:ARG:HG3   | 2.15                     | 0.47              |
| 31:BG:117:PHE:CE1  | 31:BG:119:GLY:CA   | 2.96                     | 0.47              |
| 32:BH:41:MET:HE1   | 32:BH:64:LEU:HD13  | 1.97                     | 0.47              |
| 33:BI:1:MET:O      | 33:BI:20:ASP:HB2   | 2.15                     | 0.47              |
| 34:BN:1:MET:C      | 34:BN:2:LYS:HD2    | 2.38                     | 0.47              |
| 34:BN:14:VAL:CG1   | 34:BN:15:LEU:N     | 2.77                     | 0.47              |
| 36:BP:114:ILE:HG21 | 36:BP:125:VAL:HG21 | 1.95                     | 0.47              |
| 37:BQ:66:ILE:O     | 37:BQ:66:ILE:HG13  | 2.14                     | 0.47              |
| 38:BR:63:ARG:NH2   | 38:BR:80:PHE:CD2   | 2.83                     | 0.47              |
| 38:BR:107:ASP:C    | 38:BR:107:ASP:OD2  | 2.58                     | 0.47              |
| 39:BS:20:ARG:HH11  | 39:BS:20:ARG:CG    | 2.12                     | 0.47              |
| 39:BS:53:SER:C     | 39:BS:55:ALA:N     | 2.69                     | 0.47              |
| 39:BS:92:TYR:HD2   | 39:BS:94:TYR:HB2   | 1.79                     | 0.47              |
| 39:BS:106:ARG:O    | 39:BS:107:GLU:HB3  | 2.14                     | 0.47              |
| 40:BT:80:SER:O     | 40:BT:82:LEU:N     | 2.48                     | 0.47              |
| 42:BV:43:GLU:HA    | 42:BV:43:GLU:OE1   | 2.14                     | 0.47              |
| 42:BV:65:GLY:CA    | 42:BV:91:TYR:CE1   | 2.97                     | 0.47              |
| 43:BW:20:VAL:O     | 43:BW:21:VAL:C     | 2.54                     | 0.47              |
| 46:BZ:93:ASP:HA    | 46:BZ:130:PRO:CG   | 2.31                     | 0.47              |
| 46:BZ:121:HIS:CE1  | 46:BZ:169:GLU:HG2  | 2.49                     | 0.47              |
| 46:BZ:159:PRO:C    | 46:BZ:161:VAL:H    | 2.23                     | 0.47              |
| 47:B0:41:ARG:H     | 47:B0:41:ARG:CD    | 2.26                     | 0.47              |
| 52:B5:37:LYS:HG3   | 52:B5:38:ALA:N     | 2.29                     | 0.47              |
| 1:CA:102:G:O2'     | 1:CA:151:A:N3      | 2.40                     | 0.47              |
| 1:CA:275:G:O2'     | 1:CA:276:G:H5'     | 2.14                     | 0.47              |
| 1:CA:737:A:H2'     | 1:CA:738:C:H6      | 1.80                     | 0.47              |
| 1:CA:749:C:H2'     | 1:CA:750:G:H8      | 1.80                     | 0.47              |
| 1:CA:1064:G:HO2'   | 1:CA:1065:U:C5'    | 2.24                     | 0.47              |
| 1:CA:1135:U:H6     | 1:CA:1135:U:H3'    | 1.79                     | 0.47              |
| 1:CA:1347:G:C4     | 9:CI:107:ARG:NH2   | 2.83                     | 0.47              |
| 2:CB:15:VAL:C      | 2:CB:16:HIS:CG     | 2.93                     | 0.47              |
| 2:CB:24:TRP:CG     | 2:CB:25:ASN:N      | 2.79                     | 0.47              |
| 2:CB:155:LEU:HA    | 2:CB:155:LEU:HD22  | 1.55                     | 0.47              |
| 2:CB:159:PRO:C     | 2:CB:161:ALA:H     | 2.21                     | 0.47              |
| 3:CC:71:ALA:CB     | 3:CC:109:PRO:HG3   | 2.45                     | 0.47              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 4:CD:100:ARG:HH12  | 4:CD:137:SER:HA   | 1.78                     | 0.47              |
| 4:CD:124:GLY:C     | 4:CD:126:ILE:H    | 2.23                     | 0.47              |
| 4:CD:162:LEU:O     | 4:CD:163:GLU:C    | 2.57                     | 0.47              |
| 5:CE:106:PRO:HG2   | 5:CE:107:ARG:H    | 1.78                     | 0.47              |
| 5:CE:145:LYS:HD2   | 5:CE:149:GLU:OE2  | 2.15                     | 0.47              |
| 6:CF:10:LEU:CD1    | 6:CF:10:LEU:N     | 2.77                     | 0.47              |
| 7:CG:62:PHE:HA     | 7:CG:124:LEU:HD22 | 1.97                     | 0.47              |
| 7:CG:153:HIS:O     | 7:CG:155:ARG:N    | 2.48                     | 0.47              |
| 8:CH:25:ASP:HB3    | 8:CH:58:TYR:HB3   | 1.97                     | 0.47              |
| 8:CH:112:LEU:HD12  | 8:CH:112:LEU:C    | 2.40                     | 0.47              |
| 9:CI:9:ARG:HG2     | 9:CI:104:ARG:HH11 | 1.80                     | 0.47              |
| 9:CI:25:LYS:O      | 9:CI:60:ASP:HA    | 2.14                     | 0.47              |
| 11:CK:33:THR:HG22  | 11:CK:39:PRO:HA   | 1.97                     | 0.47              |
| 12:CL:7:ILE:HD12   | 17:CQ:32:TYR:HB3  | 1.97                     | 0.47              |
| 14:CN:44:LEU:C     | 14:CN:44:LEU:CD1  | 2.85                     | 0.47              |
| 18:CR:40:LEU:O     | 18:CR:41:LYS:C    | 2.58                     | 0.47              |
| 19:CS:15:LEU:O     | 19:CS:16:LEU:C    | 2.58                     | 0.47              |
| 22:CV:29:C:H2'     | 22:CV:30:G:H8     | 1.79                     | 0.47              |
| 22:CV:53:G:O6      | 22:CV:64:G:C6     | 2.68                     | 0.47              |
| 25:DA:92:A:H2'     | 25:DA:93:G:C8     | 2.50                     | 0.47              |
| 25:DA:467:G:OP1    | 54:D7:33:ARG:NH1  | 2.47                     | 0.47              |
| 25:DA:608:A:OP1    | 30:DF:100:THR:OG1 | 2.28                     | 0.47              |
| 25:DA:850:C:O3'    | 50:D3:49:LYS:NZ   | 2.48                     | 0.47              |
| 25:DA:988:A:P      | 50:D3:11:SER:HB3  | 2.55                     | 0.47              |
| 25:DA:1237:A:H4'   | 25:DA:1238:G:O5'  | 2.13                     | 0.47              |
| 25:DA:1248:G:OP1   | 30:DF:92:PRO:HG3  | 2.14                     | 0.47              |
| 25:DA:1678:G:N2    | 25:DA:1989:G:H22  | 2.13                     | 0.47              |
| 25:DA:1821:A:H8    | 25:DA:1821:A:O5'  | 1.97                     | 0.47              |
| 25:DA:1866:C:H2'   | 25:DA:1876:A:O4'  | 2.14                     | 0.47              |
| 25:DA:2562:U:H1'   | 35:DO:23:ARG:HH11 | 1.78                     | 0.47              |
| 27:DC:68:LEU:HD22  | 27:DC:180:PHE:CB  | 2.45                     | 0.47              |
| 27:DC:214:VAL:C    | 27:DC:216:THR:N   | 2.73                     | 0.47              |
| 28:DD:3:VAL:CG1    | 28:DD:17:THR:HB   | 2.44                     | 0.47              |
| 28:DD:264:LYS:CD   | 28:DD:266:SER:HB3 | 2.40                     | 0.47              |
| 29:DE:36:ARG:NH1   | 29:DE:85:ASN:OD1  | 2.48                     | 0.47              |
| 29:DE:59:VAL:HG13  | 29:DE:60:ASN:N    | 2.29                     | 0.47              |
| 29:DE:101:ARG:HH21 | 29:DE:171:GLU:HB2 | 1.75                     | 0.47              |
| 29:DE:120:TRP:CE3  | 29:DE:155:LYS:HD3 | 2.49                     | 0.47              |
| 29:DE:188:VAL:HG23 | 29:DE:189:PRO:HD2 | 1.97                     | 0.47              |
| 30:DF:23:ASP:O     | 30:DF:24:LEU:O    | 2.32                     | 0.47              |
| 30:DF:103:LYS:HA   | 30:DF:106:ARG:CG  | 2.32                     | 0.47              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 30:DF:128:ALA:O    | 30:DF:129:PHE:CG  | 2.66                     | 0.47              |
| 31:DG:122:PRO:HB3  | 31:DG:180:PHE:HD2 | 1.79                     | 0.47              |
| 32:DH:22:GLY:O     | 32:DH:37:VAL:N    | 2.48                     | 0.47              |
| 32:DH:89:ILE:O     | 32:DH:90:LYS:C    | 2.58                     | 0.47              |
| 33:DI:29:TYR:O     | 33:DI:32:PRO:HD2  | 2.14                     | 0.47              |
| 33:DI:78:THR:CG2   | 33:DI:141:LYS:HD2 | 2.45                     | 0.47              |
| 33:DI:92:VAL:O     | 33:DI:120:ILE:CG2 | 2.62                     | 0.47              |
| 37:DQ:70:PRO:HA    | 37:DQ:94:VAL:O    | 2.14                     | 0.47              |
| 38:DR:17:ARG:HG2   | 38:DR:17:ARG:NH1  | 2.18                     | 0.47              |
| 38:DR:28:LEU:HA    | 38:DR:34:ILE:CG1  | 2.45                     | 0.47              |
| 38:DR:116:LEU:HD23 | 38:DR:116:LEU:HA  | 1.69                     | 0.47              |
| 39:DS:25:ARG:HH11  | 39:DS:25:ARG:CB   | 2.27                     | 0.47              |
| 40:DT:19:LEU:H     | 40:DT:19:LEU:HD12 | 1.79                     | 0.47              |
| 40:DT:132:LYS:C    | 40:DT:134:GLU:N   | 2.69                     | 0.47              |
| 43:DW:107:LEU:HD12 | 43:DW:107:LEU:HA  | 1.79                     | 0.47              |
| 45:DY:50:ARG:C     | 45:DY:52:SER:H    | 2.22                     | 0.47              |
| 45:DY:91:GLU:HG3   | 45:DY:92:ASN:N    | 2.30                     | 0.47              |
| 46:DZ:53:ILE:N     | 46:DZ:53:ILE:HD13 | 2.29                     | 0.47              |
| 46:DZ:152:ALA:O    | 46:DZ:167:PRO:HB2 | 2.14                     | 0.47              |
| 48:D1:80:LEU:HB3   | 48:D1:82:LEU:CD2  | 2.44                     | 0.47              |
| 49:D2:5:GLU:CB     | 49:D2:9:GLN:HE22  | 2.27                     | 0.47              |
| 50:D3:2:PRO:O      | 50:D3:39:ASP:HB3  | 2.13                     | 0.47              |
| 51:D4:9:LEU:HG     | 51:D4:26:SER:CA   | 2.43                     | 0.47              |
| 52:D5:37:LYS:HG3   | 52:D5:38:ALA:H    | 1.79                     | 0.47              |
| 1:AA:49:U:O2       | 1:AA:362:G:H1'    | 2.15                     | 0.47              |
| 1:AA:366:C:O2'     | 1:AA:394:G:N2     | 2.48                     | 0.47              |
| 1:AA:1064:G:O2'    | 1:AA:1065:U:OP2   | 2.30                     | 0.47              |
| 2:AB:121:LEU:O     | 2:AB:121:LEU:HD23 | 2.15                     | 0.47              |
| 2:AB:223:ILE:O     | 2:AB:227:GLY:N    | 2.48                     | 0.47              |
| 4:AD:112:VAL:HG23  | 4:AD:113:SER:N    | 2.30                     | 0.47              |
| 5:AE:112:LEU:HD23  | 5:AE:112:LEU:HA   | 1.57                     | 0.47              |
| 10:AJ:4:ILE:HD11   | 10:AJ:77:PRO:HB3  | 1.96                     | 0.47              |
| 13:AM:96:LEU:O     | 13:AM:110:ARG:NE  | 2.47                     | 0.47              |
| 14:AN:36:PHE:CD1   | 14:AN:37:PHE:CD2  | 3.02                     | 0.47              |
| 15:AO:87:ILE:CG2   | 15:AO:88:ARG:H    | 2.28                     | 0.47              |
| 20:AT:30:LYS:HD3   | 20:AT:30:LYS:C    | 2.39                     | 0.47              |
| 25:BA:180:G:OP2    | 54:B7:32:LYS:HE3  | 2.15                     | 0.47              |
| 25:BA:234:C:H2'    | 25:BA:235:U:H6    | 1.78                     | 0.47              |
| 25:BA:481:G:OP2    | 45:BY:47:LYS:HE3  | 2.14                     | 0.47              |
| 25:BA:598:G:H5'    | 36:BP:11:GLY:HA3  | 1.97                     | 0.47              |
| 25:BA:779:U:OP1    | 28:BD:49:ILE:HG22 | 2.14                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:BA:1300:U:O2'   | 25:BA:1301:A:OP2   | 2.30                     | 0.47              |
| 25:BA:1326:U:H5    | 25:BA:1647:G:O2'   | 1.97                     | 0.47              |
| 25:BA:1899:G:O2'   | 25:BA:1900:A:H5''  | 2.14                     | 0.47              |
| 25:BA:1902:C:OP1   | 28:BD:242:ARG:HD3  | 2.15                     | 0.47              |
| 25:BA:2320:A:H61   | 25:BA:2333:A:H2'   | 1.80                     | 0.47              |
| 28:BD:24:ILE:O     | 28:BD:26:LYS:CE    | 2.62                     | 0.47              |
| 28:BD:181:GLU:OE1  | 28:BD:270:ILE:HG21 | 2.15                     | 0.47              |
| 30:BF:101:LEU:HA   | 30:BF:102:PRO:HD2  | 1.65                     | 0.47              |
| 33:BI:83:ALA:HB2   | 33:BI:88:ILE:HG23  | 1.95                     | 0.47              |
| 35:BO:19:ILE:O     | 35:BO:19:ILE:HG13  | 2.14                     | 0.47              |
| 38:BR:2:ARG:CZ     | 38:BR:5:LYS:HE3    | 2.45                     | 0.47              |
| 39:BS:19:LYS:O     | 39:BS:19:LYS:HG2   | 2.15                     | 0.47              |
| 39:BS:38:GLN:HB2   | 39:BS:47:THR:CG2   | 2.45                     | 0.47              |
| 40:BT:1:MET:H1     | 40:BT:7:ILE:HD11   | 1.80                     | 0.47              |
| 41:BU:89:GLU:O     | 41:BU:89:GLU:HG3   | 2.14                     | 0.47              |
| 46:BZ:76:LEU:N     | 46:BZ:76:LEU:HD22  | 2.29                     | 0.47              |
| 46:BZ:128:VAL:HG21 | 46:BZ:132:ASN:O    | 2.15                     | 0.47              |
| 53:B6:15:GLU:O     | 53:B6:16:CYS:C     | 2.57                     | 0.47              |
| 1:CA:246:A:H4'     | 1:CA:247:G:OP1     | 2.15                     | 0.47              |
| 1:CA:445:G:H2'     | 1:CA:446:G:H8      | 1.79                     | 0.47              |
| 1:CA:686:U:H5'     | 1:CA:686:U:C6      | 2.50                     | 0.47              |
| 1:CA:1321:C:C4     | 1:CA:1322:C:C4     | 3.02                     | 0.47              |
| 5:CE:76:ILE:HD11   | 5:CE:142:LEU:CD2   | 2.37                     | 0.47              |
| 6:CF:29:ALA:O      | 6:CF:30:LEU:C      | 2.58                     | 0.47              |
| 7:CG:57:GLU:O      | 7:CG:57:GLU:HG3    | 2.15                     | 0.47              |
| 13:CM:11:ARG:CB    | 13:CM:11:ARG:NH1   | 2.77                     | 0.47              |
| 13:CM:19:LEU:N     | 13:CM:19:LEU:HD22  | 2.30                     | 0.47              |
| 13:CM:87:TYR:C     | 13:CM:89:GLY:N     | 2.73                     | 0.47              |
| 19:CS:11:VAL:HA    | 19:CS:38:SER:HB2   | 1.96                     | 0.47              |
| 19:CS:13:ASP:O     | 19:CS:15:LEU:N     | 2.48                     | 0.47              |
| 25:DA:911:A:C5     | 37:DQ:9:TYR:CD1    | 3.03                     | 0.47              |
| 25:DA:1610:A:H4'   | 25:DA:1611:C:OP1   | 2.13                     | 0.47              |
| 25:DA:2517:C:O2'   | 25:DA:2518:A:H3'   | 2.15                     | 0.47              |
| 25:DA:2787:C:H1'   | 29:DE:61:ARG:CG    | 2.45                     | 0.47              |
| 28:DD:92:ILE:H     | 28:DD:92:ILE:HD13  | 1.79                     | 0.47              |
| 28:DD:267:SER:O    | 28:DD:268:ARG:HB2  | 2.15                     | 0.47              |
| 30:DF:115:ALA:O    | 30:DF:116:ASP:C    | 2.55                     | 0.47              |
| 30:DF:164:ARG:HG3  | 30:DF:175:THR:OG1  | 2.15                     | 0.47              |
| 31:DG:118:ARG:HA   | 31:DG:118:ARG:NE   | 2.28                     | 0.47              |
| 32:DH:124:GLU:CB   | 32:DH:132:ARG:HG3  | 2.45                     | 0.47              |
| 32:DH:164:TYR:O    | 32:DH:166:GLY:N    | 2.47                     | 0.47              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 38:DR:81:ASP:O     | 38:DR:82:GLU:CB   | 2.63                     | 0.47              |
| 39:DS:62:LYS:HB3   | 39:DS:97:ARG:CD   | 2.44                     | 0.47              |
| 40:DT:3:ARG:O      | 40:DT:6:LEU:N     | 2.46                     | 0.47              |
| 42:DV:48:GLY:O     | 42:DV:49:THR:O    | 2.32                     | 0.47              |
| 43:DW:9:TYR:CE2    | 43:DW:102:HIS:NE2 | 2.80                     | 0.47              |
| 49:D2:13:ALA:O     | 49:D2:15:LYS:N    | 2.48                     | 0.47              |
| 1:AA:56:U:H2'      | 1:AA:57:G:C8      | 2.50                     | 0.47              |
| 1:AA:274:A:O2'     | 1:AA:275:G:H8     | 1.97                     | 0.47              |
| 1:AA:656:C:H4'     | 15:AO:62:GLN:HE22 | 1.78                     | 0.47              |
| 1:AA:681:C:H2'     | 1:AA:682:G:H8     | 1.79                     | 0.47              |
| 1:AA:737:A:H2'     | 1:AA:738:C:C6     | 2.50                     | 0.47              |
| 1:AA:914:A:H2'     | 1:AA:915:A:O4'    | 2.15                     | 0.47              |
| 2:AB:77:ALA:HA     | 2:AB:80:ILE:CG2   | 2.44                     | 0.47              |
| 5:AE:11:ILE:HG22   | 5:AE:12:LEU:N     | 2.25                     | 0.47              |
| 7:AG:142:GLU:O     | 7:AG:145:ALA:HB3  | 2.15                     | 0.47              |
| 9:AI:58:HIS:HB2    | 9:AI:59:PHE:CD1   | 2.48                     | 0.47              |
| 9:AI:100:GLY:O     | 9:AI:101:PHE:CD2  | 2.68                     | 0.47              |
| 13:AM:23:TYR:CD1   | 13:AM:70:LEU:HD22 | 2.49                     | 0.47              |
| 17:AQ:27:PHE:HB2   | 17:AQ:28:PRO:CD   | 2.45                     | 0.47              |
| 18:AR:74:ARG:HH21  | 18:AR:81:PHE:CA   | 2.21                     | 0.47              |
| 20:AT:13:LEU:O     | 20:AT:16:HIS:HB3  | 2.14                     | 0.47              |
| 22:AV:53:G:O2'     | 22:AV:54:G:O5'    | 2.32                     | 0.47              |
| 23:AW:18:G:H1      | 23:AW:55:U:C1'    | 2.27                     | 0.47              |
| 25:BA:412:A:N7     | 25:BA:2411:A:H2   | 2.13                     | 0.47              |
| 25:BA:805:G:N2     | 25:BA:829:A:OP1   | 2.41                     | 0.47              |
| 25:BA:1287:A:C6    | 25:BA:1288:U:O4   | 2.65                     | 0.47              |
| 25:BA:1344:G:C6    | 25:BA:1385:G:N7   | 2.83                     | 0.47              |
| 25:BA:1566:A:OP1   | 28:BD:211:ARG:NH1 | 2.46                     | 0.47              |
| 25:BA:1658:C:OP1   | 29:BE:132:HIS:ND1 | 2.48                     | 0.47              |
| 25:BA:2320:A:C6    | 25:BA:2333:A:C8   | 3.02                     | 0.47              |
| 25:BA:2590:A:OP2   | 28:BD:238:GLY:HA2 | 2.15                     | 0.47              |
| 28:BD:33:LEU:C     | 28:BD:35:LYS:N    | 2.70                     | 0.47              |
| 30:BF:117:ARG:NH2  | 30:BF:187:VAL:HA  | 2.30                     | 0.47              |
| 31:BG:29:TRP:C     | 31:BG:31:VAL:N    | 2.73                     | 0.47              |
| 36:BP:95:VAL:HA    | 36:BP:99:LEU:HD23 | 1.97                     | 0.47              |
| 36:BP:138:LEU:HD12 | 36:BP:139:LYS:N   | 2.30                     | 0.47              |
| 37:BQ:12:GLN:HG2   | 37:BQ:73:PRO:CD   | 2.35                     | 0.47              |
| 37:BQ:30:GLY:O     | 37:BQ:134:ARG:NH1 | 2.48                     | 0.47              |
| 41:BU:115:ALA:C    | 41:BU:117:GLN:N   | 2.73                     | 0.47              |
| 49:B2:13:ALA:HA    | 49:B2:16:LEU:HG   | 1.97                     | 0.47              |
| 55:B8:62:LEU:N     | 55:B8:63:PRO:HD2  | 2.29                     | 0.47              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:CA:974:A:OP2    | 14:CN:41:ARG:NH1   | 2.48                     | 0.47              |
| 1:CA:1316:G:O6    | 19:CS:5:LEU:HD23   | 2.13                     | 0.47              |
| 3:CC:68:VAL:HG12  | 3:CC:68:VAL:O      | 2.15                     | 0.47              |
| 7:CG:15:ASP:OD2   | 7:CG:44:TYR:OH     | 2.33                     | 0.47              |
| 10:CJ:54:PHE:CD2  | 10:CJ:55:LYS:HG2   | 2.49                     | 0.47              |
| 11:CK:33:THR:HA   | 11:CK:40:ILE:HG12  | 1.96                     | 0.47              |
| 12:CL:84:LEU:HD23 | 12:CL:84:LEU:HA    | 1.36                     | 0.47              |
| 13:CM:57:ARG:HH11 | 13:CM:57:ARG:CB    | 2.20                     | 0.47              |
| 18:CR:40:LEU:HB3  | 18:CR:79:LEU:HD11  | 1.97                     | 0.47              |
| 19:CS:8:GLY:O     | 19:CS:9:VAL:HG23   | 2.15                     | 0.47              |
| 25:DA:82:G:C5     | 25:DA:83:G:O6      | 2.68                     | 0.47              |
| 25:DA:890:A:C5    | 25:DA:892:G:N7     | 2.83                     | 0.47              |
| 25:DA:942:G:H5''  | 36:DP:36:LYS:HE2   | 1.95                     | 0.47              |
| 25:DA:1128:A:C8   | 25:DA:2518:A:N6    | 2.82                     | 0.47              |
| 25:DA:1455:G:O6   | 25:DA:2705:A:N3    | 2.47                     | 0.47              |
| 25:DA:1667:G:O2'  | 25:DA:1991:U:O4    | 2.32                     | 0.47              |
| 25:DA:1805:U:O2   | 28:DD:50:THR:HB    | 2.15                     | 0.47              |
| 25:DA:1819:A:OP1  | 28:DD:161:THR:HG21 | 2.15                     | 0.47              |
| 25:DA:2009:G:N3   | 38:DR:107:ASP:HA   | 2.30                     | 0.47              |
| 28:DD:44:ASN:HB3  | 28:DD:48:ARG:O     | 2.15                     | 0.47              |
| 28:DD:77:ALA:HB2  | 28:DD:97:TYR:CG    | 2.50                     | 0.47              |
| 28:DD:112:GLN:N   | 28:DD:115:GLN:NE2  | 2.63                     | 0.47              |
| 31:DG:80:PHE:C    | 31:DG:81:LYS:HG2   | 2.40                     | 0.47              |
| 31:DG:177:GLY:O   | 31:DG:179:PRO:HD3  | 2.15                     | 0.47              |
| 32:DH:16:SER:O    | 32:DH:17:VAL:HG23  | 2.15                     | 0.47              |
| 32:DH:137:ASP:O   | 32:DH:138:LYS:HB2  | 2.15                     | 0.47              |
| 33:DI:41:GLU:O    | 33:DI:45:LYS:HB2   | 2.15                     | 0.47              |
| 33:DI:57:ARG:CA   | 33:DI:60:GLU:HB3   | 2.45                     | 0.47              |
| 36:DP:33:ARG:O    | 36:DP:34:GLY:O     | 2.33                     | 0.47              |
| 40:DT:29:ARG:HD3  | 40:DT:29:ARG:HA    | 1.58                     | 0.47              |
| 42:DV:1:MET:HG2   | 42:DV:42:GLY:H     | 1.80                     | 0.47              |
| 44:DX:11:PRO:HG2  | 49:D2:40:SER:OG    | 2.15                     | 0.47              |
| 44:DX:60:ARG:NH2  | 54:D7:47:ARG:HH21  | 2.11                     | 0.47              |
| 44:DX:64:LYS:NZ   | 44:DX:73:ARG:HH21  | 2.13                     | 0.47              |
| 46:DZ:38:TYR:C    | 46:DZ:38:TYR:CD1   | 2.92                     | 0.47              |
| 50:D3:35:ARG:HG3  | 50:D3:35:ARG:NH1   | 2.30                     | 0.47              |
| 1:AA:787:A:N6     | 1:AA:792:A:O2'     | 2.47                     | 0.47              |
| 1:AA:1224:G:N2    | 1:AA:1363:C:N3     | 2.62                     | 0.47              |
| 2:AB:8:LYS:NZ     | 2:AB:217:ARG:HH12  | 2.12                     | 0.47              |
| 2:AB:8:LYS:O      | 2:AB:12:GLU:HG3    | 2.15                     | 0.47              |
| 2:AB:118:LEU:HB2  | 2:AB:142:LEU:HD13  | 1.97                     | 0.47              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:AB:204:ASN:ND2  | 2:AB:205:ASP:N     | 2.62                     | 0.47              |
| 3:AC:101:LEU:HD23 | 3:AC:102:ASN:N     | 2.30                     | 0.47              |
| 4:AD:30:LYS:O     | 4:AD:32:ALA:N      | 2.48                     | 0.47              |
| 4:AD:134:ASP:OD2  | 4:AD:135:LEU:HD13  | 2.15                     | 0.47              |
| 14:AN:15:LYS:CD   | 14:AN:16:PHE:CE2   | 2.98                     | 0.47              |
| 19:AS:15:LEU:HD22 | 19:AS:15:LEU:N     | 2.30                     | 0.47              |
| 19:AS:64:GLU:O    | 19:AS:67:VAL:HG23  | 2.14                     | 0.47              |
| 25:BA:590:A:H2'   | 25:BA:591:C:C6     | 2.50                     | 0.47              |
| 25:BA:639:U:H2'   | 25:BA:640:C:C6     | 2.50                     | 0.47              |
| 25:BA:797:C:OP2   | 30:BF:62:ARG:HG3   | 2.15                     | 0.47              |
| 25:BA:1416:G:O2'  | 25:BA:1417:C:O4'   | 2.32                     | 0.47              |
| 25:BA:1549:C:H2'  | 25:BA:1550:C:C5    | 2.44                     | 0.47              |
| 25:BA:2453:A:C2   | 25:BA:2504:U:N3    | 2.83                     | 0.47              |
| 27:BC:22:ILE:O    | 27:BC:22:ILE:HG22  | 2.15                     | 0.47              |
| 28:BD:210:GLY:O   | 28:BD:212:SER:N    | 2.47                     | 0.47              |
| 28:BD:264:LYS:CD  | 28:BD:266:SER:HB2  | 2.41                     | 0.47              |
| 31:BG:43:LEU:HD23 | 31:BG:88:ILE:CD1   | 2.45                     | 0.47              |
| 31:BG:47:LYS:HD3  | 31:BG:82:LEU:HG    | 1.97                     | 0.47              |
| 31:BG:64:THR:HG23 | 31:BG:65:GLY:H     | 1.79                     | 0.47              |
| 31:BG:77:ILE:H    | 31:BG:83:ARG:HB3   | 1.79                     | 0.47              |
| 35:BO:93:PRO:HB3  | 35:BO:114:ILE:HD11 | 1.96                     | 0.47              |
| 38:BR:101:ALA:HB2 | 52:B5:44:THR:CB    | 2.45                     | 0.47              |
| 39:BS:57:LYS:HB3  | 39:BS:58:LEU:H     | 1.58                     | 0.47              |
| 46:BZ:91:LEU:HD12 | 46:BZ:91:LEU:N     | 2.30                     | 0.47              |
| 47:B0:45:PHE:HE1  | 47:B0:77:ARG:NH1   | 2.13                     | 0.47              |
| 52:B5:4:HIS:HB3   | 52:B5:5:PRO:HD3    | 1.96                     | 0.47              |
| 52:B5:51:TYR:HD1  | 52:B5:52:TYR:CE2   | 2.33                     | 0.47              |
| 53:B6:9:LEU:HD22  | 53:B6:26:ASN:HB2   | 1.96                     | 0.47              |
| 55:B8:52:LYS:N    | 55:B8:53:PRO:CD    | 2.78                     | 0.47              |
| 1:CA:580:U:H2'    | 1:CA:581:G:O4'     | 2.15                     | 0.47              |
| 1:CA:971:G:OP1    | 1:CA:972:C:H5''    | 2.15                     | 0.47              |
| 1:CA:1502:A:N3    | 1:CA:1505:G:N2     | 2.54                     | 0.47              |
| 2:CB:47:THR:O     | 2:CB:48:MET:C      | 2.58                     | 0.47              |
| 2:CB:115:LEU:HD12 | 2:CB:115:LEU:O     | 2.15                     | 0.47              |
| 5:CE:60:TYR:C     | 5:CE:60:TYR:CD1    | 2.92                     | 0.47              |
| 5:CE:81:GLU:HG2   | 5:CE:90:VAL:CG1    | 2.43                     | 0.47              |
| 5:CE:100:VAL:CB   | 5:CE:118:ILE:CG2   | 2.83                     | 0.47              |
| 8:CH:28:ALA:HB3   | 8:CH:57:PRO:HB2    | 1.97                     | 0.47              |
| 9:CI:5:TYR:HH     | 9:CI:7:THR:HG1     | 1.63                     | 0.47              |
| 9:CI:33:PHE:C     | 9:CI:35:GLU:H      | 2.23                     | 0.47              |
| 9:CI:43:ALA:C     | 9:CI:45:ALA:H      | 2.21                     | 0.47              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 9:CI:58:HIS:HB2   | 9:CI:59:PHE:CE1    | 2.49                     | 0.47              |
| 10:CJ:8:LEU:HA    | 10:CJ:95:GLU:O     | 2.15                     | 0.47              |
| 10:CJ:61:GLU:OE1  | 14:CN:58:LYS:CD    | 2.63                     | 0.47              |
| 11:CK:24:SER:OG   | 11:CK:25:TYR:N     | 2.47                     | 0.47              |
| 11:CK:61:ALA:O    | 11:CK:62:GLN:C     | 2.56                     | 0.47              |
| 23:CY:31:A:C2'    | 23:CY:32:U:H5'     | 2.45                     | 0.47              |
| 25:DA:413:C:H42   | 25:DA:2410:G:H1    | 1.62                     | 0.47              |
| 25:DA:787:U:H5''  | 25:DA:788:A:H5'    | 1.96                     | 0.47              |
| 25:DA:1378:A:O2'  | 25:DA:1379:A:O5'   | 2.21                     | 0.47              |
| 25:DA:2286:A:OP1  | 53:D6:30:THR:HB    | 2.13                     | 0.47              |
| 25:DA:2420:C:OP1  | 55:D8:34:TRP:HB2   | 2.14                     | 0.47              |
| 25:DA:2848:G:C3'  | 40:DT:95:ARG:O     | 2.62                     | 0.47              |
| 28:DD:68:LYS:HB2  | 28:DD:70:TRP:CH2   | 2.49                     | 0.47              |
| 30:DF:65:TRP:CZ3  | 30:DF:73:ALA:O     | 2.67                     | 0.47              |
| 30:DF:178:PRO:HB2 | 30:DF:201:VAL:CG1  | 2.42                     | 0.47              |
| 39:DS:3:ARG:CG    | 39:DS:4:LEU:N      | 2.75                     | 0.47              |
| 39:DS:5:THR:HG23  | 39:DS:8:GLU:OE2    | 2.15                     | 0.47              |
| 40:DT:104:ASN:O   | 40:DT:105:LEU:HD23 | 2.15                     | 0.47              |
| 43:DW:44:ALA:O    | 43:DW:45:TYR:C     | 2.58                     | 0.47              |
| 45:DY:63:LYS:HZ2  | 45:DY:63:LYS:CA    | 2.24                     | 0.47              |
| 52:D5:58:LEU:C    | 52:D5:59:GLU:HG2   | 2.40                     | 0.47              |
| 1:AA:173:U:H5''   | 1:AA:197:A:O4'     | 2.16                     | 0.46              |
| 1:AA:256:U:H5'    | 17:AQ:17:LYS:NZ    | 2.30                     | 0.46              |
| 1:AA:1026:G:N3    | 1:AA:1026:G:H2'    | 2.29                     | 0.46              |
| 1:AA:1499:A:OP2   | 1:AA:1505:G:OP2    | 2.34                     | 0.46              |
| 2:AB:97:TRP:HH2   | 2:AB:176:GLU:CD    | 2.22                     | 0.46              |
| 2:AB:125:PRO:O    | 2:AB:128:GLU:HB2   | 2.15                     | 0.46              |
| 7:AG:111:ARG:NH2  | 7:AG:126:ASP:OD1   | 2.47                     | 0.46              |
| 10:AJ:45:ARG:HA   | 10:AJ:45:ARG:HD3   | 1.71                     | 0.46              |
| 11:AK:48:ILE:HD11 | 11:AK:64:ALA:HA    | 1.97                     | 0.46              |
| 13:AM:20:THR:C    | 13:AM:22:ILE:N     | 2.72                     | 0.46              |
| 19:AS:14:HIS:CD2  | 19:AS:15:LEU:HD21  | 2.50                     | 0.46              |
| 19:AS:20:LEU:HA   | 19:AS:23:ASN:HB3   | 1.98                     | 0.46              |
| 25:BA:1312:U:P    | 44:BX:63:LYS:HD2   | 2.55                     | 0.46              |
| 25:BA:1313:U:H2'  | 25:BA:1610:A:C2    | 2.50                     | 0.46              |
| 25:BA:2695:C:H2'  | 25:BA:2696:U:C6    | 2.49                     | 0.46              |
| 27:BC:66:HIS:CD2  | 27:BC:187:ASP:HA   | 2.51                     | 0.46              |
| 30:BF:96:ASP:OD1  | 30:BF:97:TYR:N     | 2.48                     | 0.46              |
| 31:BG:13:GLU:O    | 31:BG:14:GLU:HB2   | 2.15                     | 0.46              |
| 31:BG:29:TRP:C    | 31:BG:31:VAL:H     | 2.23                     | 0.46              |
| 32:BH:130:ARG:O   | 32:BH:131:VAL:HG23 | 2.15                     | 0.46              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 37:BQ:134:ARG:HG3 | 37:BQ:134:ARG:NH1  | 2.30                     | 0.46              |
| 38:BR:41:ALA:C    | 38:BR:43:GLU:N     | 2.73                     | 0.46              |
| 40:BT:83:ILE:CD1  | 40:BT:84:GLN:CG    | 2.93                     | 0.46              |
| 43:BW:24:ILE:HG21 | 43:BW:36:LEU:HD21  | 1.97                     | 0.46              |
| 49:B2:67:LYS:O    | 49:B2:70:GLN:NE2   | 2.48                     | 0.46              |
| 53:B6:9:LEU:HD23  | 53:B6:9:LEU:C      | 2.40                     | 0.46              |
| 1:CA:1191:A:H5''  | 3:CC:4:LYS:NZ      | 2.30                     | 0.46              |
| 1:CA:1504:G:H4'   | 1:CA:1505:G:O5'    | 2.13                     | 0.46              |
| 2:CB:195:ASP:O    | 8:CH:68:ARG:NH2    | 2.48                     | 0.46              |
| 5:CE:63:ARG:C     | 5:CE:65:ASN:H      | 2.22                     | 0.46              |
| 6:CF:26:ILE:O     | 6:CF:30:LEU:HD12   | 2.14                     | 0.46              |
| 7:CG:149:ARG:O    | 7:CG:152:ALA:N     | 2.48                     | 0.46              |
| 8:CH:87:SER:HB2   | 8:CH:93:VAL:HB     | 1.96                     | 0.46              |
| 10:CJ:6:ILE:HG22  | 10:CJ:98:ILE:CG1   | 2.42                     | 0.46              |
| 10:CJ:49:VAL:CG2  | 10:CJ:50:ILE:H     | 2.27                     | 0.46              |
| 15:CO:27:VAL:O    | 15:CO:31:LEU:HB2   | 2.15                     | 0.46              |
| 17:CQ:22:LEU:HD12 | 17:CQ:22:LEU:HA    | 1.66                     | 0.46              |
| 17:CQ:89:LEU:O    | 17:CQ:93:GLN:HG3   | 2.14                     | 0.46              |
| 25:DA:83:G:H22    | 25:DA:102:G:C2'    | 2.27                     | 0.46              |
| 25:DA:340:A:C2'   | 25:DA:341:G:O5'    | 2.63                     | 0.46              |
| 25:DA:1227:G:OP1  | 41:DU:13:LYS:HG2   | 2.15                     | 0.46              |
| 27:DC:43:VAL:HG12 | 27:DC:43:VAL:O     | 2.15                     | 0.46              |
| 27:DC:141:LYS:O   | 27:DC:142:ALA:HB2  | 2.14                     | 0.46              |
| 28:DD:31:LYS:HB3  | 28:DD:35:LYS:HG3   | 1.97                     | 0.46              |
| 28:DD:48:ARG:NH1  | 28:DD:48:ARG:HG3   | 2.30                     | 0.46              |
| 31:DG:122:PRO:HG3 | 31:DG:182:LYS:C    | 2.40                     | 0.46              |
| 33:DI:82:ARG:O    | 33:DI:89:TYR:HD1   | 1.98                     | 0.46              |
| 34:DN:93:THR:O    | 34:DN:94:HIS:HB2   | 2.15                     | 0.46              |
| 35:DO:47:ILE:HG23 | 35:DO:48:PRO:CD    | 2.43                     | 0.46              |
| 37:DQ:12:GLN:HE21 | 37:DQ:73:PRO:CD    | 2.28                     | 0.46              |
| 37:DQ:62:GLY:H    | 37:DQ:109:VAL:HG23 | 1.79                     | 0.46              |
| 38:DR:77:ARG:C    | 38:DR:79:LEU:N     | 2.70                     | 0.46              |
| 39:DS:25:ARG:HH11 | 39:DS:25:ARG:HB3   | 1.80                     | 0.46              |
| 39:DS:100:ALA:O   | 39:DS:103:GLU:HG2  | 2.15                     | 0.46              |
| 40:DT:106:SER:HA  | 40:DT:110:ILE:CG1  | 2.42                     | 0.46              |
| 41:DU:62:ILE:HG23 | 41:DU:76:TYR:CE1   | 2.49                     | 0.46              |
| 42:DV:38:LEU:O    | 42:DV:51:VAL:HG13  | 2.15                     | 0.46              |
| 45:DY:88:LYS:C    | 45:DY:90:LEU:N     | 2.73                     | 0.46              |
| 55:D8:63:PRO:HB2  | 55:D8:64:TYR:HD1   | 1.80                     | 0.46              |
| 1:AA:243:A:N6     | 1:AA:281:G:C4      | 2.84                     | 0.46              |
| 1:AA:820:U:O2'    | 1:AA:821:G:OP1     | 2.29                     | 0.46              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:AA:1112:C:N3     | 3:AC:178:LEU:HB2  | 2.30                     | 0.46              |
| 1:AA:1126:U:C6     | 1:AA:1126:U:O5'   | 2.68                     | 0.46              |
| 1:AA:1228:C:H4'    | 13:AM:116:THR:HA  | 1.97                     | 0.46              |
| 2:AB:35:GLU:C      | 2:AB:36:ARG:HH21  | 2.23                     | 0.46              |
| 2:AB:108:ILE:HG22  | 2:AB:152:PHE:HE1  | 1.80                     | 0.46              |
| 2:AB:144:ARG:C     | 2:AB:147:LYS:H    | 2.24                     | 0.46              |
| 11:AK:41:THR:HG21  | 11:AK:71:LYS:HD2  | 1.98                     | 0.46              |
| 13:AM:20:THR:O     | 13:AM:22:ILE:N    | 2.40                     | 0.46              |
| 13:AM:57:ARG:NH1   | 51:B4:60:GLU:HG3  | 2.30                     | 0.46              |
| 13:AM:65:LYS:HA    | 13:AM:66:LEU:CG   | 2.44                     | 0.46              |
| 13:AM:69:GLU:OE1   | 13:AM:69:GLU:O    | 2.33                     | 0.46              |
| 17:AQ:53:LEU:HD12  | 17:AQ:54:GLY:N    | 2.29                     | 0.46              |
| 20:AT:63:ILE:CG2   | 20:AT:77:ALA:HB1  | 2.45                     | 0.46              |
| 25:BA:581:C:H2'    | 25:BA:582:G:C8    | 2.50                     | 0.46              |
| 25:BA:710:G:H2'    | 25:BA:711:G:C8    | 2.50                     | 0.46              |
| 25:BA:833:U:H2'    | 25:BA:834:C:C6    | 2.50                     | 0.46              |
| 25:BA:851:U:OP1    | 50:B3:49:LYS:NZ   | 2.47                     | 0.46              |
| 25:BA:1283:G:N2    | 25:BA:1285:G:H3'  | 2.29                     | 0.46              |
| 25:BA:1558:A:O2'   | 25:BA:1559:G:OP2  | 2.31                     | 0.46              |
| 25:BA:1952:A:C6    | 25:BA:1953:A:N1   | 2.84                     | 0.46              |
| 28:BD:111:LEU:HD22 | 28:BD:115:GLN:OE1 | 2.15                     | 0.46              |
| 29:BE:94:GLU:CG    | 29:BE:177:PRO:HB3 | 2.45                     | 0.46              |
| 30:BF:34:TRP:CZ3   | 36:BP:8:PRO:HB3   | 2.49                     | 0.46              |
| 36:BP:38:GLN:HG2   | 36:BP:45:LEU:HD13 | 1.97                     | 0.46              |
| 36:BP:70:GLN:C     | 36:BP:72:PRO:CD   | 2.77                     | 0.46              |
| 38:BR:88:ARG:HD2   | 38:BR:89:ASP:OD1  | 2.14                     | 0.46              |
| 38:BR:97:VAL:O     | 38:BR:97:VAL:HG12 | 2.11                     | 0.46              |
| 39:BS:58:LEU:H     | 39:BS:58:LEU:HD12 | 1.78                     | 0.46              |
| 39:BS:92:TYR:N     | 39:BS:92:TYR:HD1  | 2.12                     | 0.46              |
| 39:BS:92:TYR:O     | 39:BS:94:TYR:N    | 2.47                     | 0.46              |
| 41:BU:14:HIS:NE2   | 41:BU:32:PHE:CG   | 2.82                     | 0.46              |
| 42:BV:65:GLY:HA3   | 42:BV:91:TYR:CE1  | 2.40                     | 0.46              |
| 46:BZ:24:LEU:CB    | 46:BZ:41:LEU:HG   | 2.45                     | 0.46              |
| 48:B1:16:ASN:HA    | 48:B1:38:SER:O    | 2.15                     | 0.46              |
| 48:B1:64:ALA:C     | 48:B1:66:HIS:H    | 2.24                     | 0.46              |
| 1:CA:77:G:O6       | 1:CA:92:C:N4      | 2.48                     | 0.46              |
| 1:CA:173:U:O4'     | 1:CA:197:A:C4     | 2.68                     | 0.46              |
| 1:CA:595:G:H1'     | 1:CA:596:C:H5     | 1.79                     | 0.46              |
| 1:CA:945:G:C2      | 1:CA:946:A:C8     | 3.03                     | 0.46              |
| 1:CA:1015:A:N3     | 1:CA:1218:C:O2'   | 2.45                     | 0.46              |
| 1:CA:1434:A:H2'    | 1:CA:1435:G:O4'   | 2.15                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:CB:85:ALA:HB1   | 2:CB:92:TYR:HB3   | 1.96                     | 0.46              |
| 2:CB:105:PHE:C    | 2:CB:107:THR:H    | 2.24                     | 0.46              |
| 4:CD:19:LEU:CB    | 4:CD:21:LEU:CD1   | 2.93                     | 0.46              |
| 5:CE:76:ILE:HG12  | 5:CE:77:PRO:CD    | 2.32                     | 0.46              |
| 13:CM:108:ARG:NH1 | 13:CM:108:ARG:HG3 | 2.30                     | 0.46              |
| 17:CQ:4:LYS:C     | 17:CQ:5:VAL:CG2   | 2.88                     | 0.46              |
| 17:CQ:53:LEU:HD12 | 17:CQ:54:GLY:N    | 2.30                     | 0.46              |
| 19:CS:6:LYS:HE3   | 19:CS:6:LYS:N     | 2.29                     | 0.46              |
| 22:CV:4:G:HO2'    | 22:CV:5:G:P       | 2.38                     | 0.46              |
| 23:CW:68:C:C2     | 23:CW:69:G:C8     | 3.02                     | 0.46              |
| 25:DA:226:G:O2'   | 25:DA:227:A:C8    | 2.68                     | 0.46              |
| 25:DA:457:A:O2'   | 25:DA:458:G:OP2   | 2.31                     | 0.46              |
| 25:DA:614:U:O2    | 25:DA:614:U:O4'   | 2.30                     | 0.46              |
| 25:DA:1357:U:H2'  | 25:DA:1358:G:O4'  | 2.15                     | 0.46              |
| 25:DA:2001:A:H4'  | 25:DA:2689:U:H2'  | 1.96                     | 0.46              |
| 25:DA:2134:A:C2   | 25:DA:2159:G:H1'  | 2.49                     | 0.46              |
| 26:DB:30:C:H1'    | 26:DB:57:A:H61    | 1.80                     | 0.46              |
| 27:DC:155:GLU:O   | 27:DC:156:ILE:CB  | 2.64                     | 0.46              |
| 29:DE:31:CYS:HB3  | 29:DE:49:LEU:HB3  | 1.96                     | 0.46              |
| 29:DE:119:ARG:HD2 | 29:DE:120:TRP:CE2 | 2.49                     | 0.46              |
| 30:DF:129:PHE:O   | 30:DF:130:ALA:HB3 | 2.15                     | 0.46              |
| 31:DG:68:PRO:HG2  | 31:DG:90:LEU:HD12 | 1.97                     | 0.46              |
| 31:DG:125:PHE:HE1 | 31:DG:180:PHE:HE2 | 1.63                     | 0.46              |
| 32:DH:62:LYS:O    | 32:DH:65:HIS:HB3  | 2.15                     | 0.46              |
| 36:DP:131:SER:O   | 36:DP:132:LYS:C   | 2.59                     | 0.46              |
| 37:DQ:12:GLN:HE21 | 37:DQ:72:LYS:HA   | 1.79                     | 0.46              |
| 38:DR:3:HIS:C     | 38:DR:5:LYS:H     | 2.15                     | 0.46              |
| 39:DS:106:ARG:CA  | 39:DS:110:LEU:CD2 | 2.86                     | 0.46              |
| 41:DU:6:THR:O     | 41:DU:9:VAL:HG23  | 2.15                     | 0.46              |
| 45:DY:91:GLU:HG3  | 45:DY:92:ASN:OD1  | 2.15                     | 0.46              |
| 46:DZ:13:GLU:HB3  | 46:DZ:14:LYS:NZ   | 2.31                     | 0.46              |
| 48:D1:29:GLY:C    | 48:D1:31:GLY:N    | 2.72                     | 0.46              |
| 55:D8:57:ARG:O    | 55:D8:58:ILE:C    | 2.59                     | 0.46              |
| 1:AA:787:A:N1     | 1:AA:795:C:N4     | 2.60                     | 0.46              |
| 1:AA:1053:G:N7    | 1:AA:1200:C:H5''  | 2.30                     | 0.46              |
| 2:AB:77:ALA:O     | 2:AB:81:VAL:HG23  | 2.15                     | 0.46              |
| 3:AC:60:ALA:HB3   | 3:AC:63:ASN:OD1   | 2.15                     | 0.46              |
| 3:AC:189:ALA:HB3  | 3:AC:196:LEU:HB2  | 1.97                     | 0.46              |
| 4:AD:33:MET:HA    | 4:AD:33:MET:CE    | 2.39                     | 0.46              |
| 4:AD:118:ARG:O    | 4:AD:120:LEU:N    | 2.48                     | 0.46              |
| 5:AE:142:LEU:O    | 5:AE:143:ARG:HD3  | 2.15                     | 0.46              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 9:AI:88:TYR:O     | 9:AI:89:ASN:CB     | 2.55                     | 0.46              |
| 10:AJ:80:LYS:HD2  | 1:CA:1162:C:O2'    | 2.16                     | 0.46              |
| 11:AK:41:THR:HG21 | 11:AK:71:LYS:CD    | 2.46                     | 0.46              |
| 14:AN:58:LYS:HE3  | 14:AN:58:LYS:HB3   | 1.65                     | 0.46              |
| 16:AP:31:LYS:HG3  | 16:AP:32:TYR:N     | 2.31                     | 0.46              |
| 19:AS:9:VAL:HG12  | 19:AS:9:VAL:O      | 2.15                     | 0.46              |
| 22:AV:34:U:O2     | 22:AV:36:A:H5''    | 2.15                     | 0.46              |
| 25:BA:587:C:O2'   | 25:BA:588:U:OP2    | 2.30                     | 0.46              |
| 26:BB:56:G:H4'    | 26:BB:57:A:C8      | 2.50                     | 0.46              |
| 29:BE:61:ARG:CB   | 29:BE:62:PRO:CD    | 2.94                     | 0.46              |
| 31:BG:28:VAL:C    | 31:BG:30:GLU:N     | 2.73                     | 0.46              |
| 32:BH:116:GLU:HG2 | 32:BH:117:PRO:N    | 2.28                     | 0.46              |
| 32:BH:144:VAL:CA  | 32:BH:147:ASN:HB2  | 2.30                     | 0.46              |
| 33:BI:2:LYS:HB2   | 33:BI:39:ALA:HB3   | 1.96                     | 0.46              |
| 33:BI:3:VAL:HG12  | 33:BI:38:LEU:HA    | 1.97                     | 0.46              |
| 33:BI:53:ALA:O    | 33:BI:57:ARG:CG    | 2.63                     | 0.46              |
| 33:BI:60:GLU:C    | 33:BI:62:LYS:H     | 2.22                     | 0.46              |
| 33:BI:77:LEU:HB3  | 33:BI:140:LEU:HD13 | 1.97                     | 0.46              |
| 36:BP:24:GLY:O    | 36:BP:25:SER:CB    | 2.64                     | 0.46              |
| 37:BQ:46:GLN:O    | 37:BQ:49:ALA:N     | 2.48                     | 0.46              |
| 38:BR:75:LEU:HD23 | 38:BR:78:LYS:HD3   | 1.97                     | 0.46              |
| 43:BW:12:ILE:HG12 | 43:BW:17:VAL:CG1   | 2.44                     | 0.46              |
| 44:BX:12:VAL:CG2  | 44:BX:13:LEU:H     | 2.23                     | 0.46              |
| 45:BY:67:LEU:HD12 | 45:BY:71:LYS:CG    | 2.31                     | 0.46              |
| 45:BY:67:LEU:CD1  | 45:BY:71:LYS:CB    | 2.93                     | 0.46              |
| 51:B4:41:ILE:HA   | 51:B4:47:VAL:HG22  | 1.96                     | 0.46              |
| 51:B4:54:LYS:HA   | 51:B4:55:PRO:HD3   | 1.69                     | 0.46              |
| 1:CA:137:C:H42    | 1:CA:226:G:H1      | 1.63                     | 0.46              |
| 1:CA:189(G):G:O6  | 1:CA:264:U:H5''    | 2.14                     | 0.46              |
| 1:CA:533:A:O2'    | 1:CA:534:U:OP1     | 2.30                     | 0.46              |
| 1:CA:1201:A:HO2'  | 1:CA:1202:G:P      | 2.39                     | 0.46              |
| 1:CA:1244:C:H2'   | 1:CA:1245:A:H8     | 1.79                     | 0.46              |
| 2:CB:156:LYS:HB3  | 2:CB:156:LYS:HE2   | 1.65                     | 0.46              |
| 3:CC:22:TRP:CB    | 3:CC:59:ARG:HB2    | 2.44                     | 0.46              |
| 4:CD:71:SER:OG    | 4:CD:74:GLN:HG3    | 2.16                     | 0.46              |
| 6:CF:7:ASN:HD21   | 18:CR:34:TYR:HE1   | 1.63                     | 0.46              |
| 8:CH:2:LEU:HD22   | 8:CH:2:LEU:HA      | 1.81                     | 0.46              |
| 8:CH:103:VAL:O    | 8:CH:108:GLY:N     | 2.44                     | 0.46              |
| 10:CJ:6:ILE:O     | 10:CJ:6:ILE:HG13   | 2.15                     | 0.46              |
| 13:CM:82:MET:CE   | 13:CM:93:ARG:HA    | 2.45                     | 0.46              |
| 25:DA:457:A:O2'   | 25:DA:458:G:P      | 2.73                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:DA:532:A:H2     | 41:DU:28:ARG:HH21  | 1.63                     | 0.46              |
| 25:DA:604:G:H2'    | 25:DA:605:C:H6     | 1.77                     | 0.46              |
| 25:DA:747:U:O2     | 25:DA:2014:A:H1'   | 2.15                     | 0.46              |
| 25:DA:793:A:OP2    | 25:DA:2071:A:O2'   | 2.31                     | 0.46              |
| 25:DA:995:C:H6     | 41:DU:57:PHE:HE1   | 1.50                     | 0.46              |
| 25:DA:1937:A:N7    | 25:DA:1939:U:H2'   | 2.31                     | 0.46              |
| 25:DA:2537:U:H2'   | 25:DA:2538:C:C6    | 2.50                     | 0.46              |
| 26:DB:92:C:OP1     | 37:DQ:19:GLY:N     | 2.45                     | 0.46              |
| 28:DD:155:LEU:N    | 28:DD:155:LEU:CD1  | 2.78                     | 0.46              |
| 32:DH:89:ILE:HD13  | 32:DH:90:LYS:H     | 1.78                     | 0.46              |
| 33:DI:11:ASN:C     | 33:DI:12:LEU:HD13  | 2.40                     | 0.46              |
| 35:DO:35:VAL:HG21  | 35:DO:69:ILE:CD1   | 2.41                     | 0.46              |
| 36:DP:61:ARG:HD2   | 36:DP:61:ARG:N     | 2.31                     | 0.46              |
| 36:DP:138:LEU:HD12 | 36:DP:139:LYS:N    | 2.30                     | 0.46              |
| 36:DP:147:LEU:C    | 36:DP:148:LEU:HD23 | 2.38                     | 0.46              |
| 37:DQ:104:PHE:HE1  | 37:DQ:125:LEU:HD11 | 1.80                     | 0.46              |
| 40:DT:108:ARG:HA   | 40:DT:111:ARG:NH1  | 2.30                     | 0.46              |
| 45:DY:49:VAL:HG11  | 45:DY:50:ARG:NH2   | 2.30                     | 0.46              |
| 1:AA:250:A:C8      | 1:AA:252:U:C2      | 3.04                     | 0.46              |
| 1:AA:251:G:O2'     | 1:AA:252:U:O5'     | 2.33                     | 0.46              |
| 1:AA:355:C:O4'     | 1:AA:388:G:O2'     | 2.34                     | 0.46              |
| 1:AA:939:G:H2'     | 1:AA:940:C:C6      | 2.50                     | 0.46              |
| 1:AA:1439:C:OP1    | 20:AT:38:LYS:NZ    | 2.29                     | 0.46              |
| 2:AB:196:LEU:HD12  | 2:AB:197:VAL:HG23  | 1.97                     | 0.46              |
| 3:AC:153:VAL:HG12  | 3:AC:196:LEU:HD12  | 1.97                     | 0.46              |
| 6:AF:16:GLN:O      | 6:AF:20:ALA:N      | 2.48                     | 0.46              |
| 9:AI:116:LYS:O     | 9:AI:118:LYS:N     | 2.42                     | 0.46              |
| 12:AL:35:GLY:HA3   | 12:AL:60:LEU:HD13  | 1.98                     | 0.46              |
| 16:AP:8:ARG:C      | 16:AP:9:PHE:CD2    | 2.93                     | 0.46              |
| 22:AV:52:C:C4      | 22:AV:53:G:N7      | 2.84                     | 0.46              |
| 22:AV:54:G:N3      | 22:AV:55:U:C5      | 2.83                     | 0.46              |
| 25:BA:804:A:C5'    | 25:BA:805:G:OP1    | 2.60                     | 0.46              |
| 25:BA:820:A:H1'    | 25:BA:943:U:H1'    | 1.96                     | 0.46              |
| 25:BA:890:A:N6     | 25:BA:892:G:C6     | 2.84                     | 0.46              |
| 25:BA:1636:C:H2'   | 25:BA:1637:A:C8    | 2.51                     | 0.46              |
| 25:BA:2489:G:O6    | 25:BA:2490:G:N1    | 2.48                     | 0.46              |
| 25:BA:2646:C:H2'   | 25:BA:2647:U:O4'   | 2.14                     | 0.46              |
| 27:BC:120:MET:CB   | 27:BC:142:ALA:HA   | 2.45                     | 0.46              |
| 28:BD:3:VAL:HA     | 28:BD:18:VAL:O     | 2.15                     | 0.46              |
| 28:BD:53:PHE:CE2   | 28:BD:220:HIS:NE2  | 2.84                     | 0.46              |
| 30:BF:11:VAL:C     | 30:BF:13:SER:N     | 2.71                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 30:BF:45:ARG:CG   | 30:BF:46:ARG:N    | 2.76                     | 0.46              |
| 32:BH:21:PRO:HB2  | 32:BH:22:GLY:H    | 1.59                     | 0.46              |
| 36:BP:86:LYS:HB3  | 36:BP:117:GLU:O   | 2.16                     | 0.46              |
| 38:BR:37:THR:HG23 | 38:BR:40:LYS:CB   | 2.46                     | 0.46              |
| 45:BY:55:TYR:HD1  | 45:BY:56:PRO:CG   | 2.29                     | 0.46              |
| 45:BY:75:ILE:O    | 45:BY:76:CYS:HB2  | 2.15                     | 0.46              |
| 46:BZ:4:ARG:NH2   | 46:BZ:66:SER:OG   | 2.49                     | 0.46              |
| 46:BZ:27:VAL:O    | 46:BZ:88:PHE:N    | 2.44                     | 0.46              |
| 50:B3:40:THR:HB   | 50:B3:41:PRO:HD2  | 1.98                     | 0.46              |
| 1:CA:61:G:O6      | 1:CA:107:G:C6     | 2.69                     | 0.46              |
| 1:CA:1198:G:HO2'  | 10:CJ:54:PHE:HD2  | 1.63                     | 0.46              |
| 1:CA:1445:C:C4    | 1:CA:1446:U:C4    | 3.02                     | 0.46              |
| 1:CA:1513:A:H2'   | 1:CA:1514:C:C6    | 2.51                     | 0.46              |
| 2:CB:71:VAL:HG13  | 2:CB:93:VAL:CG2   | 2.45                     | 0.46              |
| 4:CD:4:TYR:CE1    | 4:CD:5:ILE:O      | 2.68                     | 0.46              |
| 6:CF:63:TYR:HD2   | 6:CF:63:TYR:N     | 2.12                     | 0.46              |
| 8:CH:33:GLU:O     | 8:CH:34:GLU:C     | 2.59                     | 0.46              |
| 10:CJ:47:PHE:HZ   | 14:CN:37:PHE:CZ   | 2.33                     | 0.46              |
| 10:CJ:49:VAL:CG2  | 10:CJ:50:ILE:N    | 2.78                     | 0.46              |
| 11:CK:73:MET:HG2  | 11:CK:77:MET:O    | 2.14                     | 0.46              |
| 12:CL:102:ARG:HE  | 12:CL:102:ARG:HB3 | 1.52                     | 0.46              |
| 13:CM:25:ILE:HD11 | 13:CM:66:LEU:HD21 | 1.98                     | 0.46              |
| 19:CS:6:LYS:HD2   | 19:CS:7:LYS:H     | 1.81                     | 0.46              |
| 19:CS:57:HIS:O    | 19:CS:59:PRO:HD3  | 2.15                     | 0.46              |
| 23:CY:34:G:H2'    | 23:CY:35:A:H8     | 1.76                     | 0.46              |
| 25:DA:94(A):G:H2' | 25:DA:95:G:O4'    | 2.15                     | 0.46              |
| 25:DA:197:A:H62   | 25:DA:2430:A:H2'  | 1.79                     | 0.46              |
| 25:DA:265:A:H1'   | 25:DA:266:G:C1'   | 2.46                     | 0.46              |
| 25:DA:568:U:C5'   | 25:DA:945:A:N6    | 2.78                     | 0.46              |
| 25:DA:662:G:OP1   | 36:DP:15:ARG:NE   | 2.49                     | 0.46              |
| 25:DA:1452:A:H5'' | 25:DA:1453:U:OP2  | 2.16                     | 0.46              |
| 29:DE:52:LEU:HD12 | 29:DE:52:LEU:HA   | 1.58                     | 0.46              |
| 31:DG:91:ARG:HG2  | 31:DG:92:VAL:N    | 2.30                     | 0.46              |
| 32:DH:126:PRO:HG2 | 32:DH:130:ARG:NH1 | 2.22                     | 0.46              |
| 33:DI:69:LYS:HG3  | 33:DI:136:VAL:CB  | 2.43                     | 0.46              |
| 36:DP:38:GLN:HG2  | 36:DP:45:LEU:HD13 | 1.97                     | 0.46              |
| 39:DS:15:ARG:NE   | 39:DS:88:ASP:OD1  | 2.48                     | 0.46              |
| 42:DV:64:HIS:N    | 42:DV:64:HIS:ND1  | 2.63                     | 0.46              |
| 44:DX:57:LEU:N    | 44:DX:57:LEU:CD1  | 2.79                     | 0.46              |
| 45:DY:48:ALA:HB2  | 45:DY:61:ILE:HD13 | 1.98                     | 0.46              |
| 46:DZ:28:MET:CE   | 46:DZ:37:VAL:HG11 | 2.45                     | 0.46              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 46:DZ:59:LEU:CG   | 46:DZ:69:THR:HG21  | 2.41                     | 0.46              |
| 46:DZ:116:VAL:H   | 46:DZ:174:VAL:HG13 | 1.80                     | 0.46              |
| 50:D3:10:LYS:HB3  | 50:D3:53:LEU:HA    | 1.98                     | 0.46              |
| 1:AA:284:G:H2'    | 1:AA:285:G:C8      | 2.51                     | 0.46              |
| 1:AA:923:A:N6     | 1:AA:1392:G:O6     | 2.48                     | 0.46              |
| 1:AA:1025:U:O2'   | 1:AA:1026:G:N7     | 2.45                     | 0.46              |
| 1:AA:1064:G:H21   | 1:AA:1190:G:H2'    | 1.81                     | 0.46              |
| 1:AA:1158:C:N4    | 1:AA:1181:G:H22    | 2.13                     | 0.46              |
| 1:AA:1218:C:H2'   | 1:AA:1219:U:C6     | 2.51                     | 0.46              |
| 2:AB:58:ILE:H     | 2:AB:58:ILE:HG12   | 1.40                     | 0.46              |
| 6:AF:21:LEU:HA    | 6:AF:21:LEU:HD22   | 1.59                     | 0.46              |
| 25:BA:242:G:N3    | 25:BA:254:G:C5     | 2.83                     | 0.46              |
| 25:BA:1131:G:O2'  | 25:BA:1132:A:O5'   | 2.34                     | 0.46              |
| 25:BA:1342:A:N6   | 25:BA:1397:U:C4    | 2.82                     | 0.46              |
| 25:BA:1427:A:H4'  | 25:BA:1428:C:O4'   | 2.16                     | 0.46              |
| 25:BA:1428:C:N4   | 25:BA:1569:A:H3'   | 2.31                     | 0.46              |
| 25:BA:1494:A:N3   | 25:BA:1494:A:C5'   | 2.70                     | 0.46              |
| 25:BA:2198:A:H5'' | 25:BA:2199:A:OP1   | 2.16                     | 0.46              |
| 25:BA:2848:G:H5'' | 25:BA:2849:U:OP1   | 2.15                     | 0.46              |
| 29:BE:152:LYS:HB3 | 34:BN:78:TYR:CG    | 2.49                     | 0.46              |
| 30:BF:133:ASN:HA  | 30:BF:162:LEU:HD23 | 1.98                     | 0.46              |
| 31:BG:76:SER:CA   | 31:BG:83:ARG:HB2   | 2.45                     | 0.46              |
| 33:BI:86:THR:O    | 33:BI:123:LEU:HD12 | 2.15                     | 0.46              |
| 33:BI:110:ASP:OD1 | 33:BI:113:ARG:HG2  | 2.15                     | 0.46              |
| 33:BI:131:LYS:HG3 | 33:BI:132:PRO:CD   | 2.46                     | 0.46              |
| 34:BN:56:ASN:HA   | 34:BN:125:GLY:N    | 2.15                     | 0.46              |
| 34:BN:56:ASN:O    | 34:BN:57:ALA:O     | 2.33                     | 0.46              |
| 35:BO:63:VAL:HG12 | 35:BO:106:LEU:HD11 | 1.98                     | 0.46              |
| 35:BO:80:ASP:H    | 40:BT:70:VAL:HG12  | 1.81                     | 0.46              |
| 38:BR:2:ARG:NH2   | 38:BR:5:LYS:CE     | 2.78                     | 0.46              |
| 41:BU:22:LYS:HD3  | 41:BU:22:LYS:HA    | 1.66                     | 0.46              |
| 46:BZ:71:VAL:HG22 | 46:BZ:88:PHE:CD2   | 2.51                     | 0.46              |
| 1:CA:115:G:H1'    | 1:CA:116:A:N7      | 2.30                     | 0.46              |
| 1:CA:284:G:H2'    | 1:CA:285:G:C8      | 2.51                     | 0.46              |
| 1:CA:1239:A:H1'   | 1:CA:1241:G:C4     | 2.50                     | 0.46              |
| 2:CB:8:LYS:HD3    | 2:CB:8:LYS:N       | 2.31                     | 0.46              |
| 2:CB:55:PHE:C     | 2:CB:57:PHE:N      | 2.72                     | 0.46              |
| 4:CD:19:LEU:HB3   | 4:CD:21:LEU:HD12   | 1.97                     | 0.46              |
| 4:CD:189:PRO:CB   | 4:CD:194:LEU:HD21  | 2.46                     | 0.46              |
| 5:CE:68:GLU:OE2   | 5:CE:68:GLU:O      | 2.33                     | 0.46              |
| 7:CG:44:TYR:O     | 7:CG:48:LYS:HG3    | 2.15                     | 0.46              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 7:CG:116:ALA:O    | 7:CG:119:ARG:N     | 2.48                     | 0.46              |
| 10:CJ:56:HIS:O    | 10:CJ:57:LYS:C     | 2.57                     | 0.46              |
| 18:CR:59:SER:HB3  | 18:CR:62:GLU:CG    | 2.46                     | 0.46              |
| 19:CS:20:LEU:HA   | 19:CS:23:ASN:HB2   | 1.98                     | 0.46              |
| 20:CT:24:LEU:C    | 20:CT:24:LEU:HD13  | 2.41                     | 0.46              |
| 22:CV:35:C:O2'    | 22:CV:36:A:OP1     | 2.32                     | 0.46              |
| 23:CW:72:C:C2'    | 23:CW:73:A:H5'     | 2.45                     | 0.46              |
| 25:DA:604:G:C6    | 25:DA:605:C:N4     | 2.83                     | 0.46              |
| 25:DA:686:G:H4'   | 25:DA:687:C:OP2    | 2.16                     | 0.46              |
| 25:DA:695:G:C6    | 25:DA:768:G:O6     | 2.68                     | 0.46              |
| 25:DA:773:U:H4'   | 28:DD:47:GLY:HA3   | 1.98                     | 0.46              |
| 25:DA:1028:A:N6   | 25:DA:1125:G:H2'   | 2.30                     | 0.46              |
| 25:DA:1654:A:OP2  | 38:DR:1:MET:O      | 2.34                     | 0.46              |
| 25:DA:2033:A:H4'  | 25:DA:2034:U:OP1   | 2.16                     | 0.46              |
| 25:DA:2287:A:N6   | 25:DA:2344:U:C2    | 2.84                     | 0.46              |
| 25:DA:2327:A:H2'  | 25:DA:2328:A:C8    | 2.50                     | 0.46              |
| 28:DD:132:PRO:O   | 28:DD:136:ILE:HG13 | 2.15                     | 0.46              |
| 28:DD:133:LEU:HB3 | 28:DD:173:VAL:HG11 | 1.98                     | 0.46              |
| 28:DD:270:ILE:C   | 28:DD:271:ILE:CG1  | 2.89                     | 0.46              |
| 29:DE:108:SER:HB3 | 29:DE:165:VAL:HG21 | 1.97                     | 0.46              |
| 30:DF:161:GLU:O   | 30:DF:164:ARG:HB3  | 2.15                     | 0.46              |
| 31:DG:26:GLN:HE21 | 31:DG:27:ASN:HB2   | 1.80                     | 0.46              |
| 32:DH:151:ILE:O   | 32:DH:152:ARG:O    | 2.34                     | 0.46              |
| 35:DO:29:ASN:HD22 | 35:DO:29:ASN:C     | 2.24                     | 0.46              |
| 37:DQ:14:ARG:HG2  | 37:DQ:41:TRP:HH2   | 1.79                     | 0.46              |
| 37:DQ:112:GLU:HG3 | 37:DQ:113:GLN:N    | 2.30                     | 0.46              |
| 39:DS:7:TYR:HA    | 39:DS:10:ARG:HH11  | 1.81                     | 0.46              |
| 41:DU:105:VAL:HA  | 42:DV:44:LYS:HD3   | 1.98                     | 0.46              |
| 43:DW:8:ARG:O     | 43:DW:9:TYR:HB2    | 2.15                     | 0.46              |
| 45:DY:51:VAL:CG2  | 45:DY:57:GLN:HA    | 2.46                     | 0.46              |
| 45:DY:84:ARG:HH22 | 45:DY:97:ARG:CB    | 2.28                     | 0.46              |
| 4:AD:25:ARG:C     | 4:AD:27:TYR:N      | 2.72                     | 0.46              |
| 5:AE:77:PRO:HG2   | 5:AE:142:LEU:HD22  | 1.96                     | 0.46              |
| 7:AG:44:TYR:C     | 7:AG:46:ALA:H      | 2.24                     | 0.46              |
| 7:AG:99:LEU:O     | 7:AG:100:ALA:C     | 2.58                     | 0.46              |
| 7:AG:155:ARG:O    | 7:AG:156:TRP:C     | 2.59                     | 0.46              |
| 8:AH:134:ILE:O    | 8:AH:135:CYS:HB3   | 2.15                     | 0.46              |
| 9:AI:53:VAL:HB    | 9:AI:92:TYR:HE2    | 1.81                     | 0.46              |
| 13:AM:86:CYS:HA   | 19:AS:73:GLU:O     | 2.15                     | 0.46              |
| 25:BA:340:A:H2'   | 25:BA:341:G:C8     | 2.49                     | 0.46              |
| 25:BA:454:A:H4'   | 25:BA:455:C:OP2    | 2.14                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:BA:725:G:C6    | 25:BA:726:G:N1    | 2.84                     | 0.46              |
| 25:BA:1204:A:H1'  | 25:BA:1206:G:N7   | 2.31                     | 0.46              |
| 25:BA:1452:A:N6   | 25:BA:2703:C:H5   | 2.13                     | 0.46              |
| 25:BA:1653:G:O2'  | 25:BA:1654:A:OP2  | 2.33                     | 0.46              |
| 25:BA:2126:A:O2'  | 25:BA:2127:G:O5'  | 2.34                     | 0.46              |
| 25:BA:2152:G:H2'  | 25:BA:2153:G:H8   | 1.80                     | 0.46              |
| 25:BA:2287:A:N6   | 25:BA:2344:U:N3   | 2.63                     | 0.46              |
| 25:BA:2368:C:H2'  | 25:BA:2369:A:H8   | 1.80                     | 0.46              |
| 25:BA:2420:C:OP2  | 55:B8:32:LEU:O    | 2.33                     | 0.46              |
| 26:BB:105:A:O2'   | 46:BZ:30:ASN:HA   | 2.16                     | 0.46              |
| 27:BC:36:LYS:HD3  | 27:BC:37:PHE:H    | 1.80                     | 0.46              |
| 28:BD:244:ARG:HA  | 28:BD:245:PRO:HA  | 1.56                     | 0.46              |
| 29:BE:173:VAL:HB  | 29:BE:183:LEU:HB3 | 1.98                     | 0.46              |
| 30:BF:139:PHE:O   | 30:BF:142:TRP:HB3 | 2.15                     | 0.46              |
| 30:BF:182:ASN:C   | 30:BF:184:TYR:N   | 2.74                     | 0.46              |
| 31:BG:45:GLU:HA   | 31:BG:45:GLU:OE1  | 2.15                     | 0.46              |
| 32:BH:142:GLY:O   | 32:BH:145:ALA:HB3 | 2.15                     | 0.46              |
| 32:BH:163:TYR:N   | 32:BH:163:TYR:CD1 | 2.83                     | 0.46              |
| 35:BO:87:ILE:HG21 | 35:BO:91:LEU:HA   | 1.96                     | 0.46              |
| 39:BS:33:LYS:HD2  | 39:BS:33:LYS:HA   | 1.68                     | 0.46              |
| 39:BS:62:LYS:O    | 39:BS:65:VAL:HB   | 2.15                     | 0.46              |
| 40:BT:80:SER:CB   | 40:BT:81:PRO:CD   | 2.93                     | 0.46              |
| 43:BW:88:ARG:HG3  | 43:BW:94:ASP:OD1  | 2.16                     | 0.46              |
| 48:B1:45:ASN:HD21 | 48:B1:47:GLN:NE2  | 2.04                     | 0.46              |
| 48:B1:53:VAL:HG12 | 48:B1:53:VAL:O    | 2.14                     | 0.46              |
| 50:B3:4:LEU:O     | 50:B3:36:VAL:HA   | 2.16                     | 0.46              |
| 1:CA:61:G:H2'     | 1:CA:62:U:O4'     | 2.16                     | 0.46              |
| 1:CA:128:G:C2'    | 1:CA:129:U:C5'    | 2.87                     | 0.46              |
| 1:CA:406:G:H2'    | 1:CA:407:G:H8     | 1.80                     | 0.46              |
| 1:CA:951:G:C6     | 1:CA:1231:G:C6    | 3.04                     | 0.46              |
| 1:CA:1218:C:H2'   | 1:CA:1219:U:C6    | 2.50                     | 0.46              |
| 1:CA:1240:U:H4'   | 1:CA:1241:G:OP2   | 2.16                     | 0.46              |
| 3:CC:32:LEU:HD22  | 3:CC:59:ARG:HH12  | 1.79                     | 0.46              |
| 5:CE:7:GLU:HG2    | 5:CE:112:LEU:HD22 | 1.96                     | 0.46              |
| 5:CE:67:VAL:HG13  | 5:CE:69:VAL:HG23  | 1.97                     | 0.46              |
| 9:CI:16:ARG:NH2   | 9:CI:64:THR:HG21  | 2.31                     | 0.46              |
| 11:CK:54:ARG:NH2  | 23:CW:40:C:OP1    | 2.36                     | 0.46              |
| 15:CO:38:ARG:HH11 | 15:CO:38:ARG:HG2  | 1.80                     | 0.46              |
| 19:CS:10:PHE:HE2  | 19:CS:37:ARG:O    | 1.98                     | 0.46              |
| 22:CV:20:G:C4     | 22:CV:58:A:C2     | 3.04                     | 0.46              |
| 23:CW:36:A:C2'    | 23:CW:37:A:H5''   | 2.33                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:CY:40:C:O5'     | 23:CY:40:C:H6      | 1.99                     | 0.46              |
| 25:DA:1612:C:H4'   | 54:D7:5:TRP:O      | 2.16                     | 0.46              |
| 25:DA:1799:G:HO2'  | 25:DA:1800:C:P     | 2.37                     | 0.46              |
| 27:DC:182:PRO:O    | 27:DC:183:GLU:CB   | 2.64                     | 0.46              |
| 28:DD:85:ASP:HB2   | 28:DD:92:ILE:HD12  | 1.98                     | 0.46              |
| 31:DG:44:GLY:O     | 31:DG:47:LYS:HB2   | 2.16                     | 0.46              |
| 31:DG:75:LYS:HD2   | 31:DG:77:ILE:CD1   | 2.45                     | 0.46              |
| 31:DG:125:PHE:HB3  | 31:DG:166:ASP:HB2  | 1.98                     | 0.46              |
| 32:DH:9:ILE:HG22   | 32:DH:51:ARG:CG    | 2.42                     | 0.46              |
| 33:DI:78:THR:O     | 33:DI:79:ILE:CB    | 2.63                     | 0.46              |
| 36:DP:56:SER:O     | 36:DP:57:THR:CB    | 2.63                     | 0.46              |
| 37:DQ:43:THR:OG1   | 37:DQ:45:GLN:HG2   | 2.16                     | 0.46              |
| 37:DQ:141:GLN:OXT  | 46:DZ:99:TYR:O     | 2.34                     | 0.46              |
| 41:DU:65:ILE:HG12  | 41:DU:96:ALA:HB1   | 1.98                     | 0.46              |
| 45:DY:91:GLU:O     | 45:DY:92:ASN:HB3   | 2.16                     | 0.46              |
| 50:D3:5:LYS:CG     | 50:D3:36:VAL:HG12  | 2.45                     | 0.46              |
| 51:D4:14:ILE:HG13  | 51:D4:31:ILE:CG2   | 2.39                     | 0.46              |
| 52:D5:6:VAL:HG22   | 52:D5:7:PRO:HD2    | 1.98                     | 0.46              |
| 55:D8:26:LYS:NZ    | 55:D8:47:LYS:HD3   | 2.31                     | 0.46              |
| 1:AA:1281:U:H6     | 1:AA:1281:U:O5'    | 1.98                     | 0.46              |
| 1:AA:1329:A:H5'    | 13:AM:29:ARG:NE    | 2.31                     | 0.46              |
| 3:AC:60:ALA:CB     | 3:AC:63:ASN:HD21   | 2.28                     | 0.46              |
| 5:AE:112:LEU:C     | 5:AE:114:GLY:N     | 2.70                     | 0.46              |
| 9:AI:8:GLY:O       | 9:AI:15:ALA:N      | 2.49                     | 0.46              |
| 10:AJ:56:HIS:O     | 10:AJ:58:ASP:N     | 2.48                     | 0.46              |
| 13:AM:60:VAL:C     | 13:AM:62:ASN:H     | 2.23                     | 0.46              |
| 16:AP:70:ALA:O     | 16:AP:71:ARG:C     | 2.59                     | 0.46              |
| 25:BA:832:G:H5'    | 36:BP:45:LEU:HD11  | 1.96                     | 0.46              |
| 25:BA:1264:G:H5'   | 52:B5:11:THR:OG1   | 2.16                     | 0.46              |
| 25:BA:1342:A:N7    | 25:BA:1397:U:C6    | 2.82                     | 0.46              |
| 25:BA:2078:C:O2'   | 25:BA:2079:U:H5'   | 2.15                     | 0.46              |
| 25:BA:2126:A:H1'   | 25:BA:2127:G:C1'   | 2.45                     | 0.46              |
| 25:BA:2402:C:H5    | 25:BA:2415:G:H22   | 1.64                     | 0.46              |
| 25:BA:2432:A:C4    | 48:B1:33:LYS:HG3   | 2.50                     | 0.46              |
| 25:BA:2876:G:O5'   | 40:BT:3:ARG:HA     | 2.16                     | 0.46              |
| 28:BD:79:VAL:HG12  | 28:BD:113:VAL:HA   | 1.97                     | 0.46              |
| 29:BE:165:VAL:HG13 | 29:BE:166:THR:N    | 2.31                     | 0.46              |
| 30:BF:89:VAL:C     | 30:BF:91:GLY:H     | 2.24                     | 0.46              |
| 31:BG:107:LEU:HD13 | 31:BG:177:GLY:O    | 2.16                     | 0.46              |
| 34:BN:47:ALA:HB2   | 34:BN:112:LEU:HD11 | 1.98                     | 0.46              |
| 34:BN:99:LEU:HD22  | 34:BN:103:VAL:CG2  | 2.45                     | 0.46              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 35:BO:122:LEU:HD23 | 40:BT:43:GLN:HE22 | 1.81                     | 0.46              |
| 36:BP:131:SER:O    | 36:BP:132:LYS:C   | 2.59                     | 0.46              |
| 40:BT:30:VAL:HG21  | 40:BT:84:GLN:CD   | 2.38                     | 0.46              |
| 41:BU:90:VAL:CG2   | 42:BV:47:VAL:HG21 | 2.45                     | 0.46              |
| 45:BY:81:LYS:HD3   | 45:BY:97:ARG:CB   | 2.33                     | 0.46              |
| 46:BZ:168:GLU:O    | 46:BZ:169:GLU:C   | 2.58                     | 0.46              |
| 53:B6:18:ARG:HD3   | 53:B6:18:ARG:N    | 2.30                     | 0.46              |
| 56:B9:29:ASN:HD22  | 56:B9:29:ASN:C    | 2.22                     | 0.46              |
| 1:CA:499:A:O2'     | 1:CA:500:G:C8     | 2.69                     | 0.46              |
| 1:CA:1162:C:H2'    | 1:CA:1163:C:C6    | 2.51                     | 0.46              |
| 1:CA:1478:C:H2'    | 1:CA:1479:C:C6    | 2.50                     | 0.46              |
| 9:CI:27:THR:O      | 9:CI:63:ILE:N     | 2.46                     | 0.46              |
| 10:CJ:37:PRO:HA    | 10:CJ:72:VAL:CG2  | 2.45                     | 0.46              |
| 11:CK:34:ASP:HB2   | 11:CK:35:PRO:CD   | 2.45                     | 0.46              |
| 11:CK:61:ALA:HA    | 11:CK:64:ALA:HB3  | 1.96                     | 0.46              |
| 13:CM:15:VAL:O     | 13:CM:19:LEU:HD23 | 2.15                     | 0.46              |
| 13:CM:120:LYS:HD3  | 13:CM:120:LYS:H   | 1.76                     | 0.46              |
| 15:CO:10:LYS:HG3   | 15:CO:11:VAL:H    | 1.79                     | 0.46              |
| 17:CQ:6:LEU:O      | 17:CQ:58:GLU:HA   | 2.15                     | 0.46              |
| 18:CR:50:ILE:CD1   | 18:CR:70:ILE:HG21 | 2.46                     | 0.46              |
| 19:CS:23:ASN:OD1   | 19:CS:44:MET:HE1  | 2.16                     | 0.46              |
| 19:CS:39:THR:HA    | 19:CS:70:LYS:HD3  | 1.97                     | 0.46              |
| 19:CS:40:ILE:HG21  | 19:CS:62:ILE:HD11 | 1.97                     | 0.46              |
| 20:CT:93:GLU:OE1   | 20:CT:94:ALA:N    | 2.49                     | 0.46              |
| 22:CV:20:G:C6      | 22:CV:58:A:C2     | 3.04                     | 0.46              |
| 25:DA:85:G:OP2     | 45:DY:9:LYS:HG3   | 2.15                     | 0.46              |
| 25:DA:528:A:O2'    | 25:DA:529:A:P     | 2.74                     | 0.46              |
| 25:DA:915:C:C4     | 25:DA:916:G:C5    | 3.03                     | 0.46              |
| 25:DA:956:G:C4'    | 37:DQ:83:MET:HE1  | 2.45                     | 0.46              |
| 25:DA:2402:C:H5    | 25:DA:2415:G:H22  | 1.64                     | 0.46              |
| 27:DC:49:ILE:HG22  | 27:DC:50:ASP:N    | 2.30                     | 0.46              |
| 28:DD:68:LYS:O     | 28:DD:68:LYS:HG3  | 2.15                     | 0.46              |
| 28:DD:183:ARG:HH11 | 28:DD:183:ARG:HG2 | 1.81                     | 0.46              |
| 30:DF:24:LEU:O     | 30:DF:25:PRO:C    | 2.58                     | 0.46              |
| 32:DH:89:ILE:HD12  | 32:DH:129:THR:O   | 2.15                     | 0.46              |
| 33:DI:9:LEU:O      | 33:DI:10:GLU:O    | 2.34                     | 0.46              |
| 33:DI:139:GLN:NE2  | 33:DI:139:GLN:O   | 2.48                     | 0.46              |
| 34:DN:28:THR:HG23  | 34:DN:29:LYS:HG3  | 1.98                     | 0.46              |
| 36:DP:71:VAL:HG23  | 36:DP:72:PRO:CD   | 2.45                     | 0.46              |
| 36:DP:84:ASN:N     | 36:DP:84:ASN:HD22 | 2.12                     | 0.46              |
| 36:DP:138:LEU:HD13 | 36:DP:144:GLU:HG2 | 1.98                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 37:DQ:25:ASP:OD2   | 46:DZ:78:LYS:HD2   | 2.16                     | 0.46              |
| 38:DR:74:LYS:HD2   | 38:DR:77:ARG:HH21  | 1.80                     | 0.46              |
| 38:DR:87:TYR:HE1   | 38:DR:117:VAL:O    | 1.99                     | 0.46              |
| 39:DS:62:LYS:HB3   | 39:DS:97:ARG:HD3   | 1.96                     | 0.46              |
| 40:DT:65:LYS:CD    | 40:DT:66:VAL:H     | 2.28                     | 0.46              |
| 41:DU:104:GLN:NE2  | 41:DU:104:GLN:CA   | 2.77                     | 0.46              |
| 41:DU:111:GLU:C    | 41:DU:113:ALA:N    | 2.72                     | 0.46              |
| 42:DV:30:GLY:N     | 42:DV:61:VAL:HG13  | 2.31                     | 0.46              |
| 43:DW:76:VAL:CG2   | 43:DW:102:HIS:O    | 2.64                     | 0.46              |
| 44:DX:27:THR:CG2   | 44:DX:80:ILE:HB    | 2.45                     | 0.46              |
| 46:DZ:124:ILE:HG23 | 46:DZ:165:VAL:CG2  | 2.45                     | 0.46              |
| 1:AA:413:G:N2      | 1:AA:429:U:OP2     | 2.40                     | 0.46              |
| 1:AA:1148:U:H2'    | 1:AA:1149:C:O4'    | 2.16                     | 0.46              |
| 2:AB:27:LYS:C      | 2:AB:29:ALA:H      | 2.24                     | 0.46              |
| 3:AC:21:ARG:O      | 3:AC:22:TRP:HD1    | 1.98                     | 0.46              |
| 4:AD:38:TYR:HD1    | 4:AD:38:TYR:O      | 1.99                     | 0.46              |
| 8:AH:29:SER:HB3    | 8:AH:32:LYS:CG     | 2.44                     | 0.46              |
| 11:AK:24:SER:OG    | 11:AK:25:TYR:N     | 2.47                     | 0.46              |
| 11:AK:82:VAL:CG1   | 11:AK:108:ILE:HG12 | 2.46                     | 0.46              |
| 15:AO:70:LEU:HD23  | 15:AO:78:TYR:HB2   | 1.98                     | 0.46              |
| 17:AQ:79:SER:O     | 17:AQ:80:GLY:O     | 2.33                     | 0.46              |
| 20:AT:71:THR:CG2   | 20:AT:72:LEU:H     | 2.08                     | 0.46              |
| 25:BA:320:A:H3'    | 30:BF:136:THR:HG22 | 1.96                     | 0.46              |
| 25:BA:679:C:H2'    | 25:BA:680:G:C8     | 2.51                     | 0.46              |
| 25:BA:954:G:H4'    | 37:BQ:13:GLN:NE2   | 2.31                     | 0.46              |
| 25:BA:1337:G:H2'   | 25:BA:1338:G:H8    | 1.81                     | 0.46              |
| 25:BA:1448:G:H5'   | 25:BA:1449:A:OP1   | 2.15                     | 0.46              |
| 25:BA:2074:U:H2'   | 25:BA:2075:U:C6    | 2.51                     | 0.46              |
| 25:BA:2355:C:H4'   | 47:B0:36:ILE:HD11  | 1.97                     | 0.46              |
| 25:BA:2431:U:N3    | 25:BA:2434:A:OP2   | 2.44                     | 0.46              |
| 29:BE:134:ILE:HB   | 29:BE:137:HIS:HB2  | 1.98                     | 0.46              |
| 35:BO:64:ARG:NH1   | 40:BT:70:VAL:HG21  | 2.31                     | 0.46              |
| 36:BP:85:LEU:HD22  | 36:BP:115:LEU:O    | 2.16                     | 0.46              |
| 41:BU:27:LEU:C     | 41:BU:34:LYS:HB3   | 2.41                     | 0.46              |
| 45:BY:61:ILE:O     | 45:BY:62:GLU:HB2   | 2.16                     | 0.46              |
| 47:B0:51:VAL:N     | 47:B0:62:LEU:HD12  | 2.30                     | 0.46              |
| 52:B5:40:LYS:NZ    | 52:B5:46:CYS:HB2   | 2.31                     | 0.46              |
| 53:B6:28:ARG:O     | 53:B6:29:ASN:C     | 2.59                     | 0.46              |
| 1:CA:100:C:C2'     | 1:CA:101:A:O4'     | 2.64                     | 0.46              |
| 1:CA:119:A:H4'     | 1:CA:120:A:OP2     | 2.15                     | 0.46              |
| 1:CA:123:C:OP1     | 1:CA:311:C:O2'     | 2.32                     | 0.46              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:CA:689:C:H2'    | 1:CA:690:G:O4'     | 2.16                     | 0.46              |
| 1:CA:1002:G:C2    | 1:CA:1003:G:H1'    | 2.51                     | 0.46              |
| 1:CA:1065:U:H4'   | 1:CA:1066:C:C4'    | 2.39                     | 0.46              |
| 1:CA:1359:C:OP1   | 14:CN:22:THR:OG1   | 2.32                     | 0.46              |
| 1:CA:1456:G:N3    | 1:CA:1456:G:H3'    | 2.31                     | 0.46              |
| 2:CB:84:GLU:HB3   | 2:CB:219:VAL:CG2   | 2.45                     | 0.46              |
| 2:CB:96:ARG:HH11  | 2:CB:148:TYR:HE1   | 1.63                     | 0.46              |
| 2:CB:187:LEU:HD23 | 2:CB:201:ILE:HG22  | 1.97                     | 0.46              |
| 3:CC:113:ALA:O    | 3:CC:116:VAL:N     | 2.49                     | 0.46              |
| 4:CD:18:LYS:HE3   | 4:CD:31:CYS:CB     | 2.46                     | 0.46              |
| 9:CI:58:HIS:HB2   | 9:CI:59:PHE:CD1    | 2.50                     | 0.46              |
| 10:CJ:17:ASP:OD1  | 10:CJ:70:ARG:NH1   | 2.49                     | 0.46              |
| 11:CK:126:ARG:HB3 | 11:CK:126:ARG:NH1  | 2.31                     | 0.46              |
| 13:CM:119:GLY:CA  | 13:CM:120:LYS:HD3  | 2.44                     | 0.46              |
| 15:CO:34:LEU:C    | 15:CO:34:LEU:HD12  | 2.41                     | 0.46              |
| 22:CV:3:C:H2'     | 22:CV:4:G:C5'      | 2.45                     | 0.46              |
| 25:DA:9274:U:O3'  | 25:DA:9275:C:H6    | 1.98                     | 0.46              |
| 25:DA:476:G:H4'   | 25:DA:502:A:N1     | 2.31                     | 0.46              |
| 25:DA:819:A:C5    | 25:DA:1189:A:C4    | 3.04                     | 0.46              |
| 25:DA:2689:U:O2'  | 25:DA:2690:C:OP2   | 2.30                     | 0.46              |
| 25:DA:2823:A:OP1  | 29:DE:113:PHE:HB2  | 2.16                     | 0.46              |
| 27:DC:64:LEU:O    | 27:DC:66:HIS:N     | 2.49                     | 0.46              |
| 27:DC:77:ILE:HG21 | 27:DC:123:VAL:N    | 2.31                     | 0.46              |
| 28:DD:245:PRO:O   | 28:DD:246:PRO:C    | 2.59                     | 0.46              |
| 37:DQ:25:ASP:OD2  | 46:DZ:78:LYS:CD    | 2.63                     | 0.46              |
| 37:DQ:26:TYR:CD1  | 37:DQ:26:TYR:C     | 2.94                     | 0.46              |
| 39:DS:56:LEU:HG   | 39:DS:58:LEU:HD22  | 1.98                     | 0.46              |
| 40:DT:50:ILE:O    | 40:DT:99:LEU:HD12  | 2.16                     | 0.46              |
| 41:DU:88:ILE:CD1  | 41:DU:109:LEU:HD22 | 2.42                     | 0.46              |
| 43:DW:88:ARG:HH11 | 43:DW:88:ARG:HG3   | 1.80                     | 0.46              |
| 49:D2:16:LEU:O    | 49:D2:17:SER:HB3   | 2.15                     | 0.46              |
| 52:D5:3:LYS:HD2   | 52:D5:3:LYS:HA     | 1.53                     | 0.46              |
| 55:D8:2:PRO:O     | 55:D8:3:LYS:C      | 2.58                     | 0.46              |
| 1:AA:335:C:O2'    | 1:AA:1433:A:N3     | 2.42                     | 0.46              |
| 1:AA:644:G:H5'    | 8:AH:92:ARG:HH22   | 1.80                     | 0.46              |
| 1:AA:1190:G:OP1   | 3:AC:5:ILE:HG13    | 2.16                     | 0.46              |
| 1:AA:1235:U:O2'   | 1:AA:1305:G:O5'    | 2.34                     | 0.46              |
| 1:AA:1392:G:N2    | 1:AA:1502:A:C8     | 2.82                     | 0.46              |
| 4:AD:8:VAL:O      | 4:AD:10:ARG:N      | 2.49                     | 0.46              |
| 4:AD:56:VAL:O     | 4:AD:59:ARG:N      | 2.49                     | 0.46              |
| 7:AG:85:TYR:CE1   | 7:AG:154:TYR:HE1   | 2.32                     | 0.46              |

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| Atom-1              | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|-------------------|--------------------------|-------------------|
| 10:AJ:63:PHE:HB3    | 14:AN:58:LYS:HA   | 1.98                     | 0.46              |
| 11:AK:98:LEU:O      | 11:AK:99:GLN:C    | 2.58                     | 0.46              |
| 14:AN:41:ARG:HG3    | 14:AN:42:ILE:H    | 1.79                     | 0.46              |
| 15:AO:67:LEU:O      | 15:AO:68:ARG:C    | 2.59                     | 0.46              |
| 16:AP:43:LYS:HG2    | 16:AP:48:TRP:CD2  | 2.51                     | 0.46              |
| 20:AT:33:ILE:CD1    | 20:AT:62:LEU:HB3  | 2.45                     | 0.46              |
| 25:BA:762:U:H4'     | 25:BA:763:G:O5'   | 2.16                     | 0.46              |
| 25:BA:1032:A:O3'    | 56:B9:16:VAL:HG11 | 2.15                     | 0.46              |
| 25:BA:1251:C:C3'    | 25:BA:1252:G:H5'' | 2.45                     | 0.46              |
| 27:BC:39:GLU:CD     | 27:BC:70:LYS:HZ3  | 2.24                     | 0.46              |
| 33:BI:65:ALA:O      | 33:BI:69:LYS:HB2  | 2.16                     | 0.46              |
| 35:BO:77:ILE:HD11   | 40:BT:72:VAL:HG11 | 1.98                     | 0.46              |
| 39:BS:47:THR:HG22   | 39:BS:49:VAL:O    | 2.16                     | 0.46              |
| 40:BT:3:ARG:C       | 40:BT:5:ALA:N     | 2.72                     | 0.46              |
| 43:BW:46:PHE:C      | 43:BW:48:ALA:N    | 2.74                     | 0.46              |
| 46:BZ:5:LEU:HD22    | 46:BZ:47:VAL:HG21 | 1.97                     | 0.46              |
| 49:B2:16:LEU:HA     | 49:B2:16:LEU:HD23 | 1.66                     | 0.46              |
| 1:CA:729:A:H2'      | 1:CA:730:G:H8     | 1.80                     | 0.46              |
| 1:CA:1389:C:H2'     | 1:CA:1390:U:O4'   | 2.16                     | 0.46              |
| 2:CB:155:LEU:CD1    | 2:CB:159:PRO:HD3  | 2.46                     | 0.46              |
| 5:CE:50:GLU:OE2     | 5:CE:51:VAL:HG23  | 2.15                     | 0.46              |
| 7:CG:149:ARG:O      | 7:CG:150:ALA:C    | 2.59                     | 0.46              |
| 8:CH:35:ILE:HG23    | 8:CH:111:ILE:HD12 | 1.97                     | 0.46              |
| 9:CI:65:VAL:HG21    | 9:CI:73:GLN:HB3   | 1.97                     | 0.46              |
| 10:CJ:67:THR:O      | 10:CJ:67:THR:OG1  | 2.31                     | 0.46              |
| 11:CK:32:ILE:CD1    | 11:CK:68:ALA:HB1  | 2.46                     | 0.46              |
| 13:CM:32:GLU:O      | 13:CM:35:GLU:HG2  | 2.16                     | 0.46              |
| 19:CS:45:VAL:HG23   | 19:CS:46:GLY:N    | 2.31                     | 0.46              |
| 19:CS:73:GLU:HB2    | 19:CS:74:PHE:CE2  | 2.51                     | 0.46              |
| 25:DA:242:G:HO2'    | 25:DA:243:U:P     | 2.38                     | 0.46              |
| 25:DA:271(M):G:H5'' | 33:DI:53:ALA:HB1  | 1.97                     | 0.46              |
| 25:DA:969:U:H2'     | 25:DA:970:C:C6    | 2.51                     | 0.46              |
| 25:DA:2317:C:H2'    | 25:DA:2318:G:H5'  | 1.98                     | 0.46              |
| 25:DA:2787:C:O2     | 29:DE:61:ARG:NH1  | 2.45                     | 0.46              |
| 26:DB:66:A:N1       | 26:DB:108:U:C2    | 2.84                     | 0.46              |
| 28:DD:94:LEU:C      | 28:DD:94:LEU:CD2  | 2.86                     | 0.46              |
| 28:DD:134:ARG:CG    | 28:DD:135:PHE:CE2 | 2.95                     | 0.46              |
| 32:DH:13:LYS:HA     | 32:DH:13:LYS:CE   | 2.30                     | 0.46              |
| 32:DH:26:VAL:CG1    | 32:DH:33:LEU:HB2  | 2.45                     | 0.46              |
| 36:DP:64:LYS:CB     | 55:D8:25:MET:HG3  | 2.38                     | 0.46              |
| 36:DP:123:LEU:HD23  | 36:DP:123:LEU:N   | 2.31                     | 0.46              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 40:DT:3:ARG:HH11    | 40:DT:6:LEU:HD12   | 1.81                     | 0.46              |
| 45:DY:8:LYS:O       | 45:DY:27:VAL:HG21  | 2.15                     | 0.46              |
| 45:DY:19:LYS:O      | 45:DY:19:LYS:CG    | 2.64                     | 0.46              |
| 46:DZ:28:MET:HB2    | 46:DZ:90:VAL:HG23  | 1.98                     | 0.46              |
| 49:D2:10:LEU:O      | 49:D2:14:ARG:CG    | 2.64                     | 0.46              |
| 49:D2:40:SER:C      | 49:D2:42:GLY:H     | 2.24                     | 0.46              |
| 1:AA:142:G:O2'      | 1:AA:196:A:N1      | 2.48                     | 0.46              |
| 1:AA:428:G:H4'      | 1:AA:429:U:O5'     | 2.16                     | 0.46              |
| 1:AA:992:U:HO2'     | 1:AA:993:G:P       | 2.39                     | 0.46              |
| 1:AA:1305:G:N2      | 1:AA:1331:G:H2'    | 2.30                     | 0.46              |
| 5:AE:61:TYR:HA      | 5:AE:64:ARG:HB3    | 1.97                     | 0.46              |
| 7:AG:49:ILE:HG22    | 7:AG:49:ILE:O      | 2.15                     | 0.46              |
| 7:AG:86:GLN:HB2     | 7:AG:148:ASN:HD22  | 1.79                     | 0.46              |
| 8:AH:121:ASP:OD1    | 8:AH:121:ASP:N     | 2.49                     | 0.46              |
| 9:AI:37:PHE:HB3     | 9:AI:43:ALA:CB     | 2.46                     | 0.46              |
| 11:AK:34:ASP:O      | 11:AK:35:PRO:C     | 2.57                     | 0.46              |
| 15:AO:48:LYS:HD3    | 15:AO:48:LYS:HA    | 1.65                     | 0.46              |
| 15:AO:67:LEU:O      | 15:AO:71:GLN:HB2   | 2.16                     | 0.46              |
| 20:AT:33:ILE:HD13   | 20:AT:62:LEU:HB3   | 1.97                     | 0.46              |
| 20:AT:93:GLU:O      | 20:AT:93:GLU:CG    | 2.64                     | 0.46              |
| 22:AV:34:U:H3       | 22:AV:36:A:H5''    | 1.80                     | 0.46              |
| 23:AW:16:U:H5       | 23:AW:18:G:O5'     | 2.00                     | 0.46              |
| 25:BA:311:A:O4'     | 25:BA:332:A:O4'    | 2.34                     | 0.46              |
| 25:BA:603:A:H1'     | 25:BA:604:G:O4'    | 2.15                     | 0.46              |
| 25:BA:627:A:N7      | 36:BP:84:ASN:ND2   | 2.62                     | 0.46              |
| 25:BA:727:A:N6      | 25:BA:728:G:N1     | 2.63                     | 0.46              |
| 25:BA:910:A:C8      | 37:BQ:13:GLN:HG3   | 2.51                     | 0.46              |
| 25:BA:1558:A:HO2'   | 25:BA:1559:G:P     | 2.39                     | 0.46              |
| 25:BA:2037:G:H2'    | 25:BA:2038:G:C8    | 2.51                     | 0.46              |
| 25:BA:2801(A):A:H4' | 25:BA:2802:G:H8    | 1.80                     | 0.46              |
| 28:BD:85:ASP:OD1    | 28:BD:87:ASN:ND2   | 2.48                     | 0.46              |
| 29:BE:21:VAL:HA     | 29:BE:22:PRO:HD2   | 1.52                     | 0.46              |
| 31:BG:17:PRO:HA     | 31:BG:20:ILE:HD12  | 1.97                     | 0.46              |
| 37:BQ:43:THR:HA     | 37:BQ:94:VAL:HA    | 1.98                     | 0.46              |
| 38:BR:59:ASP:OD2    | 38:BR:59:ASP:N     | 2.47                     | 0.46              |
| 39:BS:49:VAL:CG1    | 39:BS:50:SER:H     | 2.28                     | 0.46              |
| 40:BT:23:ARG:NH2    | 40:BT:120:ARG:HD3  | 2.31                     | 0.46              |
| 40:BT:32:TYR:HB3    | 40:BT:81:PRO:HB2   | 1.91                     | 0.46              |
| 40:BT:57:PHE:C      | 40:BT:59:THR:N     | 2.74                     | 0.46              |
| 45:BY:35:TYR:CE2    | 45:BY:69:ALA:HB3   | 2.51                     | 0.46              |
| 46:BZ:125:LEU:O     | 46:BZ:126:VAL:HG13 | 2.16                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 47:B0:42:GLY:O     | 47:B0:57:PHE:CG    | 2.69                     | 0.46              |
| 1:CA:262:A:H5'     | 20:CT:74:LYS:HG3   | 1.98                     | 0.46              |
| 1:CA:1352:C:OP1    | 21:CU:3:LYS:NZ     | 2.39                     | 0.46              |
| 1:CA:1397:C:H41    | 24:CX:22:A:H3'     | 1.81                     | 0.46              |
| 2:CB:188:ALA:C     | 2:CB:189:ASP:OD1   | 2.59                     | 0.46              |
| 2:CB:215:LEU:O     | 2:CB:218:ALA:HB3   | 2.16                     | 0.46              |
| 2:CB:220:ASP:O     | 2:CB:222:ILE:N     | 2.49                     | 0.46              |
| 3:CC:76:VAL:CG2    | 3:CC:77:ILE:N      | 2.79                     | 0.46              |
| 4:CD:104:VAL:O     | 4:CD:108:LEU:HD22  | 2.15                     | 0.46              |
| 4:CD:106:TYR:HE1   | 4:CD:112:VAL:O     | 1.98                     | 0.46              |
| 7:CG:49:ILE:HG22   | 7:CG:49:ILE:O      | 2.15                     | 0.46              |
| 8:CH:33:GLU:O      | 8:CH:36:LEU:N      | 2.48                     | 0.46              |
| 11:CK:41:THR:CG2   | 11:CK:42:TRP:N     | 2.78                     | 0.46              |
| 14:CN:39:LEU:CD1   | 14:CN:47:LEU:HD12  | 2.46                     | 0.46              |
| 20:CT:98:PRO:O     | 20:CT:100:ILE:N    | 2.50                     | 0.46              |
| 25:DA:443:A:N7     | 30:DF:45:ARG:HD2   | 2.31                     | 0.46              |
| 25:DA:598:G:O4'    | 36:DP:11:GLY:CA    | 2.64                     | 0.46              |
| 25:DA:613:G:C2     | 25:DA:615:G:C6     | 3.04                     | 0.46              |
| 25:DA:642:G:N2     | 25:DA:645:C:OP2    | 2.49                     | 0.46              |
| 25:DA:819:A:C8     | 25:DA:1189:A:C6    | 3.04                     | 0.46              |
| 25:DA:975(A):G:O2' | 25:DA:1156:A:N1    | 2.34                     | 0.46              |
| 25:DA:2415:G:O3'   | 36:DP:66:GLY:HA3   | 2.15                     | 0.46              |
| 28:DD:223:GLY:O    | 28:DD:226:MET:HG3  | 2.16                     | 0.46              |
| 31:DG:51:ARG:HB3   | 31:DG:51:ARG:NH1   | 2.31                     | 0.46              |
| 31:DG:77:ILE:HG22  | 31:DG:80:PHE:N     | 2.27                     | 0.46              |
| 31:DG:98:ARG:HA    | 31:DG:101:ILE:HG12 | 1.97                     | 0.46              |
| 32:DH:54:ARG:HB2   | 32:DH:55:PRO:HD2   | 1.97                     | 0.46              |
| 33:DI:9:LEU:C      | 33:DI:10:GLU:O     | 2.57                     | 0.46              |
| 33:DI:52:ARG:HG3   | 33:DI:53:ALA:N     | 2.31                     | 0.46              |
| 39:DS:74:ALA:O     | 39:DS:75:GLU:C     | 2.59                     | 0.46              |
| 41:DU:65:ILE:C     | 41:DU:67:ALA:N     | 2.74                     | 0.46              |
| 41:DU:92:ARG:NE    | 41:DU:95:LEU:HD12  | 2.30                     | 0.46              |
| 42:DV:39:LEU:N     | 42:DV:39:LEU:CD1   | 2.79                     | 0.46              |
| 46:DZ:51:ALA:O     | 46:DZ:52:SER:C     | 2.59                     | 0.46              |
| 48:D1:35:THR:CG2   | 48:D1:36:GLY:N     | 2.76                     | 0.46              |
| 53:D6:19:ARG:HD2   | 53:D6:19:ARG:N     | 2.31                     | 0.46              |
| 1:AA:129(A):G:C6   | 1:AA:189(E):U:H4'  | 2.51                     | 0.45              |
| 1:AA:1054:C:O2     | 1:AA:1054:C:C3'    | 2.64                     | 0.45              |
| 1:AA:1065:U:O2'    | 1:AA:1066:C:P      | 2.74                     | 0.45              |
| 1:AA:1292:U:H2'    | 1:AA:1293:G:C8     | 2.51                     | 0.45              |
| 2:AB:178:ARG:HH22  | 2:AB:196:LEU:CA    | 2.28                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:AD:153:ARG:HG2   | 4:AD:181:MET:SD    | 2.56                     | 0.45              |
| 10:AJ:9:ARG:O      | 10:AJ:94:VAL:HG13  | 2.16                     | 0.45              |
| 10:AJ:44:VAL:CG1   | 10:AJ:45:ARG:H     | 2.29                     | 0.45              |
| 11:AK:20:TYR:HA    | 11:AK:83:ILE:O     | 2.17                     | 0.45              |
| 15:AO:31:LEU:HD12  | 15:AO:31:LEU:HA    | 1.81                     | 0.45              |
| 20:AT:91:LEU:C     | 20:AT:93:GLU:N     | 2.74                     | 0.45              |
| 22:AV:31:G:C6      | 22:AV:32:G:N7      | 2.84                     | 0.45              |
| 25:BA:125:G:C2     | 54:B7:10:ARG:HA    | 2.52                     | 0.45              |
| 25:BA:726:G:C5'    | 25:BA:1432:C:O2'   | 2.64                     | 0.45              |
| 25:BA:1183:G:H4'   | 50:B3:29:ARG:HH12  | 1.81                     | 0.45              |
| 25:BA:1270:C:N3    | 25:BA:1648:C:N4    | 2.63                     | 0.45              |
| 25:BA:1754:C:N3    | 25:BA:2716:U:O2'   | 2.47                     | 0.45              |
| 25:BA:2346:A:HO2'  | 25:BA:2347:C:P     | 2.39                     | 0.45              |
| 28:BD:67:PHE:CZ    | 28:BD:157:ARG:CZ   | 2.99                     | 0.45              |
| 29:BE:103:ASP:CG   | 29:BE:201:THR:HA   | 2.41                     | 0.45              |
| 30:BF:22:ALA:C     | 30:BF:24:LEU:N     | 2.71                     | 0.45              |
| 30:BF:54:ARG:O     | 30:BF:54:ARG:CG    | 2.60                     | 0.45              |
| 30:BF:112:MET:O    | 30:BF:115:ALA:HB3  | 2.17                     | 0.45              |
| 31:BG:43:LEU:HD13  | 31:BG:43:LEU:H     | 1.76                     | 0.45              |
| 32:BH:65:HIS:O     | 32:BH:69:ARG:HD3   | 2.16                     | 0.45              |
| 32:BH:151:ILE:HD13 | 32:BH:151:ILE:H    | 1.75                     | 0.45              |
| 33:BI:104:GLN:O    | 33:BI:105:HIS:CG   | 2.69                     | 0.45              |
| 34:BN:26:LEU:CD2   | 34:BN:30:ILE:HD11  | 2.44                     | 0.45              |
| 35:BO:20:MET:HE3   | 35:BO:44:LYS:HE2   | 1.98                     | 0.45              |
| 35:BO:60:ALA:HA    | 35:BO:87:ILE:HG12  | 1.98                     | 0.45              |
| 36:BP:123:LEU:N    | 36:BP:123:LEU:HD23 | 2.31                     | 0.45              |
| 37:BQ:85:LYS:HG3   | 47:B0:7:LEU:CB     | 2.39                     | 0.45              |
| 39:BS:49:VAL:HG22  | 39:BS:80:LEU:HD22  | 1.98                     | 0.45              |
| 44:BX:23:GLU:C     | 44:BX:25:LYS:H     | 2.24                     | 0.45              |
| 44:BX:92:LEU:HD21  | 49:B2:37:PHE:CE2   | 2.51                     | 0.45              |
| 45:BY:12:THR:HG22  | 45:BY:13:VAL:N     | 2.30                     | 0.45              |
| 46:BZ:10:ARG:NH2   | 46:BZ:26:GLY:O     | 2.49                     | 0.45              |
| 47:B0:46:LYS:HB3   | 47:B0:47:PRO:HD2   | 1.98                     | 0.45              |
| 51:B4:61:VAL:O     | 51:B4:61:VAL:HG12  | 2.16                     | 0.45              |
| 55:B8:17:THR:HG23  | 55:B8:23:VAL:HG23  | 1.98                     | 0.45              |
| 1:CA:64:G:H5'      | 1:CA:66:G:OP1      | 2.17                     | 0.45              |
| 1:CA:119:A:C4'     | 1:CA:120:A:O5'     | 2.63                     | 0.45              |
| 1:CA:153:C:H42     | 1:CA:168:G:H1      | 1.64                     | 0.45              |
| 1:CA:173:U:H4'     | 1:CA:174:C:OP2     | 2.09                     | 0.45              |
| 1:CA:235:C:C5'     | 17:CQ:70:ARG:HG2   | 2.42                     | 0.45              |
| 1:CA:1443:G:N2     | 1:CA:1460:A:H1'    | 2.31                     | 0.45              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 2:CB:48:MET:CA     | 2:CB:51:LEU:HD12  | 2.43                     | 0.45              |
| 7:CG:70:LYS:HB3    | 7:CG:96:GLN:HG2   | 1.97                     | 0.45              |
| 9:CI:82:ALA:HA     | 9:CI:85:LEU:HD11  | 1.97                     | 0.45              |
| 10:CJ:62:HIS:O     | 14:CN:59:ALA:HB3  | 2.16                     | 0.45              |
| 11:CK:82:VAL:HG12  | 11:CK:108:ILE:HA  | 1.97                     | 0.45              |
| 12:CL:126:LYS:CG   | 12:CL:127:GLU:H   | 2.29                     | 0.45              |
| 16:CP:39:TYR:CD2   | 16:CP:73:LEU:HD11 | 2.50                     | 0.45              |
| 20:CT:98:PRO:C     | 20:CT:100:ILE:N   | 2.71                     | 0.45              |
| 25:DA:1028:A:N3    | 25:DA:2486:G:O2'  | 2.42                     | 0.45              |
| 25:DA:1824:G:OP1   | 28:DD:52:ARG:NH1  | 2.49                     | 0.45              |
| 28:DD:260:ARG:HD3  | 28:DD:261:LYS:O   | 2.16                     | 0.45              |
| 30:DF:194:MET:HE3  | 30:DF:199:TRP:CE3 | 2.50                     | 0.45              |
| 32:DH:19:VAL:CG1   | 32:DH:20:ALA:N    | 2.79                     | 0.45              |
| 34:DN:57:ALA:O     | 34:DN:58:ASP:C    | 2.58                     | 0.45              |
| 38:DR:63:ARG:O     | 38:DR:67:LEU:HB2  | 2.17                     | 0.45              |
| 39:DS:38:GLN:HG3   | 39:DS:47:THR:CG2  | 2.46                     | 0.45              |
| 43:DW:88:ARG:HG3   | 43:DW:88:ARG:NH1  | 2.31                     | 0.45              |
| 43:DW:111:HIS:CG   | 43:DW:112:GLY:N   | 2.77                     | 0.45              |
| 46:DZ:119:GLU:OE2  | 46:DZ:122:ARG:HB3 | 2.16                     | 0.45              |
| 46:DZ:125:LEU:HD12 | 46:DZ:126:VAL:H   | 1.80                     | 0.45              |
| 50:D3:8:LEU:CD1    | 50:D3:31:LEU:HD23 | 2.46                     | 0.45              |
| 50:D3:19:GLN:HE22  | 50:D3:52:HIS:HE1  | 1.63                     | 0.45              |
| 55:D8:26:LYS:HD3   | 55:D8:26:LYS:HA   | 1.83                     | 0.45              |
| 1:AA:8:A:H1'       | 5:AE:102:ALA:O    | 2.16                     | 0.45              |
| 1:AA:243:A:N6      | 1:AA:281:G:H1'    | 2.31                     | 0.45              |
| 1:AA:520:A:N1      | 1:AA:536:C:H1'    | 2.32                     | 0.45              |
| 1:AA:662:G:H2'     | 1:AA:663:A:C8     | 2.52                     | 0.45              |
| 1:AA:1317:C:N3     | 19:AS:37:ARG:NH2  | 2.58                     | 0.45              |
| 1:AA:1321:C:H4'    | 13:AM:87:TYR:CE2  | 2.51                     | 0.45              |
| 1:AA:1349:A:OP2    | 9:AI:118:LYS:NZ   | 2.48                     | 0.45              |
| 3:AC:15:THR:CG2    | 3:AC:181:ASN:HA   | 2.40                     | 0.45              |
| 5:AE:131:ILE:HG22  | 5:AE:132:ALA:N    | 2.31                     | 0.45              |
| 6:AF:14:LEU:HB2    | 6:AF:19:LEU:HD12  | 1.99                     | 0.45              |
| 7:AG:6:ARG:C       | 7:AG:7:ALA:O      | 2.59                     | 0.45              |
| 11:AK:31:THR:OG1   | 11:AK:42:TRP:HB3  | 2.16                     | 0.45              |
| 12:AL:126:LYS:C    | 12:AL:128:ALA:H   | 2.25                     | 0.45              |
| 13:AM:68:GLY:O     | 13:AM:71:ARG:HB3  | 2.15                     | 0.45              |
| 20:AT:20:LEU:O     | 20:AT:23:ARG:N    | 2.49                     | 0.45              |
| 25:BA:479:A:H4'    | 25:BA:480:A:O5'   | 2.16                     | 0.45              |
| 25:BA:1022:G:O2'   | 25:BA:1023:U:OP2  | 2.34                     | 0.45              |
| 25:BA:1952:A:OP1   | 35:BO:44:LYS:NZ   | 2.50                     | 0.45              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 25:BA:2052:G:H4'   | 29:BE:143:ASN:O   | 2.16                     | 0.45              |
| 25:BA:2061:G:H2'   | 25:BA:2501:C:O2'  | 2.16                     | 0.45              |
| 25:BA:2517:C:HO2'  | 25:BA:2518:A:P    | 2.40                     | 0.45              |
| 31:BG:48:GLU:O     | 31:BG:49:ASP:HB2  | 2.16                     | 0.45              |
| 31:BG:60:LEU:HD12  | 31:BG:92:VAL:HG11 | 1.99                     | 0.45              |
| 31:BG:76:SER:HA    | 31:BG:83:ARG:HB2  | 1.98                     | 0.45              |
| 31:BG:82:LEU:HD22  | 31:BG:87:PRO:HB3  | 1.98                     | 0.45              |
| 32:BH:40:GLU:O     | 32:BH:42:ARG:N    | 2.47                     | 0.45              |
| 32:BH:61:HIS:O     | 32:BH:62:LYS:C    | 2.59                     | 0.45              |
| 35:BO:73:ASP:OD1   | 35:BO:73:ASP:C    | 2.58                     | 0.45              |
| 36:BP:112:LEU:HD22 | 36:BP:112:LEU:C   | 2.41                     | 0.45              |
| 39:BS:12:PHE:CE1   | 39:BS:14:VAL:HG23 | 2.50                     | 0.45              |
| 41:BU:90:VAL:HG21  | 42:BV:47:VAL:HG21 | 1.99                     | 0.45              |
| 46:BZ:53:ILE:HG21  | 46:BZ:71:VAL:HB   | 1.95                     | 0.45              |
| 48:B1:25:LYS:O     | 48:B1:27:GLU:O    | 2.34                     | 0.45              |
| 48:B1:48:LYS:HG3   | 48:B1:61:ARG:HG2  | 1.98                     | 0.45              |
| 53:B6:42:TRP:HA    | 53:B6:42:TRP:HE3  | 1.81                     | 0.45              |
| 1:CA:76:C:N4       | 1:CA:93:G:H1      | 2.10                     | 0.45              |
| 1:CA:222:U:H2'     | 1:CA:223:U:C6     | 2.51                     | 0.45              |
| 1:CA:599:C:H4'     | 8:CH:130:GLY:O    | 2.16                     | 0.45              |
| 1:CA:1134:G:N2     | 1:CA:1141:C:C2    | 2.84                     | 0.45              |
| 1:CA:1293:G:H2'    | 1:CA:1294:G:H8    | 1.81                     | 0.45              |
| 1:CA:1356:G:H2'    | 1:CA:1357:A:C8    | 2.52                     | 0.45              |
| 1:CA:1380:U:C4     | 7:CG:3:ARG:HG3    | 2.51                     | 0.45              |
| 6:CF:1:MET:H1      | 6:CF:68:PRO:HA    | 1.81                     | 0.45              |
| 7:CG:149:ARG:O     | 7:CG:152:ALA:HB2  | 2.16                     | 0.45              |
| 9:CI:16:ARG:HE     | 9:CI:64:THR:CG2   | 2.29                     | 0.45              |
| 9:CI:102:LEU:O     | 9:CI:103:THR:OG1  | 2.30                     | 0.45              |
| 10:CJ:32:ALA:CB    | 10:CJ:76:ASN:HB3  | 2.46                     | 0.45              |
| 10:CJ:89:ASP:C     | 10:CJ:91:PRO:HD3  | 2.42                     | 0.45              |
| 12:CL:7:ILE:HD13   | 12:CL:7:ILE:HA    | 1.83                     | 0.45              |
| 12:CL:87:GLY:H     | 12:CL:98:TYR:HB3  | 1.81                     | 0.45              |
| 13:CM:88:ARG:O     | 13:CM:88:ARG:HD2  | 2.15                     | 0.45              |
| 17:CQ:29:HIS:C     | 17:CQ:31:LEU:N    | 2.74                     | 0.45              |
| 23:CW:15:G:H22     | 23:CW:59:U:H1'    | 1.81                     | 0.45              |
| 25:DA:8:A:H2'      | 25:DA:9:U:H6      | 1.80                     | 0.45              |
| 25:DA:92:A:H2'     | 25:DA:93:G:H8     | 1.81                     | 0.45              |
| 25:DA:605:C:O2     | 25:DA:657:U:O2'   | 2.34                     | 0.45              |
| 25:DA:1331:A:O2'   | 25:DA:1332:G:H8   | 2.00                     | 0.45              |
| 25:DA:2030:A:H4'   | 25:DA:2031:A:C8   | 2.50                     | 0.45              |
| 25:DA:2747:G:O6    | 25:DA:2755:C:H5'' | 2.15                     | 0.45              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 28:DD:13:ARG:HG2   | 28:DD:13:ARG:O      | 2.16                     | 0.45              |
| 30:DF:117:ARG:HH21 | 30:DF:187:VAL:HA    | 1.81                     | 0.45              |
| 36:DP:21:ARG:O     | 36:DP:22:GLY:O      | 2.35                     | 0.45              |
| 36:DP:95:VAL:HA    | 36:DP:99:LEU:HD23   | 1.97                     | 0.45              |
| 40:DT:3:ARG:CB     | 40:DT:6:LEU:HB2     | 2.46                     | 0.45              |
| 41:DU:92:ARG:HH22  | 41:DU:94:ASN:HD22   | 1.49                     | 0.45              |
| 48:D1:67:ILE:N     | 48:D1:68:PRO:CD     | 2.77                     | 0.45              |
| 51:D4:9:LEU:HG     | 51:D4:26:SER:O      | 2.16                     | 0.45              |
| 55:D8:32:LEU:CD2   | 55:D8:32:LEU:H      | 2.28                     | 0.45              |
| 1:AA:377:G:OP1     | 16:AP:3:LYS:HE3     | 2.17                     | 0.45              |
| 1:AA:426:G:H4'     | 4:AD:41:GLY:O       | 2.16                     | 0.45              |
| 1:AA:1060:C:OP1    | 14:AN:45:ARG:NH2    | 2.50                     | 0.45              |
| 1:AA:1321:C:H3'    | 1:AA:1322:C:H5''    | 1.98                     | 0.45              |
| 2:AB:24:TRP:HB3    | 2:AB:40:HIS:NE2     | 2.31                     | 0.45              |
| 2:AB:157:ARG:O     | 2:AB:158:LEU:C      | 2.59                     | 0.45              |
| 3:AC:86:VAL:O      | 3:AC:90:GLU:HG2     | 2.16                     | 0.45              |
| 5:AE:6:PHE:HB3     | 5:AE:35:GLY:O       | 2.16                     | 0.45              |
| 5:AE:11:ILE:HG22   | 5:AE:12:LEU:HB2     | 1.97                     | 0.45              |
| 7:AG:10:ARG:CG     | 7:AG:10:ARG:NH1     | 2.71                     | 0.45              |
| 8:AH:32:LYS:O      | 8:AH:33:GLU:C       | 2.59                     | 0.45              |
| 11:AK:124:LYS:CD   | 11:AK:125:PHE:HE1   | 2.26                     | 0.45              |
| 12:AL:110:VAL:O    | 12:AL:111:LYS:C     | 2.60                     | 0.45              |
| 13:AM:37:THR:HG21  | 13:AM:56:LEU:HD22   | 1.98                     | 0.45              |
| 18:AR:37:VAL:HG12  | 18:AR:79:LEU:HD21   | 1.98                     | 0.45              |
| 19:AS:24:ALA:O     | 19:AS:25:LYS:HB2    | 2.16                     | 0.45              |
| 20:AT:89:ARG:HB2   | 20:AT:104:LEU:CD1   | 2.44                     | 0.45              |
| 22:AV:60:A:H2'     | 22:AV:61:U:H5'      | 1.97                     | 0.45              |
| 25:BA:227:A:H5''   | 25:BA:228:A:OP1     | 2.16                     | 0.45              |
| 25:BA:272:G:H4'    | 25:BA:272(A):U:H5'' | 1.98                     | 0.45              |
| 25:BA:1042:G:N3    | 25:BA:1042:G:H2'    | 2.31                     | 0.45              |
| 25:BA:2689:U:H5'   | 25:BA:2689:U:H6     | 1.76                     | 0.45              |
| 25:BA:2847:U:H5    | 25:BA:2848:G:C6     | 2.27                     | 0.45              |
| 28:BD:68:LYS:O     | 28:BD:68:LYS:HG3    | 2.16                     | 0.45              |
| 29:BE:93:VAL:HG21  | 29:BE:180:ASN:O     | 2.16                     | 0.45              |
| 30:BF:20:LEU:HB3   | 30:BF:23:ASP:OD2    | 2.16                     | 0.45              |
| 30:BF:64:ILE:HD13  | 30:BF:64:ILE:HA     | 1.71                     | 0.45              |
| 33:BI:9:LEU:H      | 33:BI:13:GLY:HA2    | 1.82                     | 0.45              |
| 34:BN:58:ASP:C     | 34:BN:60:ILE:N      | 2.65                     | 0.45              |
| 38:BR:76:VAL:O     | 38:BR:80:PHE:HB2    | 2.16                     | 0.45              |
| 42:BV:23:GLU:O     | 42:BV:24:LYS:C      | 2.58                     | 0.45              |
| 46:BZ:99:TYR:HB3   | 46:BZ:123:ASP:OD1   | 2.16                     | 0.45              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 48:B1:12:PRO:HA   | 48:B1:42:GLN:O     | 2.17                     | 0.45              |
| 55:B8:50:LEU:HA   | 55:B8:53:PRO:CG    | 2.46                     | 0.45              |
| 1:CA:992:U:HO2'   | 1:CA:993:G:P       | 2.38                     | 0.45              |
| 2:CB:88:ALA:HB2   | 2:CB:219:VAL:HG12  | 1.98                     | 0.45              |
| 4:CD:8:VAL:O      | 4:CD:11:LEU:N      | 2.37                     | 0.45              |
| 4:CD:54:TYR:OH    | 4:CD:209:ARG:NH1   | 2.49                     | 0.45              |
| 5:CE:10:MET:HB2   | 5:CE:32:VAL:HG22   | 1.97                     | 0.45              |
| 9:CI:114:TYR:N    | 9:CI:114:TYR:HD2   | 2.14                     | 0.45              |
| 19:CS:43:GLU:C    | 19:CS:45:VAL:N     | 2.74                     | 0.45              |
| 19:CS:44:MET:N    | 19:CS:44:MET:SD    | 2.89                     | 0.45              |
| 20:CT:52:ALA:O    | 20:CT:56:MET:N     | 2.41                     | 0.45              |
| 20:CT:53:LEU:CB   | 20:CT:102:GLY:HA3  | 2.45                     | 0.45              |
| 20:CT:88:VAL:HG12 | 20:CT:89:ARG:N     | 2.31                     | 0.45              |
| 22:CV:41:C:O2'    | 22:CV:42:C:C5'     | 2.42                     | 0.45              |
| 25:DA:371:A:H1'   | 25:DA:373:U:C6     | 2.51                     | 0.45              |
| 25:DA:532:A:O2'   | 25:DA:2021:C:N4    | 2.49                     | 0.45              |
| 25:DA:604:G:C6    | 25:DA:605:C:C4     | 3.05                     | 0.45              |
| 25:DA:635:C:H2'   | 25:DA:636:G:O4'    | 2.17                     | 0.45              |
| 25:DA:1008:C:H5'' | 25:DA:1009:A:OP1   | 2.16                     | 0.45              |
| 25:DA:1240:U:O2'  | 25:DA:1241:A:H5'   | 2.16                     | 0.45              |
| 25:DA:1365:A:OP1  | 48:D1:41:ARG:NH1   | 2.49                     | 0.45              |
| 25:DA:2683:C:OP1  | 40:DT:53:ARG:NH2   | 2.45                     | 0.45              |
| 27:DC:61:THR:HG22 | 27:DC:163:PHE:O    | 2.17                     | 0.45              |
| 29:DE:116:VAL:O   | 29:DE:117:MET:CB   | 2.65                     | 0.45              |
| 33:DI:21:VAL:O    | 33:DI:22:LYS:C     | 2.59                     | 0.45              |
| 35:DO:7:TYR:CZ    | 35:DO:44:LYS:HG3   | 2.51                     | 0.45              |
| 36:DP:85:LEU:HD22 | 36:DP:115:LEU:O    | 2.16                     | 0.45              |
| 36:DP:110:TYR:HD2 | 36:DP:111:ARG:HH21 | 1.64                     | 0.45              |
| 40:DT:32:TYR:OH   | 40:DT:76:PHE:CD2   | 2.70                     | 0.45              |
| 41:DU:78:THR:O    | 41:DU:79:PHE:C     | 2.58                     | 0.45              |
| 41:DU:112:ARG:NH1 | 41:DU:112:ARG:CG   | 2.76                     | 0.45              |
| 43:DW:52:GLU:HA   | 43:DW:52:GLU:OE2   | 2.17                     | 0.45              |
| 45:DY:9:LYS:HA    | 45:DY:27:VAL:CG2   | 2.46                     | 0.45              |
| 45:DY:9:LYS:HE3   | 45:DY:28:LYS:O     | 2.16                     | 0.45              |
| 48:D1:64:ALA:O    | 48:D1:66:HIS:N     | 2.50                     | 0.45              |
| 51:D4:7:PRO:O     | 51:D4:8:LYS:C      | 2.58                     | 0.45              |
| 55:D8:21:LYS:HD3  | 55:D8:48:PHE:CZ    | 2.52                     | 0.45              |
| 55:D8:23:VAL:CG1  | 55:D8:46:ARG:HB3   | 2.47                     | 0.45              |
| 1:AA:9:G:H2'      | 1:AA:10:A:C8       | 2.46                     | 0.45              |
| 1:AA:344:A:H5''   | 1:AA:345:C:OP2     | 2.17                     | 0.45              |
| 1:AA:1060:C:H4'   | 10:AJ:52:GLY:H     | 1.80                     | 0.45              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 2:AB:51:LEU:HD22   | 2:AB:55:PHE:HE2     | 1.80                     | 0.45              |
| 2:AB:219:VAL:O     | 2:AB:220:ASP:C      | 2.59                     | 0.45              |
| 4:AD:110:PHE:N     | 4:AD:110:PHE:CD1    | 2.84                     | 0.45              |
| 4:AD:126:ILE:HG22  | 4:AD:127:THR:N      | 2.31                     | 0.45              |
| 5:AE:13:ILE:O      | 5:AE:13:ILE:HG22    | 2.14                     | 0.45              |
| 5:AE:107:ARG:NH1   | 5:AE:107:ARG:HB2    | 2.31                     | 0.45              |
| 6:AF:72:VAL:CG1    | 6:AF:73:ASN:N       | 2.73                     | 0.45              |
| 12:AL:55:VAL:HG12  | 12:AL:56:ALA:N      | 2.32                     | 0.45              |
| 13:AM:46:LYS:HG3   | 13:AM:47:ASP:OD1    | 2.17                     | 0.45              |
| 22:AV:40:C:C2      | 22:AV:41:C:C5       | 3.04                     | 0.45              |
| 23:AW:12:U:C2      | 23:AW:24:G:N2       | 2.84                     | 0.45              |
| 23:AY:38:A:H2'     | 23:AY:39:U:C6       | 2.51                     | 0.45              |
| 25:BA:30:G:H2'     | 25:BA:31:C:C6       | 2.52                     | 0.45              |
| 25:BA:240:G:C6     | 25:BA:241:A:C6      | 3.05                     | 0.45              |
| 25:BA:727:A:N6     | 25:BA:728:G:O6      | 2.48                     | 0.45              |
| 25:BA:729:G:O5'    | 28:BD:208:LYS:NZ    | 2.43                     | 0.45              |
| 25:BA:1548:C:N4    | 25:BA:1549:C:N4     | 2.64                     | 0.45              |
| 25:BA:2285:C:C5    | 53:B6:27:LYS:HE3    | 2.51                     | 0.45              |
| 25:BA:2415:G:H4'   | 36:BP:66:GLY:C      | 2.41                     | 0.45              |
| 25:BA:2632:A:O2'   | 29:BE:61:ARG:NH2    | 2.49                     | 0.45              |
| 25:BA:2801:A:H4'   | 25:BA:2801(A):A:O5' | 2.17                     | 0.45              |
| 26:BB:14:U:C3'     | 26:BB:14:U:C6       | 3.00                     | 0.45              |
| 28:BD:84:TYR:CD2   | 28:BD:84:TYR:C      | 2.94                     | 0.45              |
| 29:BE:32:PRO:HB3   | 29:BE:69:LYS:HD2    | 1.98                     | 0.45              |
| 30:BF:17:ARG:CG    | 30:BF:17:ARG:NH1    | 2.72                     | 0.45              |
| 30:BF:51:THR:HG23  | 30:BF:92:PRO:C      | 2.41                     | 0.45              |
| 30:BF:54:ARG:O     | 30:BF:54:ARG:HG3    | 2.16                     | 0.45              |
| 31:BG:161:THR:HG22 | 31:BG:162:THR:N     | 2.31                     | 0.45              |
| 34:BN:16:ILE:CG2   | 34:BN:54:VAL:HG22   | 2.46                     | 0.45              |
| 34:BN:70:LYS:HG3   | 34:BN:71:ILE:N      | 2.30                     | 0.45              |
| 36:BP:97:PRO:O     | 36:BP:98:GLU:CB     | 2.62                     | 0.45              |
| 39:BS:49:VAL:CG1   | 39:BS:50:SER:N      | 2.78                     | 0.45              |
| 40:BT:50:ILE:HD12  | 40:BT:50:ILE:HA     | 1.77                     | 0.45              |
| 40:BT:72:VAL:HG12  | 40:BT:73:GLU:N      | 2.32                     | 0.45              |
| 41:BU:117:GLN:O    | 41:BU:118:GLY:C     | 2.59                     | 0.45              |
| 42:BV:5:VAL:HG11   | 42:BV:57:VAL:HG11   | 1.96                     | 0.45              |
| 43:BW:79:GLY:C     | 43:BW:100:THR:HG22  | 2.41                     | 0.45              |
| 45:BY:52:SER:O     | 45:BY:53:PRO:C      | 2.60                     | 0.45              |
| 46:BZ:40:ASP:OD1   | 46:BZ:42:VAL:HG12   | 2.16                     | 0.45              |
| 48:B1:57:GLU:C     | 48:B1:58:ILE:CG2    | 2.89                     | 0.45              |
| 1:CA:344:A:H5''    | 1:CA:345:C:P        | 2.56                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:791:G:C2'     | 1:CA:792:A:H5'     | 2.43                     | 0.45              |
| 1:CA:946:A:H2'     | 1:CA:947:G:H8      | 1.82                     | 0.45              |
| 1:CA:1005:A:O2'    | 1:CA:1037:C:O2'    | 2.27                     | 0.45              |
| 2:CB:72:GLY:HA2    | 2:CB:165:VAL:CG2   | 2.45                     | 0.45              |
| 2:CB:113:HIS:C     | 2:CB:115:LEU:H     | 2.25                     | 0.45              |
| 4:CD:25:ARG:NH2    | 4:CD:30:LYS:HD2    | 2.30                     | 0.45              |
| 4:CD:148:VAL:HG21  | 4:CD:158:ILE:CG2   | 2.45                     | 0.45              |
| 5:CE:33:VAL:HG21   | 5:CE:109:ILE:CG1   | 2.46                     | 0.45              |
| 7:CG:108:ALA:HB1   | 7:CG:120:ILE:HD13  | 1.97                     | 0.45              |
| 10:CJ:45:ARG:NH1   | 10:CJ:45:ARG:CG    | 2.74                     | 0.45              |
| 12:CL:117:ARG:HD2  | 12:CL:122:THR:HG22 | 1.98                     | 0.45              |
| 16:CP:36:ILE:HG13  | 16:CP:37:GLY:N     | 2.31                     | 0.45              |
| 17:CQ:22:LEU:HD22  | 17:CQ:88:TYR:HD1   | 1.82                     | 0.45              |
| 20:CT:23:ARG:CA    | 20:CT:26:ASN:OD1   | 2.55                     | 0.45              |
| 21:CU:3:LYS:HE3    | 21:CU:3:LYS:HB2    | 1.66                     | 0.45              |
| 23:CW:49:C:H42     | 23:CW:65:G:H1      | 1.64                     | 0.45              |
| 25:DA:94(A):G:N3   | 49:D2:47:ASN:ND2   | 2.64                     | 0.45              |
| 25:DA:250:G:OP2    | 55:D8:13:ARG:NH2   | 2.49                     | 0.45              |
| 25:DA:483:A:H3'    | 25:DA:484:C:H6     | 1.81                     | 0.45              |
| 25:DA:2580:U:H4'   | 29:DE:130:GLY:CA   | 2.47                     | 0.45              |
| 26:DB:15:A:H1'     | 26:DB:110:G:C4     | 2.51                     | 0.45              |
| 28:DD:158:ALA:HB3  | 28:DD:161:THR:CG2  | 2.46                     | 0.45              |
| 28:DD:224:ALA:O    | 28:DD:225:ALA:CB   | 2.64                     | 0.45              |
| 30:DF:132:VAL:HG23 | 30:DF:133:ASN:N    | 2.31                     | 0.45              |
| 31:DG:39:ILE:HB    | 31:DG:92:VAL:CG1   | 2.47                     | 0.45              |
| 32:DH:166:GLY:O    | 32:DH:167:GLU:C    | 2.59                     | 0.45              |
| 33:DI:94:ALA:C     | 33:DI:96:ASP:N     | 2.73                     | 0.45              |
| 36:DP:86:LYS:HB3   | 36:DP:117:GLU:O    | 2.16                     | 0.45              |
| 36:DP:112:LEU:HD22 | 36:DP:112:LEU:C    | 2.41                     | 0.45              |
| 37:DQ:84:GLY:O     | 37:DQ:85:LYS:HB2   | 2.16                     | 0.45              |
| 40:DT:118:ARG:O    | 40:DT:121:ILE:N    | 2.49                     | 0.45              |
| 41:DU:111:GLU:O    | 41:DU:112:ARG:C    | 2.58                     | 0.45              |
| 46:DZ:15:PRO:O     | 46:DZ:19:ARG:HG3   | 2.17                     | 0.45              |
| 46:DZ:150:LEU:C    | 46:DZ:150:LEU:HD22 | 2.41                     | 0.45              |
| 53:D6:24:GLU:O     | 53:D6:25:LYS:HB2   | 2.15                     | 0.45              |
| 54:D7:12:ARG:HG3   | 54:D7:12:ARG:HH11  | 1.80                     | 0.45              |
| 1:AA:815:A:N6      | 1:AA:1509:C:H1'    | 2.32                     | 0.45              |
| 1:AA:1226:C:O5'    | 1:AA:1226:C:H6     | 1.99                     | 0.45              |
| 1:AA:1256:A:OP2    | 3:AC:26:LYS:NZ     | 2.48                     | 0.45              |
| 2:AB:96:ARG:HH12   | 2:AB:147:LYS:CE    | 2.28                     | 0.45              |
| 2:AB:105:PHE:CD2   | 2:AB:158:LEU:HG    | 2.51                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:AB:111:ARG:HH11 | 2:AB:111:ARG:CG   | 2.23                     | 0.45              |
| 4:AD:9:CYS:HB2    | 4:AD:22:LYS:HZ2   | 1.80                     | 0.45              |
| 6:AF:19:LEU:O     | 6:AF:23:LYS:HG3   | 2.17                     | 0.45              |
| 7:AG:54:THR:OG1   | 7:AG:56:GLN:HG2   | 2.16                     | 0.45              |
| 8:AH:89:PRO:HA    | 8:AH:92:ARG:NH1   | 2.31                     | 0.45              |
| 13:AM:86:CYS:HB2  | 19:AS:73:GLU:OE1  | 2.16                     | 0.45              |
| 16:AP:58:TYR:O    | 16:AP:61:SER:HB3  | 2.16                     | 0.45              |
| 16:AP:73:LEU:HD23 | 16:AP:73:LEU:N    | 2.31                     | 0.45              |
| 22:AV:64:G:N1     | 22:AV:65:G:C5     | 2.85                     | 0.45              |
| 25:BA:1300:U:C5'  | 25:BA:1301:A:O5'  | 2.65                     | 0.45              |
| 25:BA:1344:G:HO2' | 25:BA:1385:G:H5'' | 1.80                     | 0.45              |
| 25:BA:1464:C:H2'  | 25:BA:1465:G:C8   | 2.51                     | 0.45              |
| 25:BA:1889:A:N1   | 25:BA:2234:G:H1'  | 2.31                     | 0.45              |
| 25:BA:2051:A:H2'  | 25:BA:2614:A:H61  | 1.82                     | 0.45              |
| 25:BA:2335:A:HO2' | 25:BA:2336:A:P    | 2.40                     | 0.45              |
| 25:BA:2813:A:H2'  | 25:BA:2814:C:O4'  | 2.16                     | 0.45              |
| 25:BA:2835:A:N6   | 25:BA:2879:C:O4'  | 2.50                     | 0.45              |
| 26:BB:45:A:H1'    | 31:BG:95:ARG:CZ   | 2.46                     | 0.45              |
| 26:BB:66:A:N6     | 26:BB:108:U:C4    | 2.85                     | 0.45              |
| 27:BC:77:ILE:HB   | 27:BC:121:GLY:O   | 2.17                     | 0.45              |
| 31:BG:117:PHE:C   | 31:BG:117:PHE:CD1 | 2.94                     | 0.45              |
| 34:BN:62:VAL:O    | 34:BN:63:THR:C    | 2.60                     | 0.45              |
| 38:BR:18:LEU:HD23 | 38:BR:18:LEU:HA   | 1.47                     | 0.45              |
| 40:BT:92:GLY:O    | 40:BT:114:LEU:HA  | 2.16                     | 0.45              |
| 42:BV:24:LYS:HG2  | 42:BV:90:PRO:HB2  | 1.98                     | 0.45              |
| 42:BV:52:VAL:HG13 | 42:BV:55:ALA:HB3  | 1.99                     | 0.45              |
| 42:BV:74:LYS:HB2  | 42:BV:83:ARG:HB2  | 1.99                     | 0.45              |
| 43:BW:57:ASN:C    | 43:BW:59:VAL:N    | 2.70                     | 0.45              |
| 43:BW:84:ARG:HB2  | 43:BW:96:ILE:HG23 | 1.99                     | 0.45              |
| 49:B2:10:LEU:O    | 49:B2:14:ARG:HG3  | 2.17                     | 0.45              |
| 49:B2:16:LEU:O    | 49:B2:17:SER:HB3  | 2.15                     | 0.45              |
| 53:B6:13:CYS:SG   | 53:B6:50:ARG:O    | 2.69                     | 0.45              |
| 1:CA:8:A:OP2      | 5:CE:101:ILE:HG21 | 2.17                     | 0.45              |
| 1:CA:119:A:N6     | 1:CA:288:A:N9     | 2.65                     | 0.45              |
| 1:CA:266:G:H5''   | 1:CA:267:C:C5     | 2.52                     | 0.45              |
| 1:CA:537:G:H2'    | 1:CA:538:G:C8     | 2.52                     | 0.45              |
| 1:CA:921:U:O2     | 5:CE:19:MET:HB2   | 2.16                     | 0.45              |
| 1:CA:1126:U:H1'   | 1:CA:1280:A:C6    | 2.51                     | 0.45              |
| 1:CA:1178:G:OP2   | 9:CI:97:LYS:HE3   | 2.16                     | 0.45              |
| 2:CB:87:ARG:HE    | 2:CB:233:SER:CB   | 2.30                     | 0.45              |
| 3:CC:70:VAL:CG1   | 3:CC:72:LYS:H     | 2.24                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:CD:80:GLU:O      | 4:CD:82:ALA:N      | 2.50                     | 0.45              |
| 5:CE:11:ILE:O      | 5:CE:12:LEU:C      | 2.60                     | 0.45              |
| 5:CE:31:LEU:HD23   | 5:CE:45:PHE:CD1    | 2.51                     | 0.45              |
| 7:CG:90:GLU:H      | 7:CG:90:GLU:HG3    | 1.29                     | 0.45              |
| 7:CG:110:GLN:O     | 7:CG:111:ARG:CB    | 2.65                     | 0.45              |
| 11:CK:123:LYS:O    | 11:CK:124:LYS:C    | 2.57                     | 0.45              |
| 12:CL:24:VAL:O     | 12:CL:24:VAL:CG1   | 2.57                     | 0.45              |
| 17:CQ:63:ARG:O     | 17:CQ:64:PRO:C     | 2.60                     | 0.45              |
| 18:CR:40:LEU:C     | 18:CR:42:ARG:H     | 2.23                     | 0.45              |
| 19:CS:45:VAL:C     | 19:CS:47:HIS:H     | 2.24                     | 0.45              |
| 19:CS:62:ILE:HG23  | 19:CS:62:ILE:O     | 2.16                     | 0.45              |
| 25:DA:7:G:H2'      | 25:DA:8:A:C8       | 2.51                     | 0.45              |
| 25:DA:13:A:C6      | 25:DA:525:U:C2     | 3.04                     | 0.45              |
| 25:DA:518:G:H4'    | 43:DW:18:ARG:NH1   | 2.31                     | 0.45              |
| 25:DA:862:G:O2'    | 26:DB:78:A:N3      | 2.50                     | 0.45              |
| 25:DA:1384:A:N3    | 25:DA:1405:U:H1'   | 2.31                     | 0.45              |
| 25:DA:1664:A:C2    | 25:DA:2726:U:H1'   | 2.51                     | 0.45              |
| 25:DA:2031:A:N3    | 25:DA:2455:G:O2'   | 2.49                     | 0.45              |
| 25:DA:2350:C:H2'   | 25:DA:2351:G:O4'   | 2.17                     | 0.45              |
| 25:DA:2406:U:OP2   | 25:DA:2411:A:N6    | 2.50                     | 0.45              |
| 25:DA:2468:G:H5'   | 37:DQ:120:ILE:HD12 | 1.98                     | 0.45              |
| 25:DA:2693:A:H2'   | 25:DA:2694:G:H8    | 1.82                     | 0.45              |
| 28:DD:105:ILE:HD12 | 28:DD:106:ILE:H    | 1.81                     | 0.45              |
| 29:DE:110:GLY:CA   | 29:DE:162:ALA:H    | 2.29                     | 0.45              |
| 33:DI:3:VAL:CB     | 33:DI:37:VAL:O     | 2.65                     | 0.45              |
| 33:DI:23:PRO:O     | 33:DI:27:ARG:HG2   | 2.15                     | 0.45              |
| 36:DP:101:VAL:HG21 | 36:DP:108:LYS:H    | 1.81                     | 0.45              |
| 39:DS:24:LEU:N     | 39:DS:24:LEU:HD22  | 2.32                     | 0.45              |
| 39:DS:30:ARG:HH11  | 39:DS:30:ARG:HG2   | 1.81                     | 0.45              |
| 40:DT:30:VAL:HA    | 40:DT:44:ASP:HA    | 1.99                     | 0.45              |
| 41:DU:111:GLU:OE2  | 41:DU:111:GLU:HA   | 2.16                     | 0.45              |
| 42:DV:35:LEU:O     | 42:DV:36:PRO:C     | 2.60                     | 0.45              |
| 43:DW:59:VAL:O     | 43:DW:63:ASP:N     | 2.45                     | 0.45              |
| 43:DW:95:ILE:O     | 43:DW:95:ILE:HG13  | 2.15                     | 0.45              |
| 44:DX:3:THR:O      | 44:DX:4:ALA:HB3    | 2.17                     | 0.45              |
| 44:DX:23:GLU:CD    | 44:DX:23:GLU:H     | 2.24                     | 0.45              |
| 46:DZ:65:GLN:O     | 46:DZ:65:GLN:HG3   | 2.16                     | 0.45              |
| 51:D4:3:GLU:HG3    | 51:D4:4:GLY:N      | 2.31                     | 0.45              |
| 53:D6:11:LEU:HD13  | 53:D6:12:GLU:O     | 2.17                     | 0.45              |
| 53:D6:19:ARG:CG    | 53:D6:20:ASN:H     | 2.09                     | 0.45              |
| 1:AA:67:C:O2'      | 1:AA:171:A:N3      | 2.39                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AA:176:C:H2'    | 1:AA:177:C:H6     | 1.82                     | 0.45              |
| 1:AA:345:C:H4'    | 1:AA:346:G:O5'    | 2.17                     | 0.45              |
| 1:AA:522:C:H41    | 12:AL:53:ARG:NH2  | 2.14                     | 0.45              |
| 2:AB:60:ASP:O     | 2:AB:64:ARG:HG2   | 2.17                     | 0.45              |
| 2:AB:102:LEU:O    | 2:AB:105:PHE:HB2  | 2.16                     | 0.45              |
| 3:AC:40:ARG:CD    | 3:AC:55:VAL:HB    | 2.47                     | 0.45              |
| 8:AH:2:LEU:C      | 8:AH:2:LEU:CD1    | 2.89                     | 0.45              |
| 12:AL:79:GLU:O    | 12:AL:80:HIS:CG   | 2.69                     | 0.45              |
| 23:AW:34:G:C2     | 24:AX:14:A:N3     | 2.85                     | 0.45              |
| 25:BA:184:C:H2'   | 25:BA:185:U:C6    | 2.51                     | 0.45              |
| 25:BA:703:U:C2'   | 25:BA:704:G:H5'   | 2.47                     | 0.45              |
| 25:BA:734:A:O2'   | 25:BA:1635:G:H5'  | 2.17                     | 0.45              |
| 25:BA:773:U:H4'   | 28:BD:47:GLY:CA   | 2.46                     | 0.45              |
| 25:BA:783:A:H8    | 25:BA:784:A:H4'   | 1.82                     | 0.45              |
| 25:BA:942:G:H5''  | 36:BP:33:ARG:O    | 2.17                     | 0.45              |
| 25:BA:995:C:H42   | 34:BN:1:MET:CG    | 2.17                     | 0.45              |
| 25:BA:1456:G:N3   | 25:BA:1457:A:C8   | 2.85                     | 0.45              |
| 25:BA:1648:C:N4   | 25:BA:2010:G:N1   | 2.65                     | 0.45              |
| 25:BA:2839:G:H5'  | 38:BR:46:GLY:HA2  | 1.98                     | 0.45              |
| 27:BC:59:ARG:HH21 | 27:BC:199:HIS:H   | 1.65                     | 0.45              |
| 27:BC:169:GLY:O   | 27:BC:171:ILE:N   | 2.49                     | 0.45              |
| 28:BD:70:TRP:C    | 28:BD:70:TRP:CD1  | 2.95                     | 0.45              |
| 28:BD:102:LYS:C   | 28:BD:103:ARG:HG2 | 2.41                     | 0.45              |
| 29:BE:19:ARG:O    | 29:BE:19:ARG:HG3  | 2.17                     | 0.45              |
| 30:BF:110:LEU:O   | 30:BF:111:ALA:C   | 2.60                     | 0.45              |
| 31:BG:8:LYS:O     | 31:BG:11:TYR:HB3  | 2.16                     | 0.45              |
| 33:BI:41:GLU:O    | 33:BI:44:LEU:HB3  | 2.16                     | 0.45              |
| 33:BI:75:LEU:HD21 | 33:BI:105:HIS:CD2 | 2.52                     | 0.45              |
| 35:BO:8:LEU:HD13  | 35:BO:82:ASN:HB2  | 1.98                     | 0.45              |
| 46:BZ:54:HIS:HB3  | 46:BZ:101:PRO:CD  | 2.47                     | 0.45              |
| 51:B4:61:VAL:HG13 | 51:B4:62:CYS:O    | 2.17                     | 0.45              |
| 52:B5:29:THR:O    | 52:B5:30:LEU:HD23 | 2.16                     | 0.45              |
| 54:B7:5:TRP:C     | 54:B7:6:GLN:HG2   | 2.42                     | 0.45              |
| 55:B8:23:VAL:HG13 | 55:B8:46:ARG:HB3  | 1.98                     | 0.45              |
| 1:CA:49:U:O4      | 1:CA:364:A:C4     | 2.70                     | 0.45              |
| 1:CA:414:A:OP2    | 1:CA:428:G:N2     | 2.35                     | 0.45              |
| 1:CA:923:A:O2'    | 1:CA:1399:C:OP2   | 2.27                     | 0.45              |
| 1:CA:1258:G:H2'   | 1:CA:1259:C:C6    | 2.52                     | 0.45              |
| 2:CB:220:ASP:O    | 2:CB:223:ILE:N    | 2.50                     | 0.45              |
| 4:CD:18:LYS:HE3   | 4:CD:31:CYS:HB3   | 1.98                     | 0.45              |
| 5:CE:33:VAL:HG21  | 5:CE:109:ILE:HG12 | 1.98                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 5:CE:36:ASP:C      | 5:CE:36:ASP:OD2    | 2.58                     | 0.45              |
| 7:CG:146:GLU:CA    | 7:CG:149:ARG:HB2   | 2.46                     | 0.45              |
| 9:CI:3:GLN:O       | 9:CI:88:TYR:HE1    | 1.98                     | 0.45              |
| 10:CJ:49:VAL:O     | 10:CJ:60:ARG:HB3   | 2.16                     | 0.45              |
| 13:CM:67:GLU:C     | 13:CM:67:GLU:CD    | 2.85                     | 0.45              |
| 13:CM:87:TYR:C     | 13:CM:89:GLY:H     | 2.23                     | 0.45              |
| 23:CW:55:U:C6      | 23:CW:58:A:N7      | 2.85                     | 0.45              |
| 24:CX:20:U:O2'     | 24:CX:21:C:H5'     | 2.17                     | 0.45              |
| 23:CY:36:A:H5''    | 23:CY:36:A:H8      | 1.79                     | 0.45              |
| 25:DA:64:A:O3'     | 44:DX:71:GLY:HA3   | 2.16                     | 0.45              |
| 25:DA:613:G:C6     | 25:DA:615:G:O6     | 2.69                     | 0.45              |
| 25:DA:768:G:C4     | 25:DA:769:G:C8     | 3.05                     | 0.45              |
| 25:DA:1140:C:O4'   | 25:DA:1143:A:C2    | 2.70                     | 0.45              |
| 25:DA:1558:A:N7    | 25:DA:1560:G:C8    | 2.85                     | 0.45              |
| 25:DA:1566:A:O2'   | 28:DD:58:HIS:CD2   | 2.69                     | 0.45              |
| 25:DA:1614:A:H62   | 43:DW:93:ALA:HB2   | 1.82                     | 0.45              |
| 25:DA:2133:G:H21   | 25:DA:2158:A:H62   | 1.64                     | 0.45              |
| 25:DA:2445:G:OP1   | 30:DF:74:ARG:NH2   | 2.38                     | 0.45              |
| 29:DE:101:ARG:HH21 | 29:DE:171:GLU:N    | 2.14                     | 0.45              |
| 33:DI:101:LEU:CD2  | 33:DI:107:VAL:HB   | 2.42                     | 0.45              |
| 37:DQ:141:GLN:CB   | 46:DZ:98:MET:HA    | 2.45                     | 0.45              |
| 39:DS:25:ARG:HB3   | 39:DS:25:ARG:NH1   | 2.32                     | 0.45              |
| 39:DS:106:ARG:O    | 39:DS:107:GLU:CB   | 2.64                     | 0.45              |
| 40:DT:62:THR:HG22  | 40:DT:75:ILE:HG23  | 1.99                     | 0.45              |
| 41:DU:27:LEU:N     | 41:DU:27:LEU:HD23  | 2.31                     | 0.45              |
| 42:DV:25:LEU:H     | 42:DV:92:THR:CG2   | 2.30                     | 0.45              |
| 45:DY:4:LYS:O      | 45:DY:5:MET:O      | 2.35                     | 0.45              |
| 45:DY:48:ALA:O     | 45:DY:49:VAL:C     | 2.59                     | 0.45              |
| 46:DZ:23:LYS:CE    | 46:DZ:38:TYR:HE1   | 2.28                     | 0.45              |
| 46:DZ:116:VAL:N    | 46:DZ:174:VAL:HG13 | 2.32                     | 0.45              |
| 48:D1:46:LEU:C     | 48:D1:47:GLN:HG2   | 2.40                     | 0.45              |
| 48:D1:86:SER:O     | 48:D1:90:ILE:N     | 2.50                     | 0.45              |
| 56:D9:2:LYS:O      | 56:D9:34:GLN:HA    | 2.17                     | 0.45              |
| 1:AA:436:C:H2'     | 1:AA:437:U:C6      | 2.52                     | 0.45              |
| 1:AA:532:A:C2'     | 1:AA:533:A:OP1     | 2.63                     | 0.45              |
| 1:AA:687:A:O2'     | 1:AA:688:G:O4'     | 2.23                     | 0.45              |
| 1:AA:1002:G:N2     | 1:AA:1003:G:H1'    | 2.32                     | 0.45              |
| 1:AA:1280:A:O4'    | 10:AJ:41:PRO:HG3   | 2.16                     | 0.45              |
| 1:AA:1300:G:O2'    | 1:AA:1301:U:OP2    | 2.34                     | 0.45              |
| 1:AA:1325:C:O3'    | 21:AU:17:THR:HG21  | 2.16                     | 0.45              |
| 1:AA:1517:G:N3     | 25:BA:1919:A:O2'   | 2.49                     | 0.45              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 3:AC:55:VAL:O      | 3:AC:57:ILE:HG13    | 2.16                     | 0.45              |
| 7:AG:73:MET:CA     | 7:AG:91:VAL:HG23    | 2.45                     | 0.45              |
| 11:AK:34:ASP:HB2   | 11:AK:35:PRO:HD2    | 1.98                     | 0.45              |
| 12:AL:6:THR:O      | 12:AL:9:GLN:HB2     | 2.16                     | 0.45              |
| 16:AP:52:ASP:OD2   | 16:AP:54:GLU:HB2    | 2.16                     | 0.45              |
| 17:AQ:29:HIS:HA    | 17:AQ:30:PRO:HD3    | 1.84                     | 0.45              |
| 19:AS:29:ARG:NH1   | 19:AS:30:LEU:H      | 2.10                     | 0.45              |
| 23:AY:28:G:H2'     | 23:AY:29:G:H8       | 1.81                     | 0.45              |
| 25:BA:492:A:H2'    | 25:BA:493:G:O4'     | 2.16                     | 0.45              |
| 25:BA:500:G:N2     | 25:BA:502:A:H3'     | 2.32                     | 0.45              |
| 25:BA:574:C:O2     | 29:BE:145:LYS:NZ    | 2.35                     | 0.45              |
| 25:BA:774:A:H2     | 25:BA:787:U:O2'     | 1.99                     | 0.45              |
| 25:BA:1554:A:H4'   | 25:BA:1555:G:OP1    | 2.15                     | 0.45              |
| 25:BA:2046:G:O5'   | 52:B5:19:ARG:HA     | 2.17                     | 0.45              |
| 25:BA:2119:A:H8    | 25:BA:2119:A:OP1    | 2.00                     | 0.45              |
| 25:BA:2150:U:H2'   | 25:BA:2151:G:C8     | 2.51                     | 0.45              |
| 25:BA:2712:U:O2'   | 25:BA:2712(A):A:O5' | 2.31                     | 0.45              |
| 27:BC:72:VAL:HG12  | 27:BC:74:VAL:HG23   | 1.99                     | 0.45              |
| 28:BD:107:ALA:HA   | 28:BD:108:PRO:HD2   | 1.88                     | 0.45              |
| 28:BD:232:PRO:HD2  | 28:BD:249:PRO:HA    | 1.98                     | 0.45              |
| 29:BE:117:MET:HG3  | 29:BE:122:PHE:O     | 2.17                     | 0.45              |
| 30:BF:83:PHE:O     | 30:BF:84:VAL:C      | 2.58                     | 0.45              |
| 31:BG:28:VAL:O     | 31:BG:31:VAL:N      | 2.39                     | 0.45              |
| 32:BH:66:GLY:N     | 32:BH:69:ARG:HB2    | 2.32                     | 0.45              |
| 37:BQ:17:LEU:HD23  | 37:BQ:17:LEU:N      | 2.32                     | 0.45              |
| 38:BR:72:ASP:HB3   | 38:BR:75:LEU:CB     | 2.40                     | 0.45              |
| 40:BT:102:ILE:HD12 | 40:BT:102:ILE:C     | 2.41                     | 0.45              |
| 44:BX:12:VAL:H     | 44:BX:28:PHE:HA     | 1.82                     | 0.45              |
| 45:BY:3:VAL:C      | 45:BY:5:MET:H       | 2.23                     | 0.45              |
| 46:BZ:119:GLU:HB2  | 46:BZ:122:ARG:CG    | 2.47                     | 0.45              |
| 49:B2:50:ILE:O     | 49:B2:53:LEU:N      | 2.50                     | 0.45              |
| 1:CA:64:G:H5''     | 1:CA:65:U:OP1       | 2.17                     | 0.45              |
| 1:CA:80:G:H22      | 1:CA:90:U:H4'       | 1.82                     | 0.45              |
| 1:CA:254:G:OP1     | 17:CQ:68:ARG:HB3    | 2.15                     | 0.45              |
| 1:CA:324:G:OP1     | 20:CT:22:ARG:HD3    | 2.16                     | 0.45              |
| 1:CA:765:G:N2      | 1:CA:812:C:O2'      | 2.49                     | 0.45              |
| 1:CA:1201:A:O2'    | 1:CA:1202:G:P       | 2.75                     | 0.45              |
| 2:CB:97:TRP:CH2    | 2:CB:176:GLU:OE2    | 2.69                     | 0.45              |
| 2:CB:168:THR:O     | 2:CB:169:LYS:C      | 2.60                     | 0.45              |
| 7:CG:51:GLN:HA     | 7:CG:51:GLN:OE1     | 2.16                     | 0.45              |
| 7:CG:66:VAL:HG12   | 7:CG:70:LYS:HE3     | 1.98                     | 0.45              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 7:CG:93:PRO:O      | 7:CG:94:ARG:C     | 2.57                     | 0.45              |
| 8:CH:26:VAL:C      | 8:CH:58:TYR:HD2   | 2.25                     | 0.45              |
| 9:CI:28:VAL:HA     | 9:CI:63:ILE:O     | 2.16                     | 0.45              |
| 12:CL:69:TYR:O     | 12:CL:71:PRO:HD3  | 2.17                     | 0.45              |
| 13:CM:14:ARG:H     | 13:CM:44:ARG:HD2  | 1.81                     | 0.45              |
| 18:CR:67:ALA:O     | 18:CR:68:LYS:C    | 2.59                     | 0.45              |
| 20:CT:8:ARG:HH11   | 20:CT:8:ARG:HG3   | 1.82                     | 0.45              |
| 22:CV:42:C:C2      | 22:CV:43:G:C8     | 3.04                     | 0.45              |
| 22:CV:48:U:C5'     | 22:CV:49:C:H5'    | 2.47                     | 0.45              |
| 24:CX:19:U:C2'     | 24:CX:20:U:H5'    | 2.47                     | 0.45              |
| 25:DA:412:A:N7     | 25:DA:2411:A:H2   | 2.15                     | 0.45              |
| 25:DA:819:A:C4     | 25:DA:1189:A:C2   | 3.04                     | 0.45              |
| 25:DA:1223:G:H5'   | 25:DA:1224:C:OP2  | 2.16                     | 0.45              |
| 25:DA:1648:C:C4    | 25:DA:2010:G:C2   | 3.05                     | 0.45              |
| 25:DA:2249:U:H1'   | 25:DA:2275:C:N4   | 2.31                     | 0.45              |
| 25:DA:2287:A:O2'   | 25:DA:2288:A:P    | 2.74                     | 0.45              |
| 25:DA:2386:C:H4'   | 47:D0:55:ARG:O    | 2.17                     | 0.45              |
| 25:DA:2405:G:HO2'  | 25:DA:2406:U:P    | 2.39                     | 0.45              |
| 25:DA:2750:A:HO2'  | 25:DA:2751:G:P    | 2.39                     | 0.45              |
| 28:DD:271:ILE:O    | 28:DD:272:ALA:HB2 | 2.16                     | 0.45              |
| 29:DE:47:VAL:HG12  | 29:DE:48:GLN:N    | 2.30                     | 0.45              |
| 33:DI:114:LEU:HD22 | 33:DI:130:TYR:HD1 | 1.79                     | 0.45              |
| 34:DN:112:LEU:O    | 34:DN:115:ARG:N   | 2.50                     | 0.45              |
| 38:DR:18:LEU:HD21  | 38:DR:22:ARG:HE   | 1.80                     | 0.45              |
| 38:DR:92:GLY:HA2   | 38:DR:94:TYR:CE1  | 2.52                     | 0.45              |
| 40:DT:26:ASP:OD2   | 40:DT:26:ASP:C    | 2.60                     | 0.45              |
| 41:DU:88:ILE:O     | 41:DU:88:ILE:CG1  | 2.64                     | 0.45              |
| 43:DW:86:LEU:HG    | 43:DW:88:ARG:HD3  | 1.98                     | 0.45              |
| 46:DZ:14:LYS:HZ2   | 46:DZ:14:LYS:N    | 2.09                     | 0.45              |
| 47:D0:66:VAL:O     | 47:D0:81:VAL:HA   | 2.16                     | 0.45              |
| 49:D2:32:LEU:HB2   | 49:D2:53:LEU:HD13 | 1.99                     | 0.45              |
| 1:AA:511:C:O2'     | 1:AA:512:U:P      | 2.75                     | 0.45              |
| 1:AA:620:C:H2'     | 1:AA:621:A:O4'    | 2.17                     | 0.45              |
| 2:AB:63:MET:HG3    | 2:AB:64:ARG:N     | 2.32                     | 0.45              |
| 3:AC:19:GLU:O      | 3:AC:19:GLU:HG2   | 2.16                     | 0.45              |
| 5:AE:75:THR:HA     | 5:AE:115:VAL:CG1  | 2.44                     | 0.45              |
| 20:AT:45:GLN:C     | 20:AT:47:GLY:N    | 2.74                     | 0.45              |
| 22:AV:19:G:C6      | 22:AV:58:A:C6     | 3.04                     | 0.45              |
| 25:BA:449:A:OP1    | 30:BF:84:VAL:O    | 2.35                     | 0.45              |
| 25:BA:549:G:H2'    | 25:BA:551:G:H5''  | 1.99                     | 0.45              |
| 25:BA:627:A:O2'    | 25:BA:628:G:C8    | 2.69                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:BA:1310:G:H2'  | 25:BA:1311:G:O4'  | 2.17                     | 0.45              |
| 25:BA:1653:G:HO2' | 25:BA:1654:A:P    | 2.38                     | 0.45              |
| 25:BA:2097:C:H2'  | 25:BA:2098:U:O4'  | 2.16                     | 0.45              |
| 25:BA:2114:A:H2'  | 25:BA:2115:G:O4'  | 2.17                     | 0.45              |
| 25:BA:2377:A:H2'  | 25:BA:2378:A:C8   | 2.52                     | 0.45              |
| 27:BC:41:VAL:C    | 27:BC:178:ALA:HB3 | 2.41                     | 0.45              |
| 30:BF:102:PRO:O   | 30:BF:105:VAL:N   | 2.48                     | 0.45              |
| 30:BF:185:ASP:HA  | 30:BF:188:ARG:HB2 | 1.99                     | 0.45              |
| 31:BG:51:ARG:HH11 | 31:BG:53:LEU:HD21 | 1.82                     | 0.45              |
| 32:BH:34:GLU:O    | 32:BH:36:PRO:HD3  | 2.17                     | 0.45              |
| 33:BI:42:SER:O    | 33:BI:45:LYS:HG2  | 2.17                     | 0.45              |
| 34:BN:14:VAL:HG11 | 34:BN:137:LYS:HG3 | 1.95                     | 0.45              |
| 34:BN:55:VAL:O    | 34:BN:56:ASN:C    | 2.60                     | 0.45              |
| 34:BN:70:LYS:O    | 34:BN:71:ILE:HD12 | 2.17                     | 0.45              |
| 35:BO:53:LYS:HD2  | 35:BO:53:LYS:N    | 2.32                     | 0.45              |
| 35:BO:119:PRO:HB2 | 40:BT:68:TYR:HE1  | 1.80                     | 0.45              |
| 37:BQ:140:ALA:HA  | 46:BZ:99:TYR:CD2  | 2.52                     | 0.45              |
| 38:BR:63:ARG:NH2  | 38:BR:80:PHE:HD2  | 2.15                     | 0.45              |
| 40:BT:16:ARG:O    | 40:BT:17:THR:HB   | 2.16                     | 0.45              |
| 40:BT:59:THR:O    | 40:BT:77:PRO:O    | 2.34                     | 0.45              |
| 40:BT:64:ARG:HD2  | 40:BT:73:GLU:CG   | 2.47                     | 0.45              |
| 41:BU:39:LEU:O    | 41:BU:41:ALA:N    | 2.50                     | 0.45              |
| 41:BU:60:LEU:O    | 41:BU:61:TRP:C    | 2.58                     | 0.45              |
| 42:BV:19:LYS:HZ1  | 42:BV:20:LEU:HD13 | 1.81                     | 0.45              |
| 42:BV:54:GLY:O    | 42:BV:101:GLY:HA2 | 2.17                     | 0.45              |
| 42:BV:97:LYS:HD3  | 42:BV:97:LYS:HA   | 1.68                     | 0.45              |
| 44:BX:29:TRP:CZ2  | 44:BX:76:ARG:NH2  | 2.85                     | 0.45              |
| 45:BY:28:LYS:HB2  | 45:BY:37:VAL:CA   | 2.40                     | 0.45              |
| 45:BY:47:LYS:O    | 45:BY:48:ALA:C    | 2.60                     | 0.45              |
| 46:BZ:39:VAL:HG21 | 46:BZ:44:PHE:CD2  | 2.51                     | 0.45              |
| 54:B7:12:ARG:HE   | 54:B7:46:VAL:CG2  | 2.29                     | 0.45              |
| 54:B7:13:ALA:O    | 54:B7:17:GLY:HA3  | 2.17                     | 0.45              |
| 1:CA:15:G:H4'     | 5:CE:24:ARG:NH1   | 2.31                     | 0.45              |
| 1:CA:687:A:C2     | 1:CA:704:A:C4     | 3.04                     | 0.45              |
| 1:CA:715:A:H2'    | 1:CA:716:A:C8     | 2.51                     | 0.45              |
| 1:CA:860:A:H2'    | 1:CA:861:G:O4'    | 2.17                     | 0.45              |
| 2:CB:57:PHE:CD2   | 2:CB:185:ILE:HD11 | 2.52                     | 0.45              |
| 3:CC:172:ARG:NH2  | 3:CC:174:PRO:HG3  | 2.32                     | 0.45              |
| 4:CD:94:LEU:HD23  | 4:CD:97:LEU:HD12  | 1.97                     | 0.45              |
| 4:CD:206:PHE:CD2  | 4:CD:207:TYR:HE2  | 2.33                     | 0.45              |
| 7:CG:137:LYS:HE2  | 7:CG:137:LYS:HB3  | 1.62                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 15:CO:74:ASP:HB3   | 15:CO:77:ARG:HG2   | 1.98                     | 0.45              |
| 17:CQ:9:VAL:HA     | 17:CQ:55:ASP:O     | 2.17                     | 0.45              |
| 23:CW:19:G:C2      | 23:CW:57:G:O6      | 2.70                     | 0.45              |
| 25:DA:242:G:O2'    | 25:DA:243:U:OP2    | 2.30                     | 0.45              |
| 25:DA:331:A:O2'    | 25:DA:332:A:OP1    | 2.33                     | 0.45              |
| 25:DA:452:G:H5'    | 30:DF:59:TYR:CE2   | 2.52                     | 0.45              |
| 25:DA:1113:U:H2'   | 25:DA:1114:G:C8    | 2.51                     | 0.45              |
| 25:DA:1485:G:H2'   | 25:DA:1486:A:C8    | 2.52                     | 0.45              |
| 25:DA:1790:C:H5''  | 25:DA:1791:A:OP1   | 2.16                     | 0.45              |
| 25:DA:2021:C:H4'   | 25:DA:2022:U:OP1   | 2.10                     | 0.45              |
| 25:DA:2331:G:O2'   | 25:DA:2336:A:N1    | 2.41                     | 0.45              |
| 27:DC:59:ARG:HB2   | 27:DC:62:VAL:CG2   | 2.40                     | 0.45              |
| 27:DC:208:PHE:O    | 27:DC:209:LEU:CB   | 2.65                     | 0.45              |
| 29:DE:3:GLY:CA     | 29:DE:81:ILE:HG21  | 2.38                     | 0.45              |
| 29:DE:173:VAL:O    | 29:DE:174:ASP:C    | 2.59                     | 0.45              |
| 30:DF:155:LEU:HD12 | 30:DF:174:VAL:HG22 | 1.99                     | 0.45              |
| 32:DH:124:GLU:CB   | 32:DH:132:ARG:HD2  | 2.41                     | 0.45              |
| 33:DI:96:ASP:C     | 33:DI:98:ALA:H     | 2.25                     | 0.45              |
| 34:DN:112:LEU:HD12 | 34:DN:112:LEU:HA   | 1.70                     | 0.45              |
| 35:DO:2:ILE:HD11   | 35:DO:82:ASN:HD22  | 1.82                     | 0.45              |
| 35:DO:34:THR:HG22  | 35:DO:37:ASP:OD2   | 2.17                     | 0.45              |
| 36:DP:106:LEU:HD11 | 36:DP:112:LEU:CD2  | 2.40                     | 0.45              |
| 39:DS:85:VAL:HG23  | 39:DS:112:PHE:CE1  | 2.51                     | 0.45              |
| 45:DY:5:MET:HE2    | 45:DY:32:PRO:HB3   | 1.98                     | 0.45              |
| 46:DZ:166:SER:HB2  | 46:DZ:168:GLU:HB2  | 1.99                     | 0.45              |
| 49:D2:36:ARG:C     | 49:D2:38:GLN:H     | 2.24                     | 0.45              |
| 53:D6:48:VAL:O     | 53:D6:49:HIS:HB2   | 2.16                     | 0.45              |
| 55:D8:49:VAL:O     | 55:D8:53:PRO:HG3   | 2.16                     | 0.45              |
| 56:D9:19:ARG:O     | 56:D9:24:TYR:CE1   | 2.70                     | 0.45              |
| 1:AA:80:G:N2       | 1:AA:90:U:H4'      | 2.32                     | 0.45              |
| 1:AA:460:G:N2      | 1:AA:471:G:OP2     | 2.45                     | 0.45              |
| 1:AA:640:A:O2'     | 8:AH:115:SER:O     | 2.28                     | 0.45              |
| 1:AA:1086:U:H3     | 1:AA:1099:G:H22    | 1.65                     | 0.45              |
| 1:AA:1373:G:H5''   | 7:AG:36:LYS:HB2    | 1.99                     | 0.45              |
| 1:AA:1388:C:H2'    | 1:AA:1389:C:C6     | 2.51                     | 0.45              |
| 2:AB:52:GLU:HG3    | 2:AB:56:ARG:CZ     | 2.47                     | 0.45              |
| 2:AB:83:MET:C      | 2:AB:85:ALA:H      | 2.25                     | 0.45              |
| 4:AD:39:PRO:O      | 4:AD:44:GLY:HA3    | 2.17                     | 0.45              |
| 5:AE:42:GLY:HA2    | 5:AE:66:MET:HA     | 1.99                     | 0.45              |
| 5:AE:113:ALA:HB3   | 5:AE:115:VAL:HG23  | 1.98                     | 0.45              |
| 9:AI:4:TYR:CB      | 9:AI:19:LEU:HD12   | 2.47                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 14:AN:46:GLU:O     | 14:AN:49:HIS:HB2   | 2.17                     | 0.45              |
| 17:AQ:17:LYS:O     | 17:AQ:46:ASP:N     | 2.49                     | 0.45              |
| 20:AT:96:GLY:O     | 20:AT:97:ALA:O     | 2.34                     | 0.45              |
| 22:AV:57:C:O2      | 31:BG:78:SER:HB2   | 2.17                     | 0.45              |
| 25:BA:196:A:N3     | 25:BA:805:G:C6     | 2.85                     | 0.45              |
| 25:BA:474:G:O2'    | 25:BA:475:U:OP1    | 2.31                     | 0.45              |
| 25:BA:669:G:H5''   | 25:BA:670:A:OP2    | 2.17                     | 0.45              |
| 25:BA:675:A:OP1    | 30:BF:76:GLY:HA2   | 2.16                     | 0.45              |
| 25:BA:1111:A:O3'   | 25:BA:1112:G:H4'   | 2.16                     | 0.45              |
| 25:BA:1246:A:C2    | 25:BA:1247:A:H1'   | 2.52                     | 0.45              |
| 25:BA:1721:G:N1    | 25:BA:1739:U:OP2   | 2.50                     | 0.45              |
| 25:BA:2118:U:H5    | 25:BA:2149:G:H5'   | 1.81                     | 0.45              |
| 25:BA:2161:C:H2'   | 25:BA:2162:G:H8    | 1.81                     | 0.45              |
| 25:BA:2364:C:H4'   | 47:B0:56:ASP:OD2   | 2.16                     | 0.45              |
| 28:BD:146:GLU:HA   | 28:BD:152:GLY:O    | 2.16                     | 0.45              |
| 28:BD:147:LEU:HD13 | 28:BD:155:LEU:HD21 | 1.99                     | 0.45              |
| 31:BG:16:ARG:HD3   | 31:BG:16:ARG:HA    | 1.75                     | 0.45              |
| 31:BG:63:ILE:HD12  | 31:BG:141:PHE:CG   | 2.51                     | 0.45              |
| 32:BH:26:VAL:O     | 32:BH:79:VAL:HG11  | 2.17                     | 0.45              |
| 33:BI:88:ILE:HD13  | 33:BI:123:LEU:HG   | 1.99                     | 0.45              |
| 35:BO:47:ILE:HG13  | 35:BO:48:PRO:HD2   | 1.97                     | 0.45              |
| 38:BR:52:ILE:O     | 38:BR:55:ALA:HB3   | 2.16                     | 0.45              |
| 45:BY:47:LYS:HD2   | 45:BY:47:LYS:H     | 1.82                     | 0.45              |
| 46:BZ:125:LEU:HD12 | 46:BZ:126:VAL:H    | 1.81                     | 0.45              |
| 53:B6:19:ARG:H     | 53:B6:19:ARG:CD    | 2.24                     | 0.45              |
| 1:CA:46:G:H2'      | 1:CA:366:C:H41     | 1.81                     | 0.45              |
| 1:CA:324:G:P       | 20:CT:22:ARG:HD3   | 2.57                     | 0.45              |
| 1:CA:407:G:H1      | 1:CA:435:C:N4      | 2.11                     | 0.45              |
| 1:CA:451:A:H4'     | 1:CA:452:A:O4'     | 2.17                     | 0.45              |
| 1:CA:484:G:HO2'    | 1:CA:485:G:P       | 2.39                     | 0.45              |
| 1:CA:901:A:C5      | 1:CA:902:G:H1'     | 2.52                     | 0.45              |
| 1:CA:1064:G:O6     | 1:CA:1193:G:C2     | 2.70                     | 0.45              |
| 1:CA:1298:C:H1'    | 1:CA:1299:A:C6     | 2.52                     | 0.45              |
| 2:CB:19:HIS:CE1    | 2:CB:20:GLU:CG     | 3.00                     | 0.45              |
| 2:CB:55:PHE:C      | 2:CB:57:PHE:H      | 2.25                     | 0.45              |
| 2:CB:122:PHE:HA    | 2:CB:139:LYS:HZ2   | 1.82                     | 0.45              |
| 3:CC:118:GLN:HA    | 3:CC:121:ALA:HB3   | 1.99                     | 0.45              |
| 5:CE:12:LEU:C      | 5:CE:12:LEU:HD13   | 2.41                     | 0.45              |
| 8:CH:106:GLY:O     | 8:CH:122:ARG:NH2   | 2.50                     | 0.45              |
| 11:CK:57:THR:HG22  | 11:CK:58:PRO:HD2   | 1.99                     | 0.45              |
| 12:CL:25:PRO:C     | 12:CL:27:LEU:N     | 2.69                     | 0.45              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 20:CT:18:GLN:O    | 20:CT:19:SER:C     | 2.60                     | 0.45              |
| 23:CY:36:A:C8     | 23:CY:36:A:C4'     | 3.00                     | 0.45              |
| 25:DA:340:A:H2'   | 25:DA:341:G:C5'    | 2.47                     | 0.45              |
| 25:DA:613:G:N2    | 25:DA:615:G:C8     | 2.85                     | 0.45              |
| 25:DA:1266:G:O2'  | 25:DA:2012:G:N1    | 2.45                     | 0.45              |
| 27:DC:122:ALA:HB1 | 27:DC:129:ARG:CB   | 2.46                     | 0.45              |
| 28:DD:232:PRO:HD2 | 28:DD:249:PRO:HA   | 1.99                     | 0.45              |
| 31:DG:2:PRO:C     | 31:DG:4:ASP:H      | 2.25                     | 0.45              |
| 31:DG:35:GLU:O    | 31:DG:35:GLU:CD    | 2.60                     | 0.45              |
| 31:DG:41:GLN:HB3  | 31:DG:43:LEU:HD11  | 1.99                     | 0.45              |
| 31:DG:83:ARG:H    | 31:DG:86:MET:HE3   | 1.82                     | 0.45              |
| 32:DH:35:VAL:CG2  | 32:DH:75:ALA:HB2   | 2.47                     | 0.45              |
| 34:DN:66:LYS:O    | 34:DN:70:LYS:HB3   | 2.17                     | 0.45              |
| 36:DP:49:ARG:NH2  | 36:DP:50:ARG:HH22  | 2.15                     | 0.45              |
| 38:DR:33:ARG:HG3  | 38:DR:115:GLU:HB3  | 1.99                     | 0.45              |
| 38:DR:48:VAL:O    | 38:DR:49:ASP:C     | 2.60                     | 0.45              |
| 39:DS:38:GLN:HG3  | 39:DS:47:THR:HG21  | 1.98                     | 0.45              |
| 40:DT:91:ARG:C    | 40:DT:93:ARG:H     | 2.25                     | 0.45              |
| 41:DU:15:LYS:HD3  | 41:DU:15:LYS:N     | 2.30                     | 0.45              |
| 41:DU:91:ASP:O    | 41:DU:92:ARG:C     | 2.60                     | 0.45              |
| 43:DW:19:LEU:O    | 52:D5:25:LEU:HD12  | 2.16                     | 0.45              |
| 43:DW:64:MET:HE3  | 43:DW:109:GLU:HG2  | 1.97                     | 0.45              |
| 43:DW:88:ARG:NH1  | 43:DW:94:ASP:OD1   | 2.50                     | 0.45              |
| 55:D8:44:LYS:HD2  | 55:D8:44:LYS:N     | 2.29                     | 0.45              |
| 1:AA:33:A:H61     | 1:AA:551:U:H3      | 1.64                     | 0.45              |
| 1:AA:368:U:OP1    | 33:DI:91:SER:OG    | 2.30                     | 0.45              |
| 1:AA:779:C:O2'    | 11:AK:120:ARG:HD3  | 2.17                     | 0.45              |
| 1:AA:1299:A:N7    | 1:AA:1301:U:C2     | 2.85                     | 0.45              |
| 1:AA:1368:G:H2'   | 1:AA:1369:C:C6     | 2.52                     | 0.45              |
| 2:AB:112:VAL:O    | 2:AB:115:LEU:HB3   | 2.17                     | 0.45              |
| 5:AE:76:ILE:CG1   | 5:AE:142:LEU:HD13  | 2.44                     | 0.45              |
| 8:AH:86:ILE:CG1   | 8:AH:133:LEU:HD22  | 2.47                     | 0.45              |
| 9:AI:55:ALA:HB1   | 9:AI:59:PHE:CE1    | 2.52                     | 0.45              |
| 12:AL:83:VAL:HG21 | 12:AL:100:ILE:HD13 | 1.99                     | 0.45              |
| 15:AO:17:ARG:N    | 15:AO:21:ASP:OD1   | 2.44                     | 0.45              |
| 16:AP:72:ARG:O    | 16:AP:75:ARG:N     | 2.50                     | 0.45              |
| 18:AR:58:LEU:H    | 18:AR:58:LEU:CD1   | 2.30                     | 0.45              |
| 20:AT:73:HIS:O    | 20:AT:76:ALA:HB3   | 2.17                     | 0.45              |
| 22:AV:70:C:H2'    | 22:AV:71:G:O4'     | 2.16                     | 0.45              |
| 24:AX:16:A:H2'    | 24:AX:17:U:O4'     | 2.17                     | 0.45              |
| 25:BA:636:G:O2'   | 25:BA:638:G:O2'    | 2.28                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:BA:1149:G:H2'   | 25:BA:1150:C:C6    | 2.52                     | 0.45              |
| 25:BA:1312:U:H4'   | 25:BA:1313:U:O5'   | 2.16                     | 0.45              |
| 25:BA:1414:G:H1    | 25:BA:1588:C:H42   | 1.65                     | 0.45              |
| 25:BA:1488:G:H5'   | 25:BA:1489:U:OP2   | 2.17                     | 0.45              |
| 25:BA:2327:A:H2'   | 25:BA:2328:A:C8    | 2.52                     | 0.45              |
| 25:BA:2346:A:C2    | 25:BA:2383:G:C2    | 3.05                     | 0.45              |
| 25:BA:2444:G:P     | 30:BF:68:LYS:HE2   | 2.57                     | 0.45              |
| 25:BA:2578:G:C2    | 25:BA:2579:C:C4    | 3.05                     | 0.45              |
| 30:BF:53:THR:HG23  | 30:BF:56:GLU:CG    | 2.44                     | 0.45              |
| 30:BF:64:ILE:CG2   | 30:BF:65:TRP:CE2   | 3.00                     | 0.45              |
| 31:BG:131:TYR:HE2  | 31:BG:133:LEU:HD22 | 1.82                     | 0.45              |
| 36:BP:83:VAL:CG2   | 36:BP:105:LEU:HD22 | 2.45                     | 0.45              |
| 36:BP:138:LEU:HD13 | 36:BP:144:GLU:HG2  | 1.98                     | 0.45              |
| 40:BT:114:LEU:HD23 | 40:BT:114:LEU:N    | 2.29                     | 0.45              |
| 48:B1:41:ARG:HD3   | 48:B1:43:TYR:OH    | 2.17                     | 0.45              |
| 55:B8:13:ARG:O     | 55:B8:14:VAL:HB    | 2.16                     | 0.45              |
| 1:CA:197:A:O2'     | 1:CA:220:G:N2      | 2.50                     | 0.45              |
| 1:CA:993:G:H2'     | 1:CA:995:C:H41     | 1.82                     | 0.45              |
| 1:CA:1005:A:HO2'   | 1:CA:1037:C:HO2'   | 1.55                     | 0.45              |
| 1:CA:1067:A:H1'    | 1:CA:1068:G:C1'    | 2.46                     | 0.45              |
| 1:CA:1080:A:H4'    | 5:CE:16:THR:HB     | 1.97                     | 0.45              |
| 3:CC:132:ARG:O     | 3:CC:136:GLN:CB    | 2.62                     | 0.45              |
| 4:CD:7:PRO:CB      | 4:CD:10:ARG:HD2    | 2.28                     | 0.45              |
| 4:CD:162:LEU:O     | 4:CD:165:MET:N     | 2.50                     | 0.45              |
| 5:CE:10:MET:HE3    | 5:CE:10:MET:HB3    | 1.83                     | 0.45              |
| 7:CG:43:PHE:HD1    | 7:CG:43:PHE:C      | 2.24                     | 0.45              |
| 10:CJ:54:PHE:CZ    | 10:CJ:55:LYS:NZ    | 2.85                     | 0.45              |
| 12:CL:39:VAL:CG1   | 12:CL:40:VAL:N     | 2.80                     | 0.45              |
| 12:CL:40:VAL:HG22  | 12:CL:56:ALA:HB2   | 1.98                     | 0.45              |
| 12:CL:119:LYS:HB2  | 12:CL:120:TYR:CE1  | 2.52                     | 0.45              |
| 13:CM:88:ARG:HD3   | 13:CM:98:VAL:CG1   | 2.47                     | 0.45              |
| 13:CM:120:LYS:N    | 13:CM:120:LYS:CD   | 2.60                     | 0.45              |
| 18:CR:52:PRO:O     | 18:CR:56:THR:HG23  | 2.17                     | 0.45              |
| 22:CV:22:A:C5      | 22:CV:49:C:N4      | 2.85                     | 0.45              |
| 23:CY:28:G:C4      | 23:CY:29:G:C8      | 3.05                     | 0.45              |
| 25:DA:13:A:C5      | 25:DA:525:U:C4     | 3.05                     | 0.45              |
| 25:DA:480:A:H5''   | 45:DY:46:LYS:HE2   | 1.99                     | 0.45              |
| 25:DA:1103:A:H2'   | 25:DA:1104:C:H5'   | 1.99                     | 0.45              |
| 25:DA:1453:U:H1'   | 38:DR:60:LEU:HD21  | 1.98                     | 0.45              |
| 25:DA:1568:G:P     | 28:DD:63:ARG:HH12  | 2.40                     | 0.45              |
| 25:DA:2751:G:P     | 25:DA:2751:G:C8    | 3.09                     | 0.45              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 27:DC:20:TYR:CE1   | 27:DC:22:ILE:HD13 | 2.52                     | 0.45              |
| 28:DD:31:LYS:O     | 28:DD:35:LYS:CB   | 2.56                     | 0.45              |
| 29:DE:97:LYS:O     | 29:DE:98:PRO:C    | 2.59                     | 0.45              |
| 31:DG:83:ARG:O     | 31:DG:84:LYS:C    | 2.60                     | 0.45              |
| 32:DH:153:LYS:CE   | 32:DH:153:LYS:HA  | 2.47                     | 0.45              |
| 41:DU:29:SER:OG    | 41:DU:30:LYS:HE2  | 2.17                     | 0.45              |
| 45:DY:51:VAL:HG22  | 45:DY:57:GLN:HA   | 1.99                     | 0.45              |
| 46:DZ:14:LYS:C     | 46:DZ:16:SER:H    | 2.22                     | 0.45              |
| 46:DZ:38:TYR:CD1   | 46:DZ:38:TYR:O    | 2.70                     | 0.45              |
| 47:D0:25:ARG:HG3   | 47:D0:31:VAL:CG1  | 2.47                     | 0.45              |
| 1:AA:452:A:H4'     | 16:AP:72:ARG:CZ   | 2.47                     | 0.44              |
| 1:AA:1105:A:H2'    | 1:AA:1106:G:H8    | 1.82                     | 0.44              |
| 2:AB:15:VAL:N      | 2:AB:16:HIS:ND1   | 2.60                     | 0.44              |
| 2:AB:100:GLY:HA2   | 2:AB:176:GLU:OE1  | 2.17                     | 0.44              |
| 2:AB:178:ARG:HG3   | 8:AH:72:PRO:HA    | 1.99                     | 0.44              |
| 2:AB:181:PHE:O     | 2:AB:182:ILE:C    | 2.59                     | 0.44              |
| 3:AC:11:ARG:HH21   | 3:AC:180:ALA:CB   | 2.26                     | 0.44              |
| 4:AD:103:ASN:O     | 4:AD:107:ARG:HG2  | 2.17                     | 0.44              |
| 5:AE:91:LEU:HD23   | 5:AE:138:ALA:HB1  | 1.98                     | 0.44              |
| 9:AI:53:VAL:HB     | 9:AI:92:TYR:CE2   | 2.51                     | 0.44              |
| 10:AJ:45:ARG:HG3   | 10:AJ:45:ARG:NH1  | 2.31                     | 0.44              |
| 10:AJ:91:PRO:HB3   | 10:AJ:94:VAL:HB   | 1.99                     | 0.44              |
| 14:AN:2:ALA:O      | 14:AN:6:LEU:HD12  | 2.17                     | 0.44              |
| 16:AP:19:ILE:CG2   | 16:AP:36:ILE:HG13 | 2.47                     | 0.44              |
| 16:AP:82:GLN:O     | 16:AP:83:GLU:CB   | 2.65                     | 0.44              |
| 17:AQ:75:ARG:HG3   | 17:AQ:75:ARG:HH11 | 1.82                     | 0.44              |
| 22:AV:12:G:N3      | 25:BA:1923:U:O2'  | 2.48                     | 0.44              |
| 25:BA:242:G:N2     | 25:BA:254:G:C5    | 2.85                     | 0.44              |
| 25:BA:534:U:O2     | 41:BU:49:HIS:HE1  | 2.00                     | 0.44              |
| 25:BA:669:G:H5''   | 25:BA:670:A:P     | 2.57                     | 0.44              |
| 25:BA:1620:G:HO2'  | 54:B7:2:LYS:HG3   | 1.81                     | 0.44              |
| 25:BA:1653:G:O2'   | 25:BA:1654:A:O5'  | 2.35                     | 0.44              |
| 25:BA:1654:A:C8    | 25:BA:2823:A:O4'  | 2.70                     | 0.44              |
| 25:BA:1778:U:O4    | 25:BA:1784:A:H1'  | 2.18                     | 0.44              |
| 27:BC:77:ILE:O     | 27:BC:77:ILE:CG2  | 2.65                     | 0.44              |
| 28:BD:12:SER:HB2   | 28:BD:208:LYS:HB3 | 1.98                     | 0.44              |
| 28:BD:206:LEU:HD23 | 28:BD:206:LEU:HA  | 1.72                     | 0.44              |
| 29:BE:4:ILE:HG22   | 29:BE:198:VAL:O   | 2.18                     | 0.44              |
| 30:BF:42:ALA:O     | 30:BF:45:ARG:HB2  | 2.15                     | 0.44              |
| 31:BG:91:ARG:HD2   | 31:BG:92:VAL:N    | 2.33                     | 0.44              |
| 31:BG:126:ASP:O    | 31:BG:128:ARG:NE  | 2.50                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 32:BH:58:GLU:O     | 32:BH:61:HIS:N     | 2.50                     | 0.44              |
| 32:BH:102:ALA:CB   | 32:BH:117:PRO:HD3  | 2.38                     | 0.44              |
| 33:BI:136:VAL:HA   | 33:BI:137:PRO:HD3  | 1.61                     | 0.44              |
| 34:BN:123:TYR:CD1  | 34:BN:129:PRO:HD2  | 2.52                     | 0.44              |
| 35:BO:20:MET:HG2   | 35:BO:21:CYS:N     | 2.32                     | 0.44              |
| 36:BP:101:VAL:HG21 | 36:BP:108:LYS:H    | 1.81                     | 0.44              |
| 36:BP:110:TYR:HD2  | 36:BP:111:ARG:HH21 | 1.64                     | 0.44              |
| 38:BR:117:VAL:O    | 38:BR:118:GLU:HB2  | 2.16                     | 0.44              |
| 49:B2:57:ILE:O     | 49:B2:58:ALA:C     | 2.60                     | 0.44              |
| 53:B6:20:ASN:C     | 53:B6:21:TYR:CG    | 2.95                     | 0.44              |
| 53:B6:26:ASN:OD1   | 53:B6:32:ASN:OD1   | 2.35                     | 0.44              |
| 53:B6:30:THR:O     | 53:B6:31:PRO:C     | 2.60                     | 0.44              |
| 1:CA:500:G:N2      | 1:CA:546:G:H1'     | 2.32                     | 0.44              |
| 1:CA:738:C:H5''    | 6:CF:69:GLU:HB2    | 1.99                     | 0.44              |
| 1:CA:747:C:H3'     | 1:CA:748:C:C5      | 2.51                     | 0.44              |
| 1:CA:1358:U:OP1    | 14:CN:35:ARG:HG2   | 2.18                     | 0.44              |
| 1:CA:1397:C:O2'    | 1:CA:1398:A:P      | 2.75                     | 0.44              |
| 2:CB:28:PHE:HE2    | 2:CB:31:TYR:CD1    | 2.35                     | 0.44              |
| 2:CB:219:VAL:HA    | 2:CB:222:ILE:HD12  | 1.99                     | 0.44              |
| 3:CC:203:PHE:HZ    | 3:CC:206:GLU:OE1   | 2.01                     | 0.44              |
| 4:CD:88:VAL:O      | 4:CD:92:VAL:HG23   | 2.17                     | 0.44              |
| 4:CD:201:GLN:O     | 4:CD:205:GLU:HG3   | 2.16                     | 0.44              |
| 5:CE:79:GLU:H      | 5:CE:79:GLU:HG3    | 1.42                     | 0.44              |
| 7:CG:111:ARG:HG2   | 7:CG:112:PRO:HD2   | 1.99                     | 0.44              |
| 8:CH:16:ALA:O      | 8:CH:17:THR:C      | 2.60                     | 0.44              |
| 13:CM:26:GLY:O     | 13:CM:27:LYS:C     | 2.60                     | 0.44              |
| 13:CM:84:ILE:HD11  | 19:CS:66:MET:HG2   | 1.98                     | 0.44              |
| 15:CO:65:ARG:O     | 15:CO:68:ARG:N     | 2.51                     | 0.44              |
| 17:CQ:90:ILE:O     | 17:CQ:93:GLN:HB2   | 2.17                     | 0.44              |
| 18:CR:59:SER:HB3   | 18:CR:62:GLU:CB    | 2.47                     | 0.44              |
| 19:CS:49:ILE:HD13  | 19:CS:71:LEU:HD21  | 1.99                     | 0.44              |
| 20:CT:41:ILE:C     | 20:CT:43:LEU:N     | 2.73                     | 0.44              |
| 20:CT:51:GLU:O     | 20:CT:55:ILE:N     | 2.44                     | 0.44              |
| 23:CW:40:C:O5'     | 23:CW:40:C:H6      | 2.00                     | 0.44              |
| 25:DA:955:C:H5'    | 25:DA:956:G:OP2    | 2.18                     | 0.44              |
| 25:DA:1681:G:H4'   | 25:DA:1682:G:OP1   | 2.17                     | 0.44              |
| 25:DA:1935:G:H1'   | 25:DA:1964:G:N2    | 2.32                     | 0.44              |
| 25:DA:2097:C:H2'   | 25:DA:2098:U:O4'   | 2.17                     | 0.44              |
| 25:DA:2517:C:N3    | 25:DA:2542:A:N6    | 2.65                     | 0.44              |
| 25:DA:2892:A:C5    | 25:DA:2893:G:H1'   | 2.52                     | 0.44              |
| 28:DD:34:VAL:HG22  | 28:DD:34:VAL:O     | 2.17                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 28:DD:43:ARG:H     | 28:DD:43:ARG:HG3   | 1.60                     | 0.44              |
| 31:DG:151:ALA:HB3  | 31:DG:153:ARG:HH11 | 1.80                     | 0.44              |
| 33:DI:10:GLU:OE2   | 33:DI:11:ASN:N     | 2.50                     | 0.44              |
| 33:DI:72:LEU:CD1   | 33:DI:107:VAL:HG11 | 2.43                     | 0.44              |
| 34:DN:99:LEU:HD12  | 34:DN:122:VAL:HG21 | 1.98                     | 0.44              |
| 35:DO:10:VAL:HG21  | 35:DO:16:ALA:O     | 2.17                     | 0.44              |
| 35:DO:20:MET:O     | 35:DO:41:ALA:CB    | 2.65                     | 0.44              |
| 44:DX:64:LYS:HD3   | 44:DX:73:ARG:NE    | 2.31                     | 0.44              |
| 44:DX:84:ALA:HB1   | 44:DX:85:PRO:HD2   | 1.97                     | 0.44              |
| 52:D5:20:ARG:HA    | 52:D5:23:HIS:HD1   | 1.82                     | 0.44              |
| 1:AA:802:A:H3'     | 1:AA:803:G:C8      | 2.51                     | 0.44              |
| 1:AA:1002:G:N3     | 1:AA:1002:G:H2'    | 2.32                     | 0.44              |
| 1:AA:1229:A:H2'    | 1:AA:1230:C:C6     | 2.51                     | 0.44              |
| 3:AC:6:HIS:CE1     | 14:AN:49:HIS:HB3   | 2.52                     | 0.44              |
| 4:AD:58:LEU:C      | 4:AD:58:LEU:HD13   | 2.42                     | 0.44              |
| 4:AD:169:LYS:O     | 4:AD:170:VAL:HG23  | 2.16                     | 0.44              |
| 8:AH:97:VAL:CG1    | 8:AH:98:LYS:N      | 2.81                     | 0.44              |
| 9:AI:114:TYR:N     | 9:AI:114:TYR:HD2   | 2.15                     | 0.44              |
| 10:AJ:38:ILE:HA    | 10:AJ:39:PRO:HD3   | 1.78                     | 0.44              |
| 13:AM:58:GLU:O     | 13:AM:62:ASN:ND2   | 2.47                     | 0.44              |
| 15:AO:62:GLN:HA    | 15:AO:62:GLN:OE1   | 2.17                     | 0.44              |
| 19:AS:43:GLU:C     | 19:AS:45:VAL:N     | 2.75                     | 0.44              |
| 20:AT:37:SER:CB    | 20:AT:84:LEU:HD21  | 2.35                     | 0.44              |
| 23:AW:43:C:O2'     | 23:AW:44:G:H5'     | 2.17                     | 0.44              |
| 23:AY:32:U:O2      | 23:AY:32:U:C2'     | 2.56                     | 0.44              |
| 25:BA:34:C:O2'     | 25:BA:35:G:P       | 2.74                     | 0.44              |
| 25:BA:94(A):G:H2'  | 25:BA:95:G:O4'     | 2.16                     | 0.44              |
| 25:BA:350:U:H2'    | 25:BA:351:G:O4'    | 2.17                     | 0.44              |
| 25:BA:504:U:H5''   | 25:BA:505:A:H5'    | 1.99                     | 0.44              |
| 25:BA:729:G:O2'    | 25:BA:763:G:H4'    | 2.18                     | 0.44              |
| 25:BA:1468:C:H2'   | 25:BA:1469:A:H8    | 1.82                     | 0.44              |
| 25:BA:1912:A:C2    | 25:BA:1919:A:C5    | 3.04                     | 0.44              |
| 27:BC:51:PRO:CG    | 27:BC:204:ALA:HB2  | 2.46                     | 0.44              |
| 28:BD:35:LYS:NZ    | 28:BD:103:ARG:HA   | 2.32                     | 0.44              |
| 29:BE:101:ARG:HH22 | 29:BE:171:GLU:HB2  | 1.81                     | 0.44              |
| 29:BE:107:THR:O    | 29:BE:190:GLY:HA2  | 2.16                     | 0.44              |
| 32:BH:103:LEU:H    | 32:BH:103:LEU:HD23 | 1.82                     | 0.44              |
| 33:BI:64:GLU:O     | 33:BI:66:GLU:N     | 2.50                     | 0.44              |
| 34:BN:57:ALA:C     | 34:BN:58:ASP:O     | 2.60                     | 0.44              |
| 34:BN:62:VAL:HG11  | 34:BN:66:LYS:HB3   | 2.00                     | 0.44              |
| 35:BO:102:VAL:O    | 35:BO:102:VAL:HG23 | 2.16                     | 0.44              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 37:BQ:55:VAL:CG2  | 37:BQ:56:ARG:N     | 2.78                     | 0.44              |
| 37:BQ:56:ARG:CZ   | 37:BQ:56:ARG:CA    | 2.89                     | 0.44              |
| 42:BV:39:LEU:O    | 42:BV:40:LEU:CB    | 2.65                     | 0.44              |
| 44:BX:13:LEU:HD23 | 44:BX:13:LEU:HA    | 1.69                     | 0.44              |
| 1:CA:109:A:C6     | 1:CA:326:G:C6      | 3.05                     | 0.44              |
| 1:CA:484:G:H5'    | 1:CA:486:U:H5'     | 1.99                     | 0.44              |
| 1:CA:1211:U:H1'   | 1:CA:1213:A:C2     | 2.52                     | 0.44              |
| 1:CA:1232:U:OP1   | 9:CI:124:GLN:NE2   | 2.50                     | 0.44              |
| 2:CB:25:ASN:HA    | 2:CB:26:PRO:HD2    | 1.77                     | 0.44              |
| 2:CB:167:PRO:O    | 2:CB:168:THR:C     | 2.59                     | 0.44              |
| 7:CG:108:ALA:O    | 7:CG:111:ARG:HB2   | 2.17                     | 0.44              |
| 16:CP:50:LYS:C    | 16:CP:50:LYS:HD3   | 2.42                     | 0.44              |
| 16:CP:82:GLN:N    | 16:CP:82:GLN:NE2   | 2.57                     | 0.44              |
| 19:CS:35:SER:C    | 19:CS:37:ARG:H     | 2.25                     | 0.44              |
| 22:CV:55:U:H2'    | 22:CV:56:U:O4'     | 2.17                     | 0.44              |
| 25:DA:311:A:H1'   | 25:DA:332:A:C8     | 2.52                     | 0.44              |
| 25:DA:404:C:H1'   | 25:DA:406:G:C8     | 2.52                     | 0.44              |
| 25:DA:859:G:O2'   | 25:DA:860:U:OP2    | 2.28                     | 0.44              |
| 25:DA:1952:A:OP1  | 35:DO:42:SER:OG    | 2.34                     | 0.44              |
| 25:DA:2875:C:H4'  | 40:DT:5:ALA:HB2    | 1.97                     | 0.44              |
| 28:DD:70:TRP:CZ3  | 28:DD:146:GLU:OE2  | 2.70                     | 0.44              |
| 29:DE:51:PHE:O    | 29:DE:74:PRO:HB2   | 2.16                     | 0.44              |
| 29:DE:85:ASN:HA   | 29:DE:86:PRO:HD3   | 1.84                     | 0.44              |
| 30:DF:95:ARG:NH2  | 30:DF:97:TYR:HE1   | 2.15                     | 0.44              |
| 30:DF:198:ALA:C   | 30:DF:201:VAL:HG12 | 2.42                     | 0.44              |
| 31:DG:67:LYS:CE   | 51:D4:6:HIS:CE1    | 2.86                     | 0.44              |
| 32:DH:54:ARG:NH2  | 32:DH:57:ASP:OD1   | 2.47                     | 0.44              |
| 33:DI:57:ARG:C    | 33:DI:60:GLU:HB3   | 2.43                     | 0.44              |
| 34:DN:57:ALA:N    | 34:DN:124:ALA:HA   | 2.32                     | 0.44              |
| 39:DS:15:ARG:HG3  | 39:DS:19:LYS:HE2   | 2.00                     | 0.44              |
| 40:DT:87:ASP:O    | 40:DT:87:ASP:OD1   | 2.35                     | 0.44              |
| 46:DZ:119:GLU:HA  | 46:DZ:171:ILE:O    | 2.17                     | 0.44              |
| 52:D5:47:PRO:HG2  | 52:D5:48:GLU:OE1   | 2.18                     | 0.44              |
| 1:AA:243:A:C5     | 1:AA:281:G:C2      | 3.06                     | 0.44              |
| 1:AA:376:G:H5''   | 16:AP:5:ARG:HB2    | 1.99                     | 0.44              |
| 1:AA:499:A:O2'    | 1:AA:500:G:C8      | 2.70                     | 0.44              |
| 1:AA:1067:A:H1'   | 1:AA:1068:G:O4'    | 2.17                     | 0.44              |
| 2:AB:57:PHE:O     | 2:AB:61:LEU:HB3    | 2.17                     | 0.44              |
| 2:AB:70:PHE:CE2   | 2:AB:163:PHE:CD1   | 3.05                     | 0.44              |
| 3:AC:184:TYR:CE1  | 3:AC:199:LYS:HB3   | 2.51                     | 0.44              |
| 6:AF:67:MET:HE1   | 6:AF:75:LEU:HD13   | 1.99                     | 0.44              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 7:AG:51:GLN:OE1   | 7:AG:51:GLN:HA     | 2.16                     | 0.44              |
| 9:AI:11:LYS:O     | 9:AI:12:GLU:C      | 2.60                     | 0.44              |
| 9:AI:96:LEU:CG    | 9:AI:102:LEU:HB2   | 2.38                     | 0.44              |
| 10:AJ:50:ILE:H    | 10:AJ:50:ILE:CD1   | 2.30                     | 0.44              |
| 11:AK:44:SER:C    | 11:AK:46:GLY:H     | 2.25                     | 0.44              |
| 15:AO:25:THR:HG21 | 15:AO:70:LEU:HB2   | 1.99                     | 0.44              |
| 17:AQ:87:LYS:O    | 17:AQ:88:TYR:C     | 2.60                     | 0.44              |
| 19:AS:45:VAL:HA   | 19:AS:62:ILE:HG23  | 2.00                     | 0.44              |
| 22:AV:4:G:O2'     | 22:AV:5:G:P        | 2.75                     | 0.44              |
| 25:BA:636:G:C4    | 36:BP:115:LEU:HD11 | 2.52                     | 0.44              |
| 25:BA:710:G:H2'   | 25:BA:711:G:H8     | 1.83                     | 0.44              |
| 25:BA:1299:G:C5'  | 25:BA:1301:A:O4'   | 2.64                     | 0.44              |
| 25:BA:1300:U:H5'' | 25:BA:1301:A:O5'   | 2.18                     | 0.44              |
| 25:BA:1902:C:H4'  | 28:BD:244:ARG:HA   | 1.98                     | 0.44              |
| 27:BC:67:GLY:C    | 27:BC:69:GLY:H     | 2.26                     | 0.44              |
| 28:BD:61:LEU:HD12 | 28:BD:61:LEU:HA    | 1.64                     | 0.44              |
| 29:BE:116:VAL:CG2 | 29:BE:117:MET:N    | 2.77                     | 0.44              |
| 30:BF:9:ILE:CG2   | 30:BF:11:VAL:O     | 2.65                     | 0.44              |
| 31:BG:2:PRO:HG2   | 51:B4:51:TYR:CD2   | 2.52                     | 0.44              |
| 32:BH:54:ARG:NH2  | 32:BH:57:ASP:OD1   | 2.50                     | 0.44              |
| 32:BH:97:ARG:O    | 32:BH:98:LEU:HB2   | 2.18                     | 0.44              |
| 34:BN:133:GLN:O   | 34:BN:134:ARG:HG3  | 2.17                     | 0.44              |
| 35:BO:47:ILE:O    | 35:BO:48:PRO:O     | 2.35                     | 0.44              |
| 35:BO:87:ILE:HG23 | 35:BO:91:LEU:HA    | 1.98                     | 0.44              |
| 41:BU:17:ILE:HG21 | 41:BU:32:PHE:CE1   | 2.53                     | 0.44              |
| 42:BV:3:ALA:CB    | 42:BV:99:ILE:HG21  | 2.47                     | 0.44              |
| 43:BW:64:MET:O    | 43:BW:65:LEU:HB3   | 2.17                     | 0.44              |
| 46:BZ:4:ARG:HG3   | 46:BZ:58:VAL:HB    | 2.00                     | 0.44              |
| 48:B1:75:GLU:C    | 48:B1:77:ALA:H     | 2.26                     | 0.44              |
| 1:CA:401:C:H2'    | 1:CA:402:G:C8      | 2.52                     | 0.44              |
| 1:CA:483:C:C4     | 1:CA:484:G:C6      | 3.06                     | 0.44              |
| 1:CA:1000:U:H2'   | 1:CA:1001:A:C8     | 2.52                     | 0.44              |
| 1:CA:1229:A:H4'   | 22:CV:31:G:OP1     | 2.18                     | 0.44              |
| 2:CB:114:ARG:HH11 | 2:CB:118:LEU:HD11  | 1.82                     | 0.44              |
| 3:CC:94:LEU:HD12  | 3:CC:94:LEU:C      | 2.43                     | 0.44              |
| 13:CM:105:THR:O   | 13:CM:106:ASN:C    | 2.60                     | 0.44              |
| 15:CO:32:LEU:O    | 15:CO:33:THR:C     | 2.58                     | 0.44              |
| 23:CW:36:A:N1     | 23:CW:37:A:C6      | 2.86                     | 0.44              |
| 23:CY:41:C:H2'    | 23:CY:42:C:C6      | 2.52                     | 0.44              |
| 25:DA:764:A:O2'   | 25:DA:781:A:N6     | 2.50                     | 0.44              |
| 25:DA:796:C:H2'   | 25:DA:797:C:C6     | 2.51                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:DA:893:C:H2'   | 25:DA:894:C:C6    | 2.52                     | 0.44              |
| 25:DA:1157:G:O2'  | 50:D3:31:LEU:HD12 | 2.17                     | 0.44              |
| 25:DA:1341:U:H3'  | 25:DA:1397:U:O2   | 2.17                     | 0.44              |
| 25:DA:1342:A:C6   | 25:DA:1397:U:C6   | 3.06                     | 0.44              |
| 25:DA:2074:U:H2'  | 25:DA:2075:U:C6   | 2.53                     | 0.44              |
| 25:DA:2636:U:H4'  | 29:DE:80:GLU:CD   | 2.42                     | 0.44              |
| 26:DB:40:U:H1'    | 26:DB:45:A:N6     | 2.33                     | 0.44              |
| 27:DC:36:LYS:CD   | 27:DC:37:PHE:H    | 2.30                     | 0.44              |
| 27:DC:83:ILE:HG22 | 27:DC:83:ILE:O    | 2.18                     | 0.44              |
| 29:DE:176:ILE:HB  | 29:DE:181:LEU:HB2 | 2.00                     | 0.44              |
| 30:DF:74:ARG:HG2  | 30:DF:74:ARG:O    | 2.17                     | 0.44              |
| 33:DI:9:LEU:O     | 33:DI:10:GLU:HG3  | 2.17                     | 0.44              |
| 34:DN:104:LYS:HB2 | 34:DN:117:PHE:CE1 | 2.52                     | 0.44              |
| 34:DN:126:PRO:C   | 34:DN:127:ASP:OD1 | 2.61                     | 0.44              |
| 35:DO:101:PRO:HG3 | 40:DT:67:SER:OG   | 2.17                     | 0.44              |
| 40:DT:10:VAL:C    | 40:DT:12:SER:N    | 2.74                     | 0.44              |
| 45:DY:84:ARG:HH12 | 45:DY:97:ARG:HB3  | 1.80                     | 0.44              |
| 46:DZ:23:LYS:CG   | 46:DZ:38:TYR:CE1  | 2.99                     | 0.44              |
| 48:D1:46:LEU:H    | 48:D1:46:LEU:HD22 | 1.82                     | 0.44              |
| 49:D2:17:SER:HA   | 49:D2:18:PRO:HD2  | 1.83                     | 0.44              |
| 50:D3:44:ARG:O    | 50:D3:45:GLY:C    | 2.61                     | 0.44              |
| 53:D6:14:THR:O    | 53:D6:49:HIS:HA   | 2.17                     | 0.44              |
| 53:D6:44:ARG:HD3  | 53:D6:44:ARG:HA   | 1.31                     | 0.44              |
| 54:D7:31:LEU:HA   | 54:D7:31:LEU:HD23 | 1.63                     | 0.44              |
| 1:AA:339:C:H2'    | 1:AA:340:U:C6     | 2.52                     | 0.44              |
| 1:AA:405:U:OP1    | 1:AA:406:G:O2'    | 2.26                     | 0.44              |
| 1:AA:668:G:C2'    | 15:AO:46:HIS:HD2  | 2.31                     | 0.44              |
| 1:AA:742:G:P      | 15:AO:35:ARG:HH22 | 2.41                     | 0.44              |
| 1:AA:1070:U:H2'   | 1:AA:1071:C:H6    | 1.82                     | 0.44              |
| 2:AB:36:ARG:HE    | 2:AB:36:ARG:H     | 1.65                     | 0.44              |
| 4:AD:105:VAL:HG12 | 4:AD:105:VAL:O    | 2.17                     | 0.44              |
| 4:AD:155:LEU:O    | 4:AD:156:GLU:C    | 2.60                     | 0.44              |
| 5:AE:6:PHE:CD1    | 5:AE:6:PHE:N      | 2.85                     | 0.44              |
| 5:AE:139:LEU:O    | 5:AE:142:LEU:HG   | 2.18                     | 0.44              |
| 7:AG:69:VAL:O     | 7:AG:69:VAL:CG1   | 2.65                     | 0.44              |
| 7:AG:75:VAL:O     | 7:AG:75:VAL:HG23  | 2.18                     | 0.44              |
| 14:AN:15:LYS:C    | 14:AN:16:PHE:CD2  | 2.95                     | 0.44              |
| 18:AR:76:LEU:HD13 | 18:AR:76:LEU:HA   | 1.84                     | 0.44              |
| 19:AS:37:ARG:H    | 19:AS:37:ARG:HG3  | 1.61                     | 0.44              |
| 22:AV:1:C:C5      | 22:AV:2:G:C8      | 3.05                     | 0.44              |
| 22:AV:20:G:H3'    | 22:AV:21:U:O2     | 2.18                     | 0.44              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 23:AW:45:U:H6      | 23:AW:45:U:H3'    | 1.81                     | 0.44              |
| 23:AY:29:G:H5'     | 23:AY:30:G:OP2    | 2.17                     | 0.44              |
| 25:BA:469:G:O6     | 54:B7:39:ARG:NH2  | 2.51                     | 0.44              |
| 25:BA:478:A:C6     | 25:BA:480:A:C6    | 3.06                     | 0.44              |
| 25:BA:1127:A:H2'   | 25:BA:1128:A:H5'' | 1.99                     | 0.44              |
| 25:BA:1237:A:H4'   | 25:BA:1238:G:O5'  | 2.18                     | 0.44              |
| 25:BA:1409:C:H2'   | 25:BA:1410:G:C8   | 2.52                     | 0.44              |
| 25:BA:1455:G:C8    | 38:BR:60:LEU:HD11 | 2.53                     | 0.44              |
| 25:BA:1799:G:O6    | 28:BD:178:PRO:HD2 | 2.17                     | 0.44              |
| 25:BA:2437:U:H2'   | 25:BA:2438:U:C6   | 2.52                     | 0.44              |
| 25:BA:2554:U:H2'   | 25:BA:2555:U:C6   | 2.52                     | 0.44              |
| 25:BA:2556:C:H2'   | 25:BA:2557:G:O4'  | 2.17                     | 0.44              |
| 25:BA:2612:C:C4    | 25:BA:2613:U:H5   | 2.35                     | 0.44              |
| 25:BA:2681:C:C4    | 25:BA:2724:C:C5   | 3.06                     | 0.44              |
| 27:BC:46:LYS:C     | 27:BC:47:LEU:HD23 | 2.42                     | 0.44              |
| 28:BD:11:PRO:O     | 28:BD:13:ARG:N    | 2.50                     | 0.44              |
| 28:BD:248:SER:HB2  | 28:BD:250:TRP:CE3 | 2.51                     | 0.44              |
| 29:BE:117:MET:HA   | 29:BE:122:PHE:N   | 2.30                     | 0.44              |
| 32:BH:20:ALA:HB2   | 32:BH:25:LYS:HE3  | 1.98                     | 0.44              |
| 36:BP:49:ARG:NH2   | 36:BP:50:ARG:HH22 | 2.15                     | 0.44              |
| 39:BS:15:ARG:HA    | 39:BS:18:ILE:HB   | 1.98                     | 0.44              |
| 41:BU:95:LEU:HD13  | 42:BV:4:ILE:HG21  | 1.96                     | 0.44              |
| 42:BV:99:ILE:HD13  | 42:BV:99:ILE:N    | 2.32                     | 0.44              |
| 43:BW:55:ALA:C     | 43:BW:57:ASN:N    | 2.73                     | 0.44              |
| 46:BZ:128:VAL:HG22 | 46:BZ:132:ASN:HB2 | 1.99                     | 0.44              |
| 47:B0:26:TYR:O     | 47:B0:29:GLN:HG3  | 2.18                     | 0.44              |
| 49:B2:63:VAL:CA    | 49:B2:66:GLU:HG2  | 2.46                     | 0.44              |
| 55:B8:62:LEU:N     | 55:B8:63:PRO:CD   | 2.80                     | 0.44              |
| 1:CA:321:A:N6      | 1:CA:328:C:O2'    | 2.38                     | 0.44              |
| 1:CA:426:G:H2'     | 1:CA:427:U:C6     | 2.52                     | 0.44              |
| 1:CA:728:A:H2'     | 1:CA:729:A:C8     | 2.52                     | 0.44              |
| 1:CA:971:G:OP1     | 1:CA:971:G:H3'    | 2.17                     | 0.44              |
| 1:CA:1286:A:C8     | 1:CA:1287:A:H4'   | 2.51                     | 0.44              |
| 1:CA:1363(A):A:H1' | 1:CA:1365:G:N7    | 2.32                     | 0.44              |
| 2:CB:28:PHE:CD1    | 2:CB:28:PHE:O     | 2.71                     | 0.44              |
| 3:CC:90:GLU:HA     | 3:CC:93:LYS:HB3   | 1.98                     | 0.44              |
| 3:CC:91:LEU:O      | 3:CC:95:THR:HB    | 2.17                     | 0.44              |
| 5:CE:48:ALA:HB3    | 5:CE:54:ALA:H     | 1.76                     | 0.44              |
| 5:CE:118:ILE:HG13  | 5:CE:119:LEU:N    | 2.33                     | 0.44              |
| 7:CG:47:CYS:C      | 7:CG:49:ILE:N     | 2.75                     | 0.44              |
| 7:CG:117:ALA:O     | 7:CG:118:VAL:C    | 2.57                     | 0.44              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 7:CG:147:ALA:C    | 7:CG:149:ARG:H     | 2.24                     | 0.44              |
| 8:CH:73:ASP:OD2   | 8:CH:75:ARG:HD3    | 2.17                     | 0.44              |
| 8:CH:116:LYS:HD2  | 8:CH:129:VAL:CG1   | 2.38                     | 0.44              |
| 10:CJ:23:ILE:HG23 | 10:CJ:85:LEU:HD21  | 1.98                     | 0.44              |
| 15:CO:67:LEU:HA   | 15:CO:67:LEU:HD23  | 1.71                     | 0.44              |
| 17:CQ:29:HIS:N    | 17:CQ:33:GLY:O     | 2.48                     | 0.44              |
| 20:CT:92:LEU:N    | 20:CT:92:LEU:HD23  | 2.31                     | 0.44              |
| 23:CW:14:A:N1     | 23:CW:15:G:H1'     | 2.32                     | 0.44              |
| 23:CW:37:A:C5     | 23:CW:38:A:C6      | 3.05                     | 0.44              |
| 25:DA:9274:U:O2'  | 25:DA:9275:C:P     | 2.75                     | 0.44              |
| 25:DA:530:G:N2    | 25:DA:2021:C:O2'   | 2.51                     | 0.44              |
| 25:DA:555:U:O2'   | 25:DA:556:G:C8     | 2.70                     | 0.44              |
| 25:DA:606:U:H4'   | 25:DA:658:C:H4'    | 1.99                     | 0.44              |
| 25:DA:910:A:C4    | 37:DQ:13:GLN:OE1   | 2.70                     | 0.44              |
| 25:DA:1332:G:H5'  | 25:DA:1333:C:OP2   | 2.18                     | 0.44              |
| 25:DA:1339:G:N1   | 25:DA:1340:U:O4    | 2.50                     | 0.44              |
| 25:DA:1449:A:C2   | 25:DA:1529:G:H1'   | 2.53                     | 0.44              |
| 25:DA:2848:G:N2   | 25:DA:2867:G:N9    | 2.66                     | 0.44              |
| 28:DD:28:GLU:N    | 28:DD:29:PRO:CD    | 2.79                     | 0.44              |
| 29:DE:6:GLY:O     | 29:DE:195:LEU:HD12 | 2.17                     | 0.44              |
| 30:DF:46:ARG:CG   | 30:DF:46:ARG:NH1   | 2.72                     | 0.44              |
| 30:DF:52:LYS:HG2  | 30:DF:56:GLU:HB2   | 1.99                     | 0.44              |
| 32:DH:103:LEU:CD1 | 32:DH:131:VAL:HG11 | 2.48                     | 0.44              |
| 32:DH:126:PRO:HB2 | 32:DH:130:ARG:NH1  | 2.32                     | 0.44              |
| 32:DH:127:GLU:CB  | 32:DH:130:ARG:HB3  | 2.47                     | 0.44              |
| 33:DI:25:TYR:CE2  | 33:DI:29:TYR:CD2   | 2.95                     | 0.44              |
| 33:DI:71:ILE:HD13 | 33:DI:71:ILE:C     | 2.43                     | 0.44              |
| 34:DN:102:ALA:O   | 34:DN:106:MET:CE   | 2.66                     | 0.44              |
| 34:DN:128:HIS:C   | 34:DN:130:HIS:N    | 2.75                     | 0.44              |
| 39:DS:20:ARG:C    | 39:DS:22:GLY:N     | 2.74                     | 0.44              |
| 39:DS:78:LEU:HD11 | 39:DS:107:GLU:O    | 2.18                     | 0.44              |
| 41:DU:115:ALA:C   | 41:DU:117:GLN:N    | 2.75                     | 0.44              |
| 42:DV:89:GLN:HE21 | 42:DV:89:GLN:CA    | 2.07                     | 0.44              |
| 45:DY:56:PRO:O    | 45:DY:57:GLN:O     | 2.36                     | 0.44              |
| 49:D2:57:ILE:H    | 49:D2:57:ILE:HG12  | 1.56                     | 0.44              |
| 49:D2:64:LEU:C    | 49:D2:64:LEU:HD23  | 2.43                     | 0.44              |
| 53:D6:9:LEU:HD23  | 53:D6:10:LEU:O     | 2.17                     | 0.44              |
| 1:AA:384:G:H2'    | 1:AA:385:C:C6      | 2.51                     | 0.44              |
| 1:AA:422:C:H1'    | 1:AA:423:G:C2      | 2.52                     | 0.44              |
| 1:AA:1251:A:H1'   | 1:AA:1369:C:O2'    | 2.16                     | 0.44              |
| 1:AA:1507:A:H61   | 1:AA:1528:U:H3     | 1.65                     | 0.44              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 2:AB:51:LEU:O      | 2:AB:55:PHE:HD2   | 2.00                     | 0.44              |
| 2:AB:200:ILE:HG22  | 2:AB:202:PRO:CD   | 2.47                     | 0.44              |
| 2:AB:212:GLN:NE2   | 2:AB:235:SER:HB3  | 2.32                     | 0.44              |
| 4:AD:194:LEU:N     | 4:AD:194:LEU:CD2  | 2.81                     | 0.44              |
| 6:AF:14:LEU:HA     | 6:AF:14:LEU:HD23  | 1.58                     | 0.44              |
| 6:AF:61:LEU:HD23   | 6:AF:63:TYR:OH    | 2.17                     | 0.44              |
| 6:AF:72:VAL:CG1    | 6:AF:73:ASN:H     | 2.18                     | 0.44              |
| 9:AI:114:TYR:HD1   | 10:AJ:60:ARG:HD2  | 1.83                     | 0.44              |
| 10:AJ:81:THR:OG1   | 10:AJ:82:ILE:N    | 2.51                     | 0.44              |
| 16:AP:39:TYR:CZ    | 16:AP:41:PRO:HB3  | 2.53                     | 0.44              |
| 25:BA:811:U:H3'    | 36:BP:22:GLY:CA   | 2.48                     | 0.44              |
| 25:BA:817:C:H2'    | 25:BA:818:G:O4'   | 2.18                     | 0.44              |
| 25:BA:845:G:H8     | 25:BA:845:G:OP2   | 2.01                     | 0.44              |
| 25:BA:919:G:H2'    | 25:BA:920:G:H8    | 1.82                     | 0.44              |
| 25:BA:1314:C:OP1   | 25:BA:1332:G:H5'' | 2.17                     | 0.44              |
| 25:BA:1762:A:H5'   | 25:BA:1763:G:OP2  | 2.18                     | 0.44              |
| 25:BA:1769:G:O2'   | 25:BA:1958:C:OP1  | 2.25                     | 0.44              |
| 25:BA:2022:U:OP2   | 52:B5:15:ARG:NH2  | 2.50                     | 0.44              |
| 25:BA:2875:C:H2'   | 25:BA:2876:G:O4'  | 2.18                     | 0.44              |
| 27:BC:51:PRO:HB2   | 27:BC:203:GLY:O   | 2.18                     | 0.44              |
| 28:BD:213:ARG:O    | 28:BD:216:GLY:N   | 2.36                     | 0.44              |
| 30:BF:13:SER:O     | 30:BF:14:PRO:O    | 2.35                     | 0.44              |
| 33:BI:93:THR:H     | 33:BI:96:ASP:CG   | 2.25                     | 0.44              |
| 36:BP:106:LEU:HD11 | 36:BP:112:LEU:CD2 | 2.40                     | 0.44              |
| 39:BS:20:ARG:HD3   | 39:BS:20:ARG:HA   | 1.36                     | 0.44              |
| 39:BS:28:VAL:CG1   | 39:BS:89:ARG:CG   | 2.96                     | 0.44              |
| 39:BS:92:TYR:CD2   | 39:BS:94:TYR:HB2  | 2.53                     | 0.44              |
| 43:BW:29:LEU:O     | 43:BW:33:ARG:HG3  | 2.18                     | 0.44              |
| 44:BX:37:THR:O     | 44:BX:38:GLU:C    | 2.61                     | 0.44              |
| 45:BY:28:LYS:HB3   | 45:BY:37:VAL:HG23 | 2.00                     | 0.44              |
| 45:BY:41:GLY:O     | 45:BY:42:VAL:C    | 2.61                     | 0.44              |
| 46:BZ:150:LEU:HD22 | 46:BZ:150:LEU:N   | 2.33                     | 0.44              |
| 51:B4:64:LYS:C     | 51:B4:65:CYS:HG   | 2.22                     | 0.44              |
| 52:B5:56:LYS:HG3   | 52:B5:59:GLU:CG   | 2.47                     | 0.44              |
| 1:CA:1205:U:H5''   | 3:CC:190:ARG:NH2  | 2.32                     | 0.44              |
| 2:CB:15:VAL:CG2    | 2:CB:209:ARG:HE   | 2.27                     | 0.44              |
| 2:CB:62:ALA:O      | 2:CB:63:MET:C     | 2.61                     | 0.44              |
| 3:CC:43:LEU:CD2    | 3:CC:47:LEU:HD22  | 2.48                     | 0.44              |
| 5:CE:122:GLU:HG2   | 5:CE:131:ILE:CD1  | 2.47                     | 0.44              |
| 9:CI:46:ALA:HB1    | 9:CI:77:ILE:CG2   | 2.47                     | 0.44              |
| 12:CL:31:PRO:O     | 12:CL:32:PHE:CG   | 2.69                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 12:CL:79:GLU:N     | 12:CL:79:GLU:OE2   | 2.50                     | 0.44              |
| 13:CM:25:ILE:HG13  | 13:CM:66:LEU:HD23  | 2.00                     | 0.44              |
| 22:CV:4:G:O2'      | 22:CV:5:G:P        | 2.76                     | 0.44              |
| 22:CV:20:G:C5      | 22:CV:58:A:C2      | 3.05                     | 0.44              |
| 25:DA:532:A:N6     | 25:DA:2020:A:H1'   | 2.32                     | 0.44              |
| 25:DA:587:C:O2'    | 25:DA:588:U:OP2    | 2.32                     | 0.44              |
| 25:DA:589:C:H2'    | 25:DA:590:A:C8     | 2.53                     | 0.44              |
| 25:DA:747:U:H5     | 52:D5:3:LYS:HB2    | 1.79                     | 0.44              |
| 25:DA:1902:C:H1'   | 28:DD:244:ARG:HG3  | 1.99                     | 0.44              |
| 25:DA:2020:A:O2'   | 25:DA:2021:C:O5'   | 2.33                     | 0.44              |
| 25:DA:2331:G:H4'   | 47:D0:43:THR:N     | 2.29                     | 0.44              |
| 25:DA:2335:A:C8    | 25:DA:2337:G:C5    | 3.06                     | 0.44              |
| 30:DF:165:ARG:HH11 | 30:DF:165:ARG:HB3  | 1.83                     | 0.44              |
| 30:DF:204:ASN:C    | 30:DF:206:ILE:H    | 2.24                     | 0.44              |
| 32:DH:9:ILE:O      | 32:DH:10:PRO:O     | 2.36                     | 0.44              |
| 32:DH:23:ARG:HD2   | 32:DH:34:GLU:OE2   | 2.17                     | 0.44              |
| 33:DI:112:LYS:O    | 33:DI:113:ARG:CB   | 2.65                     | 0.44              |
| 36:DP:21:ARG:O     | 36:DP:22:GLY:C     | 2.60                     | 0.44              |
| 39:DS:83:LYS:HE2   | 39:DS:84:GLN:HG3   | 1.99                     | 0.44              |
| 41:DU:92:ARG:CD    | 42:DV:11:GLN:NE2   | 2.58                     | 0.44              |
| 42:DV:98:GLU:HA    | 42:DV:98:GLU:OE1   | 2.18                     | 0.44              |
| 43:DW:22:ASP:HA    | 43:DW:25:ARG:NH1   | 2.32                     | 0.44              |
| 44:DX:12:VAL:CG1   | 44:DX:27:THR:OG1   | 2.57                     | 0.44              |
| 45:DY:46:LYS:NZ    | 45:DY:63:LYS:HG2   | 2.33                     | 0.44              |
| 46:DZ:14:LYS:HB2   | 46:DZ:17:ALA:HB3   | 1.99                     | 0.44              |
| 46:DZ:25:PRO:O     | 46:DZ:85:HIS:CD2   | 2.70                     | 0.44              |
| 47:D0:54:GLY:O     | 47:D0:56:ASP:N     | 2.50                     | 0.44              |
| 50:D3:19:GLN:HE22  | 50:D3:52:HIS:CE1   | 2.35                     | 0.44              |
| 52:D5:36:CYS:HB2   | 52:D5:49:CYS:SG    | 2.58                     | 0.44              |
| 53:D6:9:LEU:C      | 53:D6:9:LEU:CD2    | 2.90                     | 0.44              |
| 56:D9:24:TYR:CE2   | 56:D9:35:ARG:HG3   | 2.51                     | 0.44              |
| 1:AA:686:U:HO2'    | 11:AK:42:TRP:NE1   | 2.16                     | 0.44              |
| 1:AA:913:A:C4'     | 1:AA:914:A:O5'     | 2.43                     | 0.44              |
| 5:AE:47:LYS:O      | 5:AE:57:LYS:NZ     | 2.41                     | 0.44              |
| 8:AH:25:ASP:N      | 8:AH:25:ASP:OD1    | 2.50                     | 0.44              |
| 8:AH:87:SER:HB2    | 8:AH:93:VAL:HB     | 1.98                     | 0.44              |
| 10:AJ:99:LYS:O     | 10:AJ:100:THR:HG23 | 2.17                     | 0.44              |
| 13:AM:60:VAL:HG12  | 13:AM:66:LEU:HD11  | 1.99                     | 0.44              |
| 16:AP:75:ARG:C     | 16:AP:77:ALA:H     | 2.26                     | 0.44              |
| 17:AQ:62:SER:O     | 17:AQ:63:ARG:C     | 2.61                     | 0.44              |
| 17:AQ:68:ARG:CG    | 17:AQ:68:ARG:HH11  | 2.30                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 17:AQ:68:ARG:HH11 | 17:AQ:68:ARG:HG2  | 1.83                     | 0.44              |
| 25:BA:319:C:C2    | 25:BA:333:G:N2    | 2.86                     | 0.44              |
| 25:BA:613:G:C2    | 25:BA:615:G:C5    | 3.05                     | 0.44              |
| 25:BA:1394:U:O4   | 25:BA:1395:A:N6   | 2.51                     | 0.44              |
| 25:BA:1395:A:O2'  | 25:BA:1397:U:C6   | 2.71                     | 0.44              |
| 25:BA:1654:A:OP2  | 38:BR:3:HIS:CG    | 2.71                     | 0.44              |
| 25:BA:2155:G:H2'  | 25:BA:2156:G:O4'  | 2.17                     | 0.44              |
| 25:BA:2225:A:H4'  | 25:BA:2226:C:H5'  | 2.00                     | 0.44              |
| 25:BA:2561:A:H2   | 35:BO:23:ARG:NH1  | 2.16                     | 0.44              |
| 25:BA:2575:C:H2'  | 25:BA:2578:G:O6   | 2.17                     | 0.44              |
| 25:BA:2875:C:O2'  | 40:BT:5:ALA:HB3   | 2.17                     | 0.44              |
| 28:BD:85:ASP:OD2  | 28:BD:88:ARG:NH1  | 2.40                     | 0.44              |
| 28:BD:268:ARG:O   | 28:BD:268:ARG:NH1 | 2.51                     | 0.44              |
| 29:BE:47:VAL:HG23 | 29:BE:84:PHE:O    | 2.18                     | 0.44              |
| 33:BI:127:VAL:CG2 | 33:BI:139:GLN:HG3 | 2.48                     | 0.44              |
| 36:BP:46:LYS:HB3  | 36:BP:51:PHE:CD2  | 2.53                     | 0.44              |
| 38:BR:51:LEU:CD2  | 38:BR:66:VAL:HG13 | 2.48                     | 0.44              |
| 41:BU:26:GLY:C    | 41:BU:28:ARG:H    | 2.24                     | 0.44              |
| 43:BW:46:PHE:O    | 43:BW:50:VAL:HG12 | 2.18                     | 0.44              |
| 45:BY:13:VAL:HG21 | 45:BY:72:VAL:HG11 | 2.00                     | 0.44              |
| 46:BZ:39:VAL:HG21 | 46:BZ:44:PHE:HD2  | 1.83                     | 0.44              |
| 49:B2:6:VAL:C     | 49:B2:8:LYS:N     | 2.75                     | 0.44              |
| 1:CA:992:U:O2'    | 1:CA:993:G:O5'    | 2.35                     | 0.44              |
| 1:CA:1062:U:H2'   | 1:CA:1063:C:C6    | 2.53                     | 0.44              |
| 1:CA:1151:A:H5''  | 10:CJ:42:THR:OG1  | 2.17                     | 0.44              |
| 2:CB:32:ILE:HD11  | 2:CB:40:HIS:HB3   | 2.00                     | 0.44              |
| 2:CB:166:ASP:CG   | 2:CB:169:LYS:HB2  | 2.43                     | 0.44              |
| 3:CC:63:ASN:C     | 3:CC:64:VAL:HG22  | 2.43                     | 0.44              |
| 3:CC:189:ALA:O    | 3:CC:190:ARG:C    | 2.61                     | 0.44              |
| 4:CD:12:CYS:SG    | 4:CD:21:LEU:HD12  | 2.58                     | 0.44              |
| 4:CD:198:VAL:CG1  | 4:CD:199:ASN:N    | 2.76                     | 0.44              |
| 5:CE:115:VAL:CG1  | 5:CE:116:THR:N    | 2.81                     | 0.44              |
| 8:CH:56:LYS:HA    | 8:CH:57:PRO:HD2   | 1.83                     | 0.44              |
| 13:CM:11:ARG:NH1  | 13:CM:11:ARG:HB2  | 2.32                     | 0.44              |
| 13:CM:45:VAL:O    | 13:CM:48:LEU:HD22 | 2.17                     | 0.44              |
| 16:CP:6:LEU:HB3   | 16:CP:17:TYR:CD2  | 2.53                     | 0.44              |
| 17:CQ:26:GLN:HB3  | 17:CQ:37:LYS:HG2  | 2.00                     | 0.44              |
| 18:CR:56:THR:HB   | 18:CR:58:LEU:CD1  | 2.48                     | 0.44              |
| 19:CS:45:VAL:CA   | 19:CS:62:ILE:HG23 | 2.46                     | 0.44              |
| 25:DA:17:G:H4'    | 41:DU:25:TRP:CZ3  | 2.53                     | 0.44              |
| 25:DA:144:C:H2'   | 25:DA:145:G:H8    | 1.83                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:DA:196:A:H2'   | 25:DA:805:G:O6    | 2.18                     | 0.44              |
| 25:DA:709:U:H2'   | 25:DA:710:G:C8    | 2.53                     | 0.44              |
| 25:DA:987:G:O2'   | 25:DA:1000:A:N3   | 2.44                     | 0.44              |
| 25:DA:995:C:O2'   | 25:DA:996:A:OP2   | 2.31                     | 0.44              |
| 25:DA:1359:A:OP2  | 25:DA:1371:G:N2   | 2.43                     | 0.44              |
| 25:DA:2010:G:H5'' | 43:DW:42:ARG:HB2  | 1.98                     | 0.44              |
| 25:DA:2330:G:O3'  | 47:D0:44:ARG:NH1  | 2.49                     | 0.44              |
| 28:DD:28:GLU:H    | 28:DD:29:PRO:CD   | 2.24                     | 0.44              |
| 31:DG:181:ARG:O   | 31:DG:181:ARG:CG  | 2.65                     | 0.44              |
| 32:DH:12:PRO:HG3  | 32:DH:48:GLY:C    | 2.42                     | 0.44              |
| 34:DN:9:VAL:CG1   | 34:DN:10:GLU:H    | 2.23                     | 0.44              |
| 37:DQ:141:GLN:CD  | 46:DZ:72:ARG:HD3  | 2.43                     | 0.44              |
| 39:DS:35:ILE:CG2  | 39:DS:69:VAL:HG11 | 2.48                     | 0.44              |
| 40:DT:76:PHE:HA   | 40:DT:77:PRO:HD3  | 1.70                     | 0.44              |
| 40:DT:106:SER:C   | 40:DT:107:ASP:OD1 | 2.60                     | 0.44              |
| 40:DT:115:ARG:HA  | 40:DT:115:ARG:HE  | 1.83                     | 0.44              |
| 41:DU:69:CYS:CB   | 41:DU:79:PHE:CD1  | 3.00                     | 0.44              |
| 41:DU:103:PRO:O   | 41:DU:106:PHE:CB  | 2.66                     | 0.44              |
| 45:DY:50:ARG:C    | 45:DY:52:SER:N    | 2.72                     | 0.44              |
| 46:DZ:5:LEU:HB3   | 46:DZ:59:LEU:CD2  | 2.48                     | 0.44              |
| 46:DZ:86:VAL:HG12 | 46:DZ:87:ASP:O    | 2.17                     | 0.44              |
| 48:D1:51:VAL:O    | 48:D1:57:GLU:O    | 2.35                     | 0.44              |
| 51:D4:4:GLY:O     | 51:D4:5:ILE:CB    | 2.64                     | 0.44              |
| 53:D6:30:THR:O    | 53:D6:31:PRO:C    | 2.61                     | 0.44              |
| 1:AA:583:A:H2'    | 1:AA:584:G:O4'    | 2.17                     | 0.44              |
| 1:AA:1048:G:C2'   | 1:AA:1049:U:OP2   | 2.65                     | 0.44              |
| 3:AC:6:HIS:CD2    | 3:AC:6:HIS:C      | 2.96                     | 0.44              |
| 3:AC:22:TRP:CH2   | 3:AC:32:LEU:O     | 2.70                     | 0.44              |
| 3:AC:54:ARG:HG2   | 3:AC:56:ASP:H     | 1.83                     | 0.44              |
| 4:AD:98:GLU:O     | 4:AD:103:ASN:ND2  | 2.51                     | 0.44              |
| 4:AD:173:TRP:CD1  | 4:AD:174:LEU:HG   | 2.52                     | 0.44              |
| 5:AE:43:LEU:HD12  | 5:AE:44:GLY:N     | 2.32                     | 0.44              |
| 5:AE:139:LEU:O    | 5:AE:140:ARG:C    | 2.61                     | 0.44              |
| 6:AF:21:LEU:HD13  | 6:AF:24:GLU:HG2   | 1.98                     | 0.44              |
| 6:AF:45:LEU:HA    | 6:AF:45:LEU:HD13  | 1.67                     | 0.44              |
| 7:AG:49:ILE:HG23  | 7:AG:53:LYS:HG3   | 2.00                     | 0.44              |
| 7:AG:52:GLU:O     | 7:AG:54:THR:N     | 2.51                     | 0.44              |
| 7:AG:61:VAL:O     | 7:AG:64:GLN:N     | 2.50                     | 0.44              |
| 9:AI:87:GLN:C     | 9:AI:89:ASN:H     | 2.25                     | 0.44              |
| 10:AJ:40:LEU:CB   | 10:AJ:41:PRO:HD2  | 2.29                     | 0.44              |
| 11:AK:59:TYR:CZ   | 11:AK:63:LEU:HD11 | 2.52                     | 0.44              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 12:AL:118:SER:C   | 12:AL:119:LYS:O    | 2.59                     | 0.44              |
| 13:AM:53:VAL:CG1  | 13:AM:57:ARG:HH21  | 2.30                     | 0.44              |
| 20:AT:20:LEU:HD23 | 20:AT:20:LEU:HA    | 1.66                     | 0.44              |
| 20:AT:42:GLN:C    | 20:AT:43:LEU:HD23  | 2.43                     | 0.44              |
| 22:AV:3:C:H6      | 22:AV:3:C:O5'      | 2.00                     | 0.44              |
| 22:AV:24:C:H2'    | 22:AV:25:U:H6      | 1.83                     | 0.44              |
| 22:AV:30:G:C2'    | 22:AV:31:G:H5'     | 2.48                     | 0.44              |
| 23:AY:30:G:H2'    | 23:AY:30:G:N3      | 2.33                     | 0.44              |
| 25:BA:958:U:O4    | 37:BQ:41:TRP:HB2   | 2.17                     | 0.44              |
| 25:BA:1204:A:O2'  | 25:BA:1205:U:P     | 2.75                     | 0.44              |
| 25:BA:1252:G:C5   | 25:BA:1253:A:N1    | 2.86                     | 0.44              |
| 25:BA:2225:A:O2'  | 25:BA:2226:C:OP2   | 2.32                     | 0.44              |
| 26:BB:50:G:OP1    | 39:BS:62:LYS:HB2   | 2.17                     | 0.44              |
| 27:BC:49:ILE:O    | 27:BC:51:PRO:HD3   | 2.18                     | 0.44              |
| 28:BD:69:ARG:HH21 | 28:BD:192:THR:HG21 | 1.82                     | 0.44              |
| 32:BH:34:GLU:HA   | 32:BH:34:GLU:OE1   | 2.16                     | 0.44              |
| 34:BN:104:LYS:HB2 | 34:BN:117:PHE:HE1  | 1.82                     | 0.44              |
| 36:BP:59:LEU:HD11 | 55:B8:13:ARG:HH21  | 1.83                     | 0.44              |
| 39:BS:34:HIS:CE1  | 39:BS:54:LEU:CG    | 3.00                     | 0.44              |
| 40:BT:88:ILE:HG22 | 40:BT:89:VAL:N     | 2.33                     | 0.44              |
| 42:BV:20:LEU:N    | 42:BV:20:LEU:HD12  | 2.33                     | 0.44              |
| 44:BX:47:PHE:O    | 44:BX:48:LYS:C     | 2.59                     | 0.44              |
| 46:BZ:163:LEU:H   | 46:BZ:163:LEU:HD12 | 1.82                     | 0.44              |
| 1:CA:48:C:C4'     | 1:CA:49:U:OP2      | 2.65                     | 0.44              |
| 1:CA:61:G:OP2     | 20:CT:10:LEU:CD2   | 2.65                     | 0.44              |
| 1:CA:129:U:H4'    | 1:CA:130:A:OP1     | 2.18                     | 0.44              |
| 1:CA:608:A:H2'    | 1:CA:609:A:O4'     | 2.18                     | 0.44              |
| 1:CA:790:A:OP1    | 22:CV:39:A:O2'     | 2.32                     | 0.44              |
| 1:CA:1295:G:O3'   | 13:CM:14:ARG:NH1   | 2.50                     | 0.44              |
| 2:CB:87:ARG:O     | 2:CB:87:ARG:HD2    | 2.17                     | 0.44              |
| 3:CC:15:THR:CG2   | 3:CC:16:ARG:H      | 2.28                     | 0.44              |
| 4:CD:49:ARG:HH11  | 4:CD:50:ARG:H      | 1.64                     | 0.44              |
| 5:CE:12:LEU:HB3   | 5:CE:31:LEU:HB2    | 2.00                     | 0.44              |
| 7:CG:66:VAL:O     | 7:CG:70:LYS:HG3    | 2.17                     | 0.44              |
| 8:CH:92:ARG:HD2   | 8:CH:92:ARG:HA     | 1.66                     | 0.44              |
| 8:CH:134:ILE:O    | 8:CH:135:CYS:HB3   | 2.17                     | 0.44              |
| 12:CL:118:SER:C   | 12:CL:119:LYS:O    | 2.59                     | 0.44              |
| 13:CM:36:LYS:C    | 13:CM:38:GLY:H     | 2.25                     | 0.44              |
| 15:CO:59:MET:O    | 15:CO:62:GLN:HB3   | 2.18                     | 0.44              |
| 16:CP:53:VAL:CG1  | 16:CP:79:VAL:HG22  | 2.47                     | 0.44              |
| 20:CT:56:MET:HE3  | 20:CT:56:MET:HB3   | 1.71                     | 0.44              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 21:CU:6:ARG:HG3    | 21:CU:15:ARG:NH1  | 2.33                     | 0.44              |
| 22:CV:40:C:C2      | 22:CV:41:C:C5     | 3.06                     | 0.44              |
| 25:DA:314:A:H2'    | 25:DA:315:G:C8    | 2.53                     | 0.44              |
| 25:DA:570:G:H2'    | 25:DA:2030:A:C5   | 2.53                     | 0.44              |
| 25:DA:1142(A):A:C5 | 25:DA:1144:G:C5   | 3.05                     | 0.44              |
| 25:DA:2414:G:N2    | 36:DP:67:MET:HE1  | 2.31                     | 0.44              |
| 26:DB:15:A:OP1     | 26:DB:108:U:O2'   | 2.20                     | 0.44              |
| 27:DC:39:GLU:HG2   | 27:DC:180:PHE:CB  | 2.48                     | 0.44              |
| 28:DD:24:ILE:HD12  | 28:DD:84:TYR:HB2  | 2.00                     | 0.44              |
| 28:DD:32:SER:O     | 28:DD:33:LEU:C    | 2.60                     | 0.44              |
| 29:DE:103:ASP:CG   | 29:DE:201:THR:HA  | 2.42                     | 0.44              |
| 30:DF:96:ASP:OD1   | 30:DF:96:ASP:C    | 2.60                     | 0.44              |
| 31:DG:25:TYR:CE2   | 31:DG:31:VAL:HA   | 2.53                     | 0.44              |
| 32:DH:83:TYR:HB2   | 32:DH:84:SER:H    | 1.46                     | 0.44              |
| 33:DI:114:LEU:HD22 | 33:DI:130:TYR:CE1 | 2.53                     | 0.44              |
| 34:DN:87:LEU:O     | 34:DN:88:GLU:C    | 2.61                     | 0.44              |
| 36:DP:46:LYS:HB3   | 36:DP:51:PHE:CD2  | 2.53                     | 0.44              |
| 38:DR:2:ARG:HG3    | 38:DR:2:ARG:HH11  | 1.83                     | 0.44              |
| 40:DT:48:ILE:HD12  | 40:DT:48:ILE:N    | 2.32                     | 0.44              |
| 40:DT:53:ARG:HG2   | 40:DT:53:ARG:NH1  | 2.31                     | 0.44              |
| 42:DV:69:LYS:HA    | 42:DV:87:HIS:O    | 2.17                     | 0.44              |
| 43:DW:1:MET:CE     | 43:DW:2:GLU:H     | 2.30                     | 0.44              |
| 46:DZ:53:ILE:O     | 46:DZ:54:HIS:CG   | 2.71                     | 0.44              |
| 46:DZ:161:VAL:HG12 | 46:DZ:162:GLU:N   | 2.33                     | 0.44              |
| 46:DZ:169:GLU:HG2  | 46:DZ:170:THR:H   | 1.82                     | 0.44              |
| 1:AA:382:A:H2'     | 1:AA:383:A:C8     | 2.52                     | 0.44              |
| 1:AA:618:C:N3      | 1:AA:622:A:N6     | 2.64                     | 0.44              |
| 1:AA:637:G:H2'     | 1:AA:638:G:C8     | 2.53                     | 0.44              |
| 1:AA:1000:U:H2'    | 1:AA:1001:A:C8    | 2.52                     | 0.44              |
| 1:AA:1054:C:O2     | 1:AA:1054:C:H3'   | 2.18                     | 0.44              |
| 1:AA:1095:U:P      | 1:AA:1108:G:H1    | 2.41                     | 0.44              |
| 1:AA:1128:C:H1'    | 1:AA:1146:A:H61   | 1.83                     | 0.44              |
| 1:AA:1241:G:H2'    | 1:AA:1242:C:C6    | 2.53                     | 0.44              |
| 3:AC:17:ASP:O      | 3:AC:18:TRP:O     | 2.35                     | 0.44              |
| 3:AC:164:ARG:HG2   | 3:AC:165:THR:H    | 1.83                     | 0.44              |
| 4:AD:152:SER:O     | 4:AD:158:ILE:HG13 | 2.18                     | 0.44              |
| 5:AE:53:LEU:HD12   | 5:AE:53:LEU:H     | 1.81                     | 0.44              |
| 9:AI:95:LYS:O      | 9:AI:99:LEU:HB3   | 2.18                     | 0.44              |
| 10:AJ:7:LYS:HB2    | 10:AJ:97:GLU:HB2  | 1.99                     | 0.44              |
| 22:AV:72:C:O5'     | 22:AV:72:C:H6     | 2.01                     | 0.44              |
| 25:BA:142(A):C:H2' | 25:BA:143:G:O4'   | 2.17                     | 0.44              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:BA:636:G:H2'   | 36:BP:115:LEU:HD11 | 1.98                     | 0.44              |
| 25:BA:1275:A:N9   | 38:BR:16:HIS:CD2   | 2.86                     | 0.44              |
| 25:BA:1286:A:H5'  | 25:BA:1287:A:OP2   | 2.18                     | 0.44              |
| 25:BA:1458:C:H5'' | 25:BA:1459:G:OP1   | 2.18                     | 0.44              |
| 25:BA:2050:C:H2'  | 25:BA:2051:A:O4'   | 2.18                     | 0.44              |
| 25:BA:2258:C:H4'  | 25:BA:2259:G:OP2   | 2.12                     | 0.44              |
| 25:BA:2503:A:O2'  | 25:BA:2504:U:OP1   | 2.36                     | 0.44              |
| 27:BC:36:LYS:O    | 27:BC:37:PHE:C     | 2.61                     | 0.44              |
| 29:BE:132:HIS:CA  | 29:BE:135:HIS:NE2  | 2.81                     | 0.44              |
| 30:BF:132:VAL:CG1 | 30:BF:133:ASN:H    | 2.20                     | 0.44              |
| 33:BI:2:LYS:HB2   | 33:BI:39:ALA:CB    | 2.47                     | 0.44              |
| 35:BO:122:LEU:HA  | 40:BT:33:LYS:NZ    | 2.33                     | 0.44              |
| 36:BP:59:LEU:O    | 36:BP:59:LEU:CG    | 2.66                     | 0.44              |
| 39:BS:98:VAL:HG22 | 39:BS:100:ALA:H    | 1.83                     | 0.44              |
| 41:BU:74:LEU:CD1  | 41:BU:78:THR:HB    | 2.47                     | 0.44              |
| 42:BV:89:GLN:HA   | 42:BV:90:PRO:HD2   | 1.85                     | 0.44              |
| 45:BY:44:ILE:HG22 | 45:BY:45:VAL:N     | 2.33                     | 0.44              |
| 45:BY:48:ALA:C    | 45:BY:50:ARG:N     | 2.75                     | 0.44              |
| 46:BZ:72:ARG:HD3  | 46:BZ:72:ARG:HA    | 1.71                     | 0.44              |
| 1:CA:8:A:H1'      | 5:CE:103:GLY:HA2   | 2.00                     | 0.44              |
| 1:CA:401:C:H2'    | 1:CA:402:G:H8      | 1.83                     | 0.44              |
| 1:CA:461:A:N6     | 1:CA:471:G:N1      | 2.66                     | 0.44              |
| 1:CA:532:A:C2'    | 1:CA:533:A:OP1     | 2.63                     | 0.44              |
| 1:CA:1268:A:N3    | 1:CA:1326:C:O2'    | 2.40                     | 0.44              |
| 1:CA:1293:G:H2'   | 1:CA:1294:G:C8     | 2.53                     | 0.44              |
| 1:CA:1297:C:O2'   | 7:CG:114:ARG:NH2   | 2.51                     | 0.44              |
| 2:CB:87:ARG:HH11  | 2:CB:223:ILE:HD11  | 1.82                     | 0.44              |
| 2:CB:159:PRO:C    | 2:CB:161:ALA:N     | 2.76                     | 0.44              |
| 2:CB:204:ASN:ND2  | 2:CB:206:ASP:H     | 2.16                     | 0.44              |
| 3:CC:23:TYR:C     | 3:CC:23:TYR:HD2    | 2.21                     | 0.44              |
| 3:CC:111:LEU:HD12 | 3:CC:204:LEU:CD2   | 2.48                     | 0.44              |
| 5:CE:106:PRO:O    | 5:CE:108:ALA:N     | 2.51                     | 0.44              |
| 5:CE:116:THR:HB   | 5:CE:117:ASP:OD2   | 2.17                     | 0.44              |
| 6:CF:48:LEU:HG    | 6:CF:57:GLN:HA     | 1.98                     | 0.44              |
| 7:CG:24:THR:O     | 7:CG:27:ILE:HB     | 2.17                     | 0.44              |
| 7:CG:43:PHE:CE1   | 7:CG:47:CYS:SG     | 3.11                     | 0.44              |
| 8:CH:104:ARG:HB3  | 8:CH:107:LEU:HB2   | 2.00                     | 0.44              |
| 9:CI:4:TYR:CD2    | 9:CI:88:TYR:CG     | 3.06                     | 0.44              |
| 12:CL:110:VAL:CG2 | 12:CL:120:TYR:HB3  | 2.47                     | 0.44              |
| 16:CP:9:PHE:CD2   | 16:CP:9:PHE:N      | 2.85                     | 0.44              |
| 19:CS:10:PHE:CE1  | 19:CS:70:LYS:HE2   | 2.52                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:DA:586:A:H5'   | 30:DF:89:VAL:HG21 | 1.99                     | 0.44              |
| 25:DA:1128:A:C5   | 25:DA:2518:A:N6   | 2.85                     | 0.44              |
| 25:DA:2145:C:H4'  | 25:DA:2146:C:OP2  | 2.18                     | 0.44              |
| 25:DA:2377:A:C4'  | 39:DS:112:PHE:HA  | 2.47                     | 0.44              |
| 25:DA:2838:G:H2'  | 25:DA:2839:G:H8   | 1.82                     | 0.44              |
| 29:DE:28:ALA:O    | 29:DE:29:GLY:C    | 2.60                     | 0.44              |
| 29:DE:43:GLY:O    | 29:DE:44:TYR:HB3  | 2.17                     | 0.44              |
| 29:DE:46:ALA:HA   | 29:DE:82:ARG:O    | 2.18                     | 0.44              |
| 29:DE:79:ARG:HH11 | 29:DE:79:ARG:HG2  | 1.83                     | 0.44              |
| 31:DG:2:PRO:O     | 31:DG:4:ASP:N     | 2.50                     | 0.44              |
| 32:DH:16:SER:OG   | 32:DH:17:VAL:N    | 2.51                     | 0.44              |
| 32:DH:41:MET:HA   | 32:DH:53:GLU:O    | 2.18                     | 0.44              |
| 33:DI:118:LYS:O   | 33:DI:119:PRO:C   | 2.60                     | 0.44              |
| 34:DN:29:LYS:C    | 34:DN:31:ALA:N    | 2.74                     | 0.44              |
| 41:DU:96:ALA:C    | 41:DU:98:LEU:N    | 2.75                     | 0.44              |
| 41:DU:97:ASP:OD1  | 41:DU:97:ASP:C    | 2.61                     | 0.44              |
| 42:DV:41:GLY:CA   | 42:DV:46:VAL:CG1  | 2.96                     | 0.44              |
| 45:DY:97:ARG:NE   | 45:DY:97:ARG:C    | 2.75                     | 0.44              |
| 46:DZ:48:PHE:HE2  | 46:DZ:71:VAL:HG21 | 1.82                     | 0.44              |
| 46:DZ:61:LEU:HG   | 46:DZ:67:LEU:CD1  | 2.47                     | 0.44              |
| 48:D1:52:ARG:HG3  | 48:D1:53:VAL:N    | 2.25                     | 0.44              |
| 1:AA:109:A:C6     | 1:AA:327:A:C6     | 3.05                     | 0.44              |
| 1:AA:251:G:H1'    | 1:AA:252:U:H6     | 1.80                     | 0.44              |
| 1:AA:1004:A:H5''  | 1:AA:1025:U:H3    | 1.83                     | 0.44              |
| 1:AA:1053:G:O6    | 1:AA:1199:U:H2'   | 2.17                     | 0.44              |
| 1:AA:1495:U:O2'   | 25:BA:1919:A:N1   | 2.45                     | 0.44              |
| 4:AD:99:SER:O     | 4:AD:140:VAL:HG23 | 2.17                     | 0.44              |
| 5:AE:79:GLU:H     | 5:AE:79:GLU:HG3   | 1.47                     | 0.44              |
| 8:AH:97:VAL:HG13  | 8:AH:98:LYS:HG3   | 2.00                     | 0.44              |
| 11:AK:124:LYS:C   | 11:AK:125:PHE:HD1 | 2.26                     | 0.44              |
| 13:AM:35:GLU:O    | 13:AM:38:GLY:N    | 2.51                     | 0.44              |
| 13:AM:49:THR:C    | 13:AM:51:ALA:N    | 2.75                     | 0.44              |
| 22:AV:60:A:H2'    | 22:AV:61:U:C5'    | 2.48                     | 0.44              |
| 23:AW:34:G:N3     | 24:AX:14:A:C2     | 2.78                     | 0.44              |
| 25:BA:1212:G:H1'  | 25:BA:1237:A:N6   | 2.33                     | 0.44              |
| 25:BA:1287:A:OP1  | 38:BR:104:ARG:HG3 | 2.18                     | 0.44              |
| 25:BA:1353:A:H4'  | 28:BD:38:LYS:HE3  | 2.00                     | 0.44              |
| 25:BA:2236:C:H2'  | 25:BA:2237:G:O4'  | 2.18                     | 0.44              |
| 25:BA:2447:G:H1'  | 25:BA:2501:C:N4   | 2.32                     | 0.44              |
| 26:BB:83:G:H5''   | 50:B3:52:HIS:NE2  | 2.32                     | 0.44              |
| 27:BC:22:ILE:HD13 | 27:BC:24:GLU:OE2  | 2.17                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:BC:41:VAL:HG23  | 27:BC:178:ALA:HB3  | 2.00                     | 0.44              |
| 28:BD:245:PRO:O    | 28:BD:246:PRO:C    | 2.61                     | 0.44              |
| 30:BF:10:PRO:HD2   | 30:BF:13:SER:O     | 2.17                     | 0.44              |
| 34:BN:120:LEU:HD22 | 34:BN:121:LYS:N    | 2.33                     | 0.44              |
| 35:BO:29:ASN:O     | 35:BO:29:ASN:ND2   | 2.51                     | 0.44              |
| 35:BO:115:VAL:O    | 35:BO:116:SER:C    | 2.61                     | 0.44              |
| 36:BP:59:LEU:CD1   | 55:B8:13:ARG:NH2   | 2.80                     | 0.44              |
| 38:BR:77:ARG:O     | 38:BR:78:LYS:C     | 2.61                     | 0.44              |
| 38:BR:100:LEU:CB   | 38:BR:111:LEU:O    | 2.44                     | 0.44              |
| 39:BS:28:VAL:HG12  | 39:BS:89:ARG:HG2   | 2.00                     | 0.44              |
| 40:BT:122:ASP:C    | 40:BT:124:ASP:H    | 2.24                     | 0.44              |
| 42:BV:2:PHE:HB3    | 42:BV:42:GLY:H     | 1.81                     | 0.44              |
| 43:BW:65:LEU:CD2   | 43:BW:67:ASP:HB2   | 2.47                     | 0.44              |
| 45:BY:12:THR:C     | 45:BY:13:VAL:HG13  | 2.42                     | 0.44              |
| 47:B0:19:LYS:O     | 47:B0:20:ARG:C     | 2.61                     | 0.44              |
| 1:CA:821:G:H2'     | 1:CA:822:C:C6      | 2.53                     | 0.44              |
| 1:CA:914:A:H2'     | 1:CA:915:A:H8      | 1.83                     | 0.44              |
| 1:CA:1054:C:H2'    | 1:CA:1055:A:H5''   | 1.99                     | 0.44              |
| 1:CA:1074:G:O2'    | 1:CA:1101:A:N1     | 2.48                     | 0.44              |
| 1:CA:1131:G:H2'    | 1:CA:1132:C:C6     | 2.53                     | 0.44              |
| 2:CB:208:ILE:HA    | 2:CB:211:ILE:HD12  | 1.99                     | 0.44              |
| 3:CC:29:TYR:C      | 3:CC:31:HIS:N      | 2.76                     | 0.44              |
| 3:CC:127:ARG:HH11  | 3:CC:127:ARG:HG2   | 1.82                     | 0.44              |
| 4:CD:166:LYS:HE3   | 4:CD:166:LYS:HB2   | 1.60                     | 0.44              |
| 5:CE:16:THR:O      | 5:CE:17:ALA:CB     | 2.65                     | 0.44              |
| 8:CH:27:PRO:N      | 8:CH:58:TYR:HD2    | 2.15                     | 0.44              |
| 10:CJ:38:ILE:HG13  | 10:CJ:71:LEU:HB3   | 2.00                     | 0.44              |
| 11:CK:58:PRO:HB3   | 11:CK:90:GLY:HA2   | 2.00                     | 0.44              |
| 11:CK:59:TYR:O     | 11:CK:63:LEU:HB2   | 2.18                     | 0.44              |
| 13:CM:40:ASN:ND2   | 13:CM:42:ALA:HB3   | 2.33                     | 0.44              |
| 13:CM:54:VAL:O     | 13:CM:58:GLU:HG3   | 2.17                     | 0.44              |
| 13:CM:123:ALA:HA   | 13:CM:124:PRO:HD3  | 1.75                     | 0.44              |
| 14:CN:13:THR:O     | 14:CN:15:LYS:N     | 2.50                     | 0.44              |
| 20:CT:71:THR:HG22  | 20:CT:72:LEU:H     | 1.81                     | 0.44              |
| 25:DA:271(R):G:H2' | 25:DA:271(S):G:H8  | 1.83                     | 0.44              |
| 25:DA:943:U:OP2    | 36:DP:36:LYS:HD3   | 2.18                     | 0.44              |
| 25:DA:1427:A:H4'   | 25:DA:1428:C:OP1   | 2.18                     | 0.44              |
| 25:DA:1782:C:H1'   | 25:DA:2609:U:O4'   | 2.18                     | 0.44              |
| 25:DA:2228:G:P     | 28:DD:263:ARG:HH12 | 2.40                     | 0.44              |
| 25:DA:2262:U:H5    | 47:D0:16:SER:HG    | 1.63                     | 0.44              |
| 28:DD:61:LEU:HB3   | 28:DD:63:ARG:NH1   | 2.33                     | 0.44              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 29:DE:200:GLU:OE2 | 29:DE:200:GLU:N    | 2.40                     | 0.44              |
| 29:DE:201:THR:OG1 | 29:DE:202:LYS:N    | 2.50                     | 0.44              |
| 30:DF:135:LYS:O   | 30:DF:138:GLU:N    | 2.49                     | 0.44              |
| 31:DG:34:LEU:HD12 | 31:DG:100:TRP:CH2  | 2.53                     | 0.44              |
| 31:DG:47:LYS:HD3  | 31:DG:81:LYS:CB    | 2.35                     | 0.44              |
| 32:DH:124:GLU:HB2 | 32:DH:132:ARG:HG3  | 1.99                     | 0.44              |
| 32:DH:146:ALA:O   | 32:DH:150:ALA:N    | 2.43                     | 0.44              |
| 34:DN:39:ARG:HE   | 34:DN:41:ASP:CG    | 2.25                     | 0.44              |
| 37:DQ:51:ARG:HH11 | 37:DQ:51:ARG:HB3   | 1.83                     | 0.44              |
| 37:DQ:133:ARG:HG3 | 37:DQ:133:ARG:NH1  | 2.33                     | 0.44              |
| 39:DS:103:GLU:C   | 39:DS:105:ALA:N    | 2.73                     | 0.44              |
| 40:DT:28:VAL:CG2  | 40:DT:46:GLU:HG3   | 2.48                     | 0.44              |
| 42:DV:1:MET:HE2   | 42:DV:43:GLU:CB    | 2.47                     | 0.44              |
| 42:DV:62:LEU:HD12 | 42:DV:62:LEU:N     | 2.32                     | 0.44              |
| 1:AA:579:G:H5'    | 1:AA:728:A:H1'     | 2.00                     | 0.43              |
| 1:AA:914:A:C5     | 1:AA:915:A:N7      | 2.86                     | 0.43              |
| 1:AA:991:U:O2'    | 1:AA:992:U:O5'     | 2.30                     | 0.43              |
| 1:AA:1347:G:N2    | 1:AA:1373:G:H2'    | 2.33                     | 0.43              |
| 2:AB:158:LEU:HD12 | 2:AB:158:LEU:N     | 2.29                     | 0.43              |
| 2:AB:187:LEU:HD22 | 2:AB:187:LEU:O     | 2.18                     | 0.43              |
| 3:AC:11:ARG:O     | 3:AC:14:ILE:O      | 2.36                     | 0.43              |
| 4:AD:168:ARG:NH2  | 6:CF:18:GLN:NE2    | 2.65                     | 0.43              |
| 5:AE:83:GLU:HA    | 5:AE:88:LYS:HA     | 2.00                     | 0.43              |
| 12:AL:34:ARG:HA   | 12:AL:84:LEU:HD23  | 2.00                     | 0.43              |
| 13:AM:22:ILE:HB   | 13:AM:25:ILE:HD13  | 1.99                     | 0.43              |
| 19:AS:28:LYS:HB3  | 19:AS:29:ARG:H     | 1.47                     | 0.43              |
| 20:AT:71:THR:CG2  | 20:AT:72:LEU:N     | 2.57                     | 0.43              |
| 22:AV:56:U:C5     | 22:AV:58:A:OP2     | 2.70                     | 0.43              |
| 25:BA:181:A:N3    | 25:BA:435:C:OP1    | 2.51                     | 0.43              |
| 25:BA:468:G:H5''  | 30:BF:60:SER:HB2   | 2.00                     | 0.43              |
| 25:BA:708:C:H5'   | 25:BA:709:U:OP2    | 2.18                     | 0.43              |
| 25:BA:1161:C:H2'  | 25:BA:1162:G:H8    | 1.83                     | 0.43              |
| 25:BA:1670:C:O2   | 29:BE:129:HIS:NE2  | 2.48                     | 0.43              |
| 25:BA:2243:U:H2'  | 25:BA:2244:U:C6    | 2.53                     | 0.43              |
| 25:BA:2352:A:N6   | 25:BA:2365:G:O2'   | 2.51                     | 0.43              |
| 25:BA:2500:U:C2   | 25:BA:2504:U:C4    | 3.06                     | 0.43              |
| 25:BA:2745:C:C6   | 25:BA:2746:U:C5    | 3.06                     | 0.43              |
| 28:BD:31:LYS:HZ1  | 28:BD:102:LYS:HZ2  | 1.66                     | 0.43              |
| 28:BD:233:HIS:CE1 | 28:BD:247:ALA:H    | 2.36                     | 0.43              |
| 29:BE:7:VAL:HG22  | 29:BE:27:LEU:HB3   | 1.99                     | 0.43              |
| 30:BF:160:ASN:CG  | 30:BF:163:VAL:HG23 | 2.43                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 34:BN:36:GLY:HA3   | 34:BN:48:MET:O     | 2.18                     | 0.43              |
| 34:BN:133:GLN:HG2  | 34:BN:135:PRO:CD   | 2.48                     | 0.43              |
| 35:BO:105:GLU:HA   | 35:BO:108:GLU:CD   | 2.42                     | 0.43              |
| 37:BQ:65:PHE:N     | 37:BQ:65:PHE:CD2   | 2.86                     | 0.43              |
| 39:BS:74:ALA:HB1   | 39:BS:103:GLU:CB   | 2.48                     | 0.43              |
| 40:BT:47:GLY:C     | 40:BT:63:VAL:HG12  | 2.43                     | 0.43              |
| 42:BV:3:ALA:CB     | 42:BV:38:LEU:HD21  | 2.47                     | 0.43              |
| 45:BY:55:TYR:HB2   | 45:BY:56:PRO:CD    | 2.12                     | 0.43              |
| 46:BZ:76:LEU:N     | 46:BZ:76:LEU:CD2   | 2.81                     | 0.43              |
| 1:CA:275:G:H2'     | 1:CA:276:G:H8      | 1.82                     | 0.43              |
| 1:CA:396:G:O2'     | 1:CA:398:C:OP1     | 2.29                     | 0.43              |
| 1:CA:963:G:N2      | 10:CJ:55:LYS:HZ3   | 2.15                     | 0.43              |
| 1:CA:1292:U:H5'    | 9:CI:38:GLN:NE2    | 2.32                     | 0.43              |
| 1:CA:1367:C:H5'    | 10:CJ:60:ARG:NH2   | 2.33                     | 0.43              |
| 2:CB:42:ILE:HD11   | 2:CB:202:PRO:C     | 2.43                     | 0.43              |
| 2:CB:62:ALA:HB3    | 2:CB:225:ALA:HB3   | 1.99                     | 0.43              |
| 2:CB:71:VAL:HB     | 2:CB:164:VAL:HG13  | 2.00                     | 0.43              |
| 2:CB:106:LYS:O     | 2:CB:110:GLN:HG3   | 2.17                     | 0.43              |
| 3:CC:7:PRO:HG2     | 3:CC:184:TYR:HB3   | 1.99                     | 0.43              |
| 3:CC:193:TYR:CD2   | 3:CC:193:TYR:N     | 2.86                     | 0.43              |
| 4:CD:33:MET:O      | 4:CD:33:MET:HG3    | 2.18                     | 0.43              |
| 4:CD:93:PHE:HB3    | 4:CD:94:LEU:H      | 1.54                     | 0.43              |
| 4:CD:106:TYR:HE1   | 4:CD:113:SER:HA    | 1.79                     | 0.43              |
| 6:CF:4:TYR:CD1     | 6:CF:92:LYS:HA     | 2.53                     | 0.43              |
| 6:CF:15:ASP:O      | 6:CF:15:ASP:OD1    | 2.35                     | 0.43              |
| 6:CF:99:ALA:HB3    | 18:CR:29:PHE:CE2   | 2.53                     | 0.43              |
| 9:CI:19:LEU:HD22   | 9:CI:59:PHE:CG     | 2.47                     | 0.43              |
| 9:CI:58:HIS:CB     | 9:CI:59:PHE:HD1    | 2.26                     | 0.43              |
| 13:CM:108:ARG:NH1  | 13:CM:112:GLY:O    | 2.51                     | 0.43              |
| 14:CN:28:GLY:O     | 14:CN:29:ARG:C     | 2.61                     | 0.43              |
| 14:CN:37:PHE:HE1   | 14:CN:53:LEU:HD13  | 1.83                     | 0.43              |
| 15:CO:87:ILE:HG22  | 15:CO:88:ARG:N     | 2.33                     | 0.43              |
| 16:CP:48:TRP:O     | 16:CP:48:TRP:HE3   | 2.01                     | 0.43              |
| 25:DA:63:U:O2'     | 25:DA:64:A:N7      | 2.51                     | 0.43              |
| 25:DA:250:G:O6     | 25:DA:251:A:C6     | 2.71                     | 0.43              |
| 25:DA:271(D):G:H1  | 25:DA:271(T):C:N4  | 2.15                     | 0.43              |
| 25:DA:458:G:H1'    | 25:DA:459:U:C5     | 2.49                     | 0.43              |
| 25:DA:1043:C:H2'   | 25:DA:1044:G:H5''  | 2.00                     | 0.43              |
| 25:DA:1142(A):A:N7 | 25:DA:1144:G:C6    | 2.86                     | 0.43              |
| 25:DA:1803:A:H4'   | 28:DD:259:THR:HG23 | 1.99                     | 0.43              |
| 25:DA:2086:U:H2'   | 25:DA:2087:G:C8    | 2.53                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:DA:2161:C:H2'   | 25:DA:2162:G:C8    | 2.53                     | 0.43              |
| 25:DA:2258:C:C4'   | 25:DA:2259:G:OP2   | 2.63                     | 0.43              |
| 25:DA:2620:C:H1'   | 29:DE:156:MET:HB2  | 1.99                     | 0.43              |
| 25:DA:2853:C:H2'   | 25:DA:2854:G:H8    | 1.83                     | 0.43              |
| 26:DB:56:G:H5'     | 31:DG:27:ASN:ND2   | 2.33                     | 0.43              |
| 28:DD:168:ARG:HA   | 28:DD:173:VAL:HA   | 2.00                     | 0.43              |
| 29:DE:176:ILE:HG22 | 29:DE:179:GLU:H    | 1.82                     | 0.43              |
| 30:DF:110:LEU:HD11 | 30:DF:181:LEU:HD13 | 2.00                     | 0.43              |
| 31:DG:51:ARG:NH1   | 31:DG:51:ARG:CB    | 2.81                     | 0.43              |
| 36:DP:96:THR:O     | 36:DP:100:LEU:HD23 | 2.19                     | 0.43              |
| 38:DR:12:ARG:HH11  | 38:DR:12:ARG:CG    | 2.26                     | 0.43              |
| 40:DT:78:LEU:O     | 40:DT:78:LEU:HD23  | 2.17                     | 0.43              |
| 41:DU:79:PHE:HE1   | 41:DU:106:PHE:CZ   | 2.36                     | 0.43              |
| 42:DV:66:ARG:HH11  | 42:DV:66:ARG:CG    | 2.30                     | 0.43              |
| 46:DZ:53:ILE:H     | 46:DZ:71:VAL:HG21  | 1.80                     | 0.43              |
| 1:AA:204:U:H4'     | 1:AA:216:G:N7      | 2.33                     | 0.43              |
| 1:AA:604:G:H2'     | 1:AA:605:U:O4'     | 2.18                     | 0.43              |
| 1:AA:828:A:H2'     | 1:AA:829:G:O4'     | 2.18                     | 0.43              |
| 1:AA:1064:G:HO2'   | 1:AA:1065:U:P      | 2.40                     | 0.43              |
| 1:AA:1189:C:O2'    | 3:AC:176:HIS:HD2   | 2.00                     | 0.43              |
| 4:AD:13:ARG:HH22   | 4:AD:36:ARG:HD3    | 1.82                     | 0.43              |
| 4:AD:110:PHE:CD2   | 4:AD:148:VAL:CG2   | 3.01                     | 0.43              |
| 6:AF:89:MET:CE     | 18:AR:76:LEU:HD22  | 2.48                     | 0.43              |
| 6:AF:100:ASN:HD22  | 18:AR:23:LYS:HE3   | 1.83                     | 0.43              |
| 11:AK:59:TYR:CZ    | 11:AK:63:LEU:CD1   | 3.02                     | 0.43              |
| 15:AO:56:LEU:C     | 15:AO:58:MET:N     | 2.73                     | 0.43              |
| 17:AQ:31:LEU:HG    | 17:AQ:32:TYR:CD2   | 2.54                     | 0.43              |
| 17:AQ:44:ALA:HA    | 17:AQ:71:PHE:O     | 2.18                     | 0.43              |
| 22:AV:53:G:C2'     | 22:AV:54:G:C5'     | 2.96                     | 0.43              |
| 25:BA:434:U:H2'    | 25:BA:436:C:H41    | 1.82                     | 0.43              |
| 25:BA:563:G:C6     | 25:BA:564:C:C4     | 3.05                     | 0.43              |
| 25:BA:943:U:OP1    | 36:BP:36:LYS:HG3   | 2.17                     | 0.43              |
| 25:BA:1006:C:H1'   | 34:BN:106:MET:HG2  | 1.99                     | 0.43              |
| 25:BA:1171:G:H5''  | 25:BA:1173:G:H4'   | 2.00                     | 0.43              |
| 25:BA:1578:U:C2'   | 25:BA:1579:A:H5'   | 2.48                     | 0.43              |
| 25:BA:1688:U:H1'   | 25:BA:1701:A:C6    | 2.53                     | 0.43              |
| 25:BA:2343:C:O2    | 25:BA:2343:C:C2'   | 2.66                     | 0.43              |
| 28:BD:57:GLY:O     | 28:BD:58:HIS:C     | 2.61                     | 0.43              |
| 28:BD:143:HIS:HD2  | 28:BD:144:ALA:HB2  | 1.83                     | 0.43              |
| 29:BE:60:ASN:O     | 29:BE:61:ARG:C     | 2.61                     | 0.43              |
| 29:BE:61:ARG:CB    | 29:BE:62:PRO:HD3   | 2.48                     | 0.43              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 29:BE:170:LEU:HB3 | 29:BE:184:VAL:HG12 | 2.01                     | 0.43              |
| 30:BF:63:LYS:HG3  | 30:BF:75:HIS:O     | 2.18                     | 0.43              |
| 35:BO:80:ASP:HB2  | 40:BT:70:VAL:CG1   | 2.48                     | 0.43              |
| 36:BP:48:PRO:HG2  | 36:BP:49:ARG:N     | 2.30                     | 0.43              |
| 37:BQ:108:GLY:HA3 | 46:BZ:116:VAL:HG11 | 1.99                     | 0.43              |
| 42:BV:47:VAL:O    | 42:BV:49:THR:O     | 2.36                     | 0.43              |
| 43:BW:69:LEU:O    | 43:BW:70:TYR:HB3   | 2.17                     | 0.43              |
| 44:BX:11:PRO:HB2  | 44:BX:12:VAL:HG22  | 2.00                     | 0.43              |
| 1:CA:337:C:H2'    | 1:CA:338:A:H8      | 1.83                     | 0.43              |
| 1:CA:963:G:H21    | 10:CJ:55:LYS:NZ    | 2.16                     | 0.43              |
| 1:CA:1314:C:H2'   | 1:CA:1315:U:C6     | 2.52                     | 0.43              |
| 1:CA:1342:C:O3'   | 9:CI:125:TYR:HB3   | 2.18                     | 0.43              |
| 1:CA:1442:G:C6    | 1:CA:1442(B):A:N6  | 2.86                     | 0.43              |
| 2:CB:24:TRP:CD1   | 2:CB:24:TRP:H      | 2.37                     | 0.43              |
| 2:CB:103:THR:OG1  | 2:CB:176:GLU:HG2   | 2.18                     | 0.43              |
| 2:CB:164:VAL:O    | 2:CB:186:ALA:HB1   | 2.19                     | 0.43              |
| 2:CB:173:ALA:O    | 2:CB:174:VAL:C     | 2.62                     | 0.43              |
| 2:CB:177:ALA:O    | 2:CB:178:ARG:C     | 2.62                     | 0.43              |
| 3:CC:154:SER:OG   | 3:CC:155:GLY:N     | 2.47                     | 0.43              |
| 5:CE:144:THR:C    | 5:CE:146:ALA:N     | 2.74                     | 0.43              |
| 6:CF:10:LEU:O     | 6:CF:11:ASN:C      | 2.61                     | 0.43              |
| 8:CH:27:PRO:HG3   | 8:CH:58:TYR:HE2    | 1.84                     | 0.43              |
| 12:CL:83:VAL:CG2  | 12:CL:100:ILE:HD13 | 2.47                     | 0.43              |
| 12:CL:90:VAL:CG1  | 12:CL:93:LEU:HG    | 2.45                     | 0.43              |
| 15:CO:24:SER:OG   | 15:CO:25:THR:N     | 2.50                     | 0.43              |
| 17:CQ:60:ILE:O    | 17:CQ:60:ILE:HG23  | 2.17                     | 0.43              |
| 21:CU:9:ARG:O     | 21:CU:13:ILE:HG13  | 2.18                     | 0.43              |
| 22:CV:24:C:N3     | 22:CV:25:U:C4      | 2.86                     | 0.43              |
| 23:CW:4:C:N4      | 23:CW:5:G:O6       | 2.51                     | 0.43              |
| 23:CW:5:G:N2      | 23:CW:6:G:C4       | 2.86                     | 0.43              |
| 25:DA:456:C:C4    | 44:DX:69:TYR:CE2   | 3.06                     | 0.43              |
| 25:DA:585:G:O6    | 25:DA:1251:C:H2'   | 2.18                     | 0.43              |
| 25:DA:2146:C:H4'  | 25:DA:2147:G:O5'   | 2.19                     | 0.43              |
| 25:DA:2425:A:H1'  | 25:DA:2427:C:C4    | 2.52                     | 0.43              |
| 29:DE:7:VAL:HA    | 29:DE:194:GLY:O    | 2.18                     | 0.43              |
| 30:DF:6:VAL:C     | 30:DF:7:TYR:CD1    | 2.95                     | 0.43              |
| 30:DF:34:TRP:CE3  | 36:DP:8:PRO:HB3    | 2.53                     | 0.43              |
| 31:DG:111:LEU:N   | 31:DG:112:PRO:CD   | 2.81                     | 0.43              |
| 31:DG:146:TYR:O   | 31:DG:149:VAL:N    | 2.50                     | 0.43              |
| 32:DH:4:ILE:O     | 32:DH:6:ARG:N      | 2.42                     | 0.43              |
| 32:DH:155:SER:O   | 32:DH:156:ALA:O    | 2.36                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 33:DI:110:ASP:OD2 | 33:DI:130:TYR:CE1 | 2.71                     | 0.43              |
| 34:DN:118:LYS:C   | 34:DN:120:LEU:H   | 2.27                     | 0.43              |
| 40:DT:93:ARG:HH11 | 40:DT:93:ARG:CG   | 2.31                     | 0.43              |
| 42:DV:38:LEU:N    | 42:DV:51:VAL:HG13 | 2.33                     | 0.43              |
| 43:DW:92:ARG:O    | 43:DW:93:ALA:HB3  | 2.18                     | 0.43              |
| 45:DY:43:ASN:CA   | 45:DY:64:GLU:HA   | 2.48                     | 0.43              |
| 45:DY:77:PRO:O    | 45:DY:78:ALA:CB   | 2.66                     | 0.43              |
| 46:DZ:23:LYS:HD3  | 46:DZ:23:LYS:HA   | 1.66                     | 0.43              |
| 47:D0:27:GLU:HG3  | 47:D0:68:GLU:HA   | 1.99                     | 0.43              |
| 52:D5:41:PRO:HA   | 52:D5:42:PRO:HD2  | 1.79                     | 0.43              |
| 55:D8:6:THR:HG21  | 55:D8:63:PRO:HD3  | 2.00                     | 0.43              |
| 1:AA:242:C:H6     | 1:AA:242:C:C3'    | 2.26                     | 0.43              |
| 1:AA:346:G:OP1    | 40:BT:41:ARG:NH2  | 2.51                     | 0.43              |
| 1:AA:591:U:H2'    | 1:AA:592:G:C8     | 2.53                     | 0.43              |
| 1:AA:1410:G:H2'   | 1:AA:1411:C:C6    | 2.53                     | 0.43              |
| 2:AB:139:LYS:C    | 2:AB:141:GLU:N    | 2.76                     | 0.43              |
| 4:AD:133:VAL:HG13 | 4:AD:135:LEU:H    | 1.83                     | 0.43              |
| 5:AE:142:LEU:O    | 5:AE:143:ARG:CD   | 2.66                     | 0.43              |
| 6:AF:11:ASN:HB3   | 6:AF:14:LEU:HG    | 1.99                     | 0.43              |
| 7:AG:92:SER:HB3   | 7:AG:95:ARG:HB3   | 2.00                     | 0.43              |
| 7:AG:146:GLU:HA   | 7:AG:149:ARG:HB2  | 2.01                     | 0.43              |
| 9:AI:26:VAL:HG13  | 9:AI:61:ALA:HB3   | 1.99                     | 0.43              |
| 9:AI:58:HIS:CB    | 9:AI:59:PHE:CD1   | 3.01                     | 0.43              |
| 13:AM:5:ALA:O     | 13:AM:7:VAL:N     | 2.51                     | 0.43              |
| 13:AM:66:LEU:HD23 | 13:AM:66:LEU:HA   | 1.73                     | 0.43              |
| 20:AT:43:LEU:O    | 20:AT:47:GLY:N    | 2.50                     | 0.43              |
| 22:AV:38:A:C2     | 24:AX:16:A:C5     | 3.07                     | 0.43              |
| 25:BA:89:G:H3'    | 25:BA:90:U:H5''   | 2.01                     | 0.43              |
| 25:BA:506:G:O3'   | 25:BA:507:A:H8    | 2.01                     | 0.43              |
| 25:BA:907:U:OP1   | 37:BQ:24:GLY:N    | 2.50                     | 0.43              |
| 25:BA:994:C:O2'   | 25:BA:996:A:OP1   | 2.24                     | 0.43              |
| 25:BA:1456:G:C4   | 25:BA:1457:A:C8   | 3.06                     | 0.43              |
| 25:BA:1464:C:O2'  | 25:BA:1528:A:H8   | 2.01                     | 0.43              |
| 25:BA:1647:G:C4'  | 25:BA:1648:C:O5'  | 2.58                     | 0.43              |
| 25:BA:1814:G:H4'  | 28:BD:51:VAL:HG21 | 2.01                     | 0.43              |
| 28:BD:211:ARG:HA  | 28:BD:214:TRP:CD2 | 2.53                     | 0.43              |
| 30:BF:63:LYS:HA   | 30:BF:76:GLY:O    | 2.19                     | 0.43              |
| 31:BG:152:LEU:HG  | 31:BG:153:ARG:H   | 1.81                     | 0.43              |
| 32:BH:37:VAL:HG11 | 32:BH:68:THR:HG21 | 2.00                     | 0.43              |
| 37:BQ:133:ARG:O   | 37:BQ:134:ARG:CB  | 2.66                     | 0.43              |
| 38:BR:11:ASN:C    | 38:BR:12:ARG:HG3  | 2.42                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 42:BV:20:LEU:HB2   | 42:BV:21:ARG:H     | 1.47                     | 0.43              |
| 43:BW:10:VAL:HG21  | 43:BW:103:ILE:HG13 | 2.00                     | 0.43              |
| 45:BY:54:LYS:O     | 45:BY:54:LYS:CG    | 2.64                     | 0.43              |
| 54:B7:18:PHE:C     | 54:B7:20:ALA:N     | 2.73                     | 0.43              |
| 1:CA:324:G:H22     | 1:CA:327:A:P       | 2.41                     | 0.43              |
| 1:CA:1059:C:H2'    | 1:CA:1060:C:H6     | 1.83                     | 0.43              |
| 1:CA:1376:U:H2'    | 1:CA:1377:A:C8     | 2.54                     | 0.43              |
| 4:CD:17:VAL:HG12   | 4:CD:18:LYS:N      | 2.33                     | 0.43              |
| 4:CD:126:ILE:HG22  | 4:CD:127:THR:N     | 2.33                     | 0.43              |
| 8:CH:4:ASP:CG      | 8:CH:85:ARG:HH12   | 2.26                     | 0.43              |
| 8:CH:105:ARG:HA    | 8:CH:105:ARG:HD3   | 1.65                     | 0.43              |
| 8:CH:109:ILE:HG12  | 8:CH:110:ALA:N     | 2.32                     | 0.43              |
| 9:CI:17:VAL:CG1    | 9:CI:81:ILE:HD13   | 2.45                     | 0.43              |
| 12:CL:126:LYS:NZ   | 12:CL:127:GLU:HB2  | 2.34                     | 0.43              |
| 13:CM:115:LYS:O    | 13:CM:116:THR:C    | 2.62                     | 0.43              |
| 25:DA:271(J):C:H5' | 25:DA:271(K):U:OP2 | 2.18                     | 0.43              |
| 25:DA:628:G:O2'    | 25:DA:651:G:O2'    | 2.35                     | 0.43              |
| 25:DA:845:G:O2'    | 25:DA:846:C:H5     | 2.02                     | 0.43              |
| 25:DA:1336:A:OP1   | 44:DX:64:LYS:HE3   | 2.18                     | 0.43              |
| 25:DA:2391:G:HO2'  | 25:DA:2424:C:N4    | 2.16                     | 0.43              |
| 25:DA:2615:U:C2    | 25:DA:2616:C:C5    | 3.06                     | 0.43              |
| 26:DB:31:C:H2'     | 26:DB:53:A:H61     | 1.83                     | 0.43              |
| 27:DC:62:VAL:O     | 27:DC:63:SER:C     | 2.60                     | 0.43              |
| 28:DD:79:VAL:HG21  | 28:DD:111:LEU:CD1  | 2.42                     | 0.43              |
| 28:DD:168:ARG:O    | 28:DD:169:GLU:HB2  | 2.18                     | 0.43              |
| 29:DE:47:VAL:CG1   | 29:DE:48:GLN:N     | 2.81                     | 0.43              |
| 29:DE:66:HIS:HD1   | 29:DE:66:HIS:C     | 2.24                     | 0.43              |
| 30:DF:9:ILE:CG2    | 30:DF:20:LEU:O     | 2.66                     | 0.43              |
| 31:DG:32:PRO:HA    | 31:DG:162:THR:OG1  | 2.18                     | 0.43              |
| 31:DG:125:PHE:CD2  | 31:DG:166:ASP:HB2  | 2.53                     | 0.43              |
| 33:DI:86:THR:O     | 33:DI:87:LYS:HB2   | 2.18                     | 0.43              |
| 33:DI:94:ALA:H     | 33:DI:116:LEU:HD13 | 1.83                     | 0.43              |
| 33:DI:121:LYS:O    | 33:DI:122:GLU:HB2  | 2.19                     | 0.43              |
| 35:DO:26:LYS:HB3   | 35:DO:27:GLY:H     | 1.59                     | 0.43              |
| 35:DO:77:ILE:HD11  | 40:DT:72:VAL:HG12  | 2.00                     | 0.43              |
| 35:DO:105:GLU:OE1  | 35:DO:105:GLU:N    | 2.44                     | 0.43              |
| 36:DP:52:GLU:O     | 36:DP:54:GLY:N     | 2.51                     | 0.43              |
| 37:DQ:58:PHE:O     | 37:DQ:59:ARG:C     | 2.61                     | 0.43              |
| 38:DR:12:ARG:NH1   | 38:DR:12:ARG:CG    | 2.80                     | 0.43              |
| 43:DW:61:ASN:N     | 43:DW:61:ASN:ND2   | 2.66                     | 0.43              |
| 50:D3:6:VAL:HG13   | 50:D3:56:VAL:HG13  | 2.00                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 55:D8:62:LEU:H     | 55:D8:62:LEU:HG    | 1.68                     | 0.43              |
| 1:AA:652:U:C5      | 1:AA:752:G:N3      | 2.86                     | 0.43              |
| 1:AA:737:A:O2'     | 6:AF:72:VAL:HG11   | 2.18                     | 0.43              |
| 1:AA:1031:G:H2'    | 1:AA:1032:G:C8     | 2.54                     | 0.43              |
| 1:AA:1305:G:O2'    | 1:AA:1306:A:H8     | 2.01                     | 0.43              |
| 1:AA:1323:G:H2'    | 1:AA:1324:A:C8     | 2.53                     | 0.43              |
| 2:AB:155:LEU:HD22  | 2:AB:155:LEU:HA    | 1.88                     | 0.43              |
| 2:AB:171:ALA:O     | 2:AB:172:ILE:C     | 2.62                     | 0.43              |
| 3:AC:107:GLN:H     | 3:AC:107:GLN:CD    | 2.26                     | 0.43              |
| 8:AH:56:LYS:HB2    | 8:AH:58:TYR:HE1    | 1.84                     | 0.43              |
| 8:AH:109:ILE:HG22  | 8:AH:137:VAL:O     | 2.18                     | 0.43              |
| 10:AJ:3:LYS:N      | 10:AJ:74:ILE:O     | 2.51                     | 0.43              |
| 10:AJ:64:GLU:OE2   | 10:AJ:66:ARG:HG3   | 2.18                     | 0.43              |
| 11:AK:127:LYS:HE2  | 11:AK:127:LYS:CA   | 2.46                     | 0.43              |
| 25:BA:34:C:H2'     | 25:BA:35:G:C5'     | 2.49                     | 0.43              |
| 25:BA:83:G:N2      | 25:BA:102:G:H2'    | 2.33                     | 0.43              |
| 25:BA:196:A:H5''   | 36:BP:46:LYS:CE    | 2.49                     | 0.43              |
| 25:BA:974:G:C4     | 25:BA:989:G:C2     | 3.07                     | 0.43              |
| 25:BA:1044:G:H1'   | 25:BA:1111:A:N1    | 2.32                     | 0.43              |
| 25:BA:1964:G:H4'   | 25:BA:1965:C:OP2   | 2.18                     | 0.43              |
| 25:BA:2078:C:H2'   | 25:BA:2079:U:C6    | 2.54                     | 0.43              |
| 25:BA:2086:U:H2'   | 25:BA:2087:G:C8    | 2.53                     | 0.43              |
| 25:BA:2291:U:H2'   | 25:BA:2292:C:C6    | 2.54                     | 0.43              |
| 25:BA:2847:U:OP1   | 40:BT:98:LYS:HD3   | 2.19                     | 0.43              |
| 28:BD:168:ARG:O    | 28:BD:169:GLU:HB2  | 2.18                     | 0.43              |
| 30:BF:7:TYR:CB     | 30:BF:16:GLY:C     | 2.91                     | 0.43              |
| 30:BF:7:TYR:HD2    | 30:BF:16:GLY:H     | 1.66                     | 0.43              |
| 30:BF:102:PRO:HB2  | 30:BF:105:VAL:HG23 | 1.99                     | 0.43              |
| 30:BF:160:ASN:HB3  | 30:BF:163:VAL:HG23 | 1.99                     | 0.43              |
| 31:BG:21:ARG:HD3   | 31:BG:21:ARG:C     | 2.44                     | 0.43              |
| 33:BI:81:VAL:HG11  | 33:BI:88:ILE:HD12  | 2.01                     | 0.43              |
| 35:BO:64:ARG:HG2   | 35:BO:79:PHE:CD1   | 2.52                     | 0.43              |
| 35:BO:86:ILE:C     | 35:BO:87:ILE:HD13  | 2.44                     | 0.43              |
| 36:BP:124:LYS:HZ2  | 36:BP:143:GLY:CA   | 2.27                     | 0.43              |
| 38:BR:59:ASP:O     | 38:BR:60:LEU:C     | 2.62                     | 0.43              |
| 38:BR:113:LEU:HD12 | 38:BR:113:LEU:HA   | 1.44                     | 0.43              |
| 39:BS:34:HIS:CE1   | 39:BS:54:LEU:CD2   | 3.02                     | 0.43              |
| 40:BT:28:VAL:HG12  | 40:BT:29:ARG:NH2   | 2.33                     | 0.43              |
| 40:BT:57:PHE:C     | 40:BT:59:THR:H     | 2.26                     | 0.43              |
| 40:BT:129:ARG:HG3  | 40:BT:129:ARG:O    | 2.18                     | 0.43              |
| 43:BW:8:ARG:HH11   | 43:BW:8:ARG:CG     | 2.32                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 45:BY:13:VAL:CG2   | 45:BY:28:LYS:HE2   | 2.43                     | 0.43              |
| 45:BY:87:LYS:O     | 45:BY:88:LYS:HB2   | 2.17                     | 0.43              |
| 45:BY:96:ILE:HD12  | 45:BY:99:CYS:HB2   | 2.01                     | 0.43              |
| 47:B0:9:SER:OG     | 47:B0:10:THR:N     | 2.52                     | 0.43              |
| 47:B0:46:LYS:O     | 47:B0:78:TYR:HA    | 2.18                     | 0.43              |
| 49:B2:69:ARG:NH1   | 49:B2:69:ARG:CG    | 2.80                     | 0.43              |
| 50:B3:31:LEU:O     | 50:B3:32:GLN:HB2   | 2.17                     | 0.43              |
| 54:B7:24:THR:HG23  | 54:B7:27:GLY:CA    | 2.47                     | 0.43              |
| 1:CA:100:C:H2'     | 1:CA:101:A:C1'     | 2.47                     | 0.43              |
| 1:CA:246:A:H61     | 1:CA:281:G:C1'     | 2.30                     | 0.43              |
| 1:CA:1238:A:N7     | 1:CA:1301:U:O4     | 2.52                     | 0.43              |
| 1:CA:1452:C:O2'    | 1:CA:1456:G:OP2    | 2.30                     | 0.43              |
| 3:CC:69:HIS:O      | 3:CC:70:VAL:HG22   | 2.18                     | 0.43              |
| 3:CC:83:ARG:C      | 3:CC:85:ARG:N      | 2.76                     | 0.43              |
| 3:CC:110:ASN:O     | 3:CC:111:LEU:HD22  | 2.18                     | 0.43              |
| 4:CD:30:LYS:O      | 4:CD:32:ALA:N      | 2.48                     | 0.43              |
| 4:CD:124:GLY:C     | 4:CD:126:ILE:N     | 2.75                     | 0.43              |
| 5:CE:41:VAL:CG1    | 5:CE:113:ALA:HA    | 2.48                     | 0.43              |
| 6:CF:99:ALA:HB2    | 18:CR:31:LEU:HD11  | 2.01                     | 0.43              |
| 9:CI:9:ARG:HG3     | 9:CI:14:VAL:HG22   | 2.00                     | 0.43              |
| 9:CI:55:ALA:CB     | 9:CI:58:HIS:CG     | 3.01                     | 0.43              |
| 10:CJ:8:LEU:HB3    | 10:CJ:16:LEU:HD21  | 2.00                     | 0.43              |
| 13:CM:10:PRO:O     | 13:CM:11:ARG:HB3   | 2.18                     | 0.43              |
| 19:CS:53:ASN:OD1   | 19:CS:53:ASN:C     | 2.62                     | 0.43              |
| 20:CT:16:HIS:O     | 20:CT:19:SER:N     | 2.52                     | 0.43              |
| 20:CT:43:LEU:HA    | 20:CT:46:GLU:HB3   | 2.00                     | 0.43              |
| 25:DA:142:A:H5'    | 25:DA:142(A):C:OP2 | 2.18                     | 0.43              |
| 25:DA:272(D):G:H1  | 25:DA:364:C:H42    | 1.65                     | 0.43              |
| 25:DA:404:C:H4'    | 25:DA:405:U:H5'    | 2.00                     | 0.43              |
| 25:DA:1024:G:C6    | 25:DA:1025:G:C6    | 3.07                     | 0.43              |
| 25:DA:1525:G:H2'   | 25:DA:1526:G:C8    | 2.54                     | 0.43              |
| 25:DA:1698:A:C8    | 25:DA:1700:A:H5''  | 2.54                     | 0.43              |
| 25:DA:2257:U:H2'   | 25:DA:2258:C:C6    | 2.53                     | 0.43              |
| 25:DA:2394:C:OP1   | 36:DP:63:PRO:HD2   | 2.18                     | 0.43              |
| 25:DA:2698:U:H2'   | 25:DA:2699:C:C6    | 2.53                     | 0.43              |
| 25:DA:2774:C:H2'   | 25:DA:2775:A:O4'   | 2.18                     | 0.43              |
| 28:DD:206:LEU:HD23 | 28:DD:206:LEU:HA   | 1.79                     | 0.43              |
| 31:DG:115:ARG:O    | 31:DG:116:ASP:HB2  | 2.18                     | 0.43              |
| 31:DG:127:GLY:HA2  | 31:DG:166:ASP:CG   | 2.44                     | 0.43              |
| 31:DG:134:GLY:C    | 31:DG:135:LEU:HD12 | 2.44                     | 0.43              |
| 32:DH:9:ILE:HD12   | 32:DH:49:VAL:HG11  | 2.00                     | 0.43              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 32:DH:144:VAL:O   | 32:DH:148:ILE:HG12 | 2.19                     | 0.43              |
| 33:DI:31:LEU:N    | 33:DI:32:PRO:CD    | 2.82                     | 0.43              |
| 33:DI:73:GLU:HB2  | 33:DI:136:VAL:CG2  | 2.48                     | 0.43              |
| 35:DO:2:ILE:HD11  | 35:DO:82:ASN:ND2   | 2.33                     | 0.43              |
| 35:DO:18:LYS:HD2  | 35:DO:45:GLU:OE1   | 2.17                     | 0.43              |
| 35:DO:80:ASP:OD2  | 40:DT:64:ARG:NH2   | 2.51                     | 0.43              |
| 37:DQ:16:ARG:O    | 37:DQ:17:LEU:HD23  | 2.18                     | 0.43              |
| 37:DQ:30:GLY:O    | 37:DQ:134:ARG:NH1  | 2.50                     | 0.43              |
| 41:DU:55:ARG:HA   | 41:DU:58:ARG:CG    | 2.49                     | 0.43              |
| 42:DV:52:VAL:O    | 42:DV:52:VAL:HG23  | 2.19                     | 0.43              |
| 45:DY:9:LYS:O     | 45:DY:10:GLY:C     | 2.61                     | 0.43              |
| 45:DY:30:VAL:HG13 | 45:DY:37:VAL:HG12  | 1.99                     | 0.43              |
| 45:DY:40:GLU:N    | 45:DY:40:GLU:CD    | 2.75                     | 0.43              |
| 46:DZ:23:LYS:N    | 46:DZ:41:LEU:HG    | 2.33                     | 0.43              |
| 46:DZ:139:VAL:O   | 46:DZ:139:VAL:HG23 | 2.19                     | 0.43              |
| 47:D0:46:LYS:HD2  | 47:D0:78:TYR:CZ    | 2.54                     | 0.43              |
| 56:D9:9:ARG:HB3   | 56:D9:9:ARG:HH11   | 1.76                     | 0.43              |
| 1:AA:376:G:OP2    | 16:AP:67:THR:HG21  | 2.19                     | 0.43              |
| 1:AA:748:C:O2'    | 1:AA:749:C:OP2     | 2.30                     | 0.43              |
| 1:AA:994:A:H2     | 14:AN:4:LYS:HG3    | 1.82                     | 0.43              |
| 1:AA:1278:U:H5''  | 1:AA:1279:A:O4'    | 2.18                     | 0.43              |
| 2:AB:18:GLY:O     | 2:AB:204:ASN:HB2   | 2.18                     | 0.43              |
| 2:AB:154:LEU:O    | 2:AB:156:LYS:HG3   | 2.18                     | 0.43              |
| 2:AB:166:ASP:HA   | 2:AB:167:PRO:HD2   | 1.59                     | 0.43              |
| 2:AB:168:THR:CG2  | 2:AB:192:SER:HA    | 2.48                     | 0.43              |
| 3:AC:24:ALA:HB1   | 3:AC:28:GLN:O      | 2.18                     | 0.43              |
| 7:AG:16:LEU:HD13  | 9:AI:44:VAL:CG2    | 2.47                     | 0.43              |
| 8:AH:23:SER:HA    | 8:AH:63:LEU:HD23   | 2.01                     | 0.43              |
| 9:AI:14:VAL:HG12  | 9:AI:15:ALA:H      | 1.83                     | 0.43              |
| 9:AI:77:ILE:O     | 9:AI:81:ILE:HG12   | 2.18                     | 0.43              |
| 10:AJ:4:ILE:HG23  | 10:AJ:100:THR:HG23 | 2.00                     | 0.43              |
| 11:AK:73:MET:CG   | 11:AK:103:LEU:HD21 | 2.49                     | 0.43              |
| 15:AO:69:TYR:CD2  | 15:AO:70:LEU:N     | 2.87                     | 0.43              |
| 18:AR:58:LEU:HB3  | 18:AR:62:GLU:HB2   | 2.01                     | 0.43              |
| 22:AV:15:G:C2     | 22:AV:49:C:H5      | 2.34                     | 0.43              |
| 22:AV:65:G:H2'    | 22:AV:66:C:O4'     | 2.18                     | 0.43              |
| 23:AW:2:C:H42     | 23:AW:71:G:H1      | 1.66                     | 0.43              |
| 23:AW:21:A:C2     | 23:AW:48:C:C2      | 3.07                     | 0.43              |
| 25:BA:250:G:C6    | 25:BA:251:A:C6     | 3.07                     | 0.43              |
| 25:BA:769:G:H4'   | 25:BA:1379:A:C6    | 2.52                     | 0.43              |
| 25:BA:861:A:N3    | 26:BB:79:C:O2'     | 2.49                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:BA:1010:A:H1'  | 25:BA:1153:C:H1'  | 2.00                     | 0.43              |
| 25:BA:1497:U:H5'  | 25:BA:1498:C:C5   | 2.54                     | 0.43              |
| 25:BA:1748:G:H2'  | 25:BA:1749:A:O4'  | 2.19                     | 0.43              |
| 25:BA:1789:A:OP1  | 28:BD:221:VAL:HA  | 2.17                     | 0.43              |
| 25:BA:2123:G:H2'  | 25:BA:2124:G:H8   | 1.83                     | 0.43              |
| 25:BA:2846:G:OP2  | 40:BT:54:ARG:HB2  | 2.18                     | 0.43              |
| 28:BD:25:THR:C    | 28:BD:27:THR:N    | 2.75                     | 0.43              |
| 28:BD:264:LYS:CG  | 28:BD:265:PRO:HD2 | 2.49                     | 0.43              |
| 29:BE:16:ARG:O    | 29:BE:17:ASP:CB   | 2.60                     | 0.43              |
| 29:BE:92:THR:C    | 29:BE:94:GLU:N    | 2.74                     | 0.43              |
| 30:BF:89:VAL:O    | 30:BF:91:GLY:N    | 2.47                     | 0.43              |
| 31:BG:58:GLN:HG3  | 31:BG:59:GLU:N    | 2.33                     | 0.43              |
| 31:BG:64:THR:OG1  | 31:BG:94:LEU:HD21 | 2.18                     | 0.43              |
| 31:BG:125:PHE:CB  | 31:BG:166:ASP:OD2 | 2.66                     | 0.43              |
| 33:BI:10:GLU:O    | 33:BI:11:ASN:HB3  | 2.17                     | 0.43              |
| 34:BN:27:ALA:HA   | 34:BN:30:ILE:CG1  | 2.47                     | 0.43              |
| 35:BO:63:VAL:O    | 35:BO:64:ARG:HG3  | 2.19                     | 0.43              |
| 38:BR:59:ASP:OD1  | 38:BR:61:HIS:HB3  | 2.19                     | 0.43              |
| 38:BR:116:LEU:O   | 38:BR:117:VAL:C   | 2.60                     | 0.43              |
| 40:BT:132:LYS:O   | 40:BT:134:GLU:N   | 2.50                     | 0.43              |
| 43:BW:68:ARG:HD2  | 43:BW:110:LYS:CB  | 2.49                     | 0.43              |
| 44:BX:37:THR:C    | 44:BX:39:ILE:N    | 2.74                     | 0.43              |
| 44:BX:92:LEU:HD21 | 49:B2:37:PHE:HE2  | 1.83                     | 0.43              |
| 45:BY:36:ALA:HB1  | 45:BY:67:LEU:C    | 2.43                     | 0.43              |
| 53:B6:15:GLU:O    | 53:B6:18:ARG:HG2  | 2.18                     | 0.43              |
| 55:B8:50:LEU:CA   | 55:B8:53:PRO:CD   | 2.97                     | 0.43              |
| 1:CA:49:U:C2      | 1:CA:362:G:H1'    | 2.54                     | 0.43              |
| 1:CA:243:A:H5'    | 1:CA:245:C:OP1    | 2.18                     | 0.43              |
| 1:CA:676:A:H1'    | 11:CK:115:PRO:HB3 | 1.99                     | 0.43              |
| 1:CA:764:C:H2'    | 1:CA:765:G:O4'    | 2.19                     | 0.43              |
| 1:CA:828:A:H62    | 1:CA:858:G:N2     | 2.14                     | 0.43              |
| 1:CA:991:U:O2     | 1:CA:993:G:H8     | 2.02                     | 0.43              |
| 1:CA:1198:G:O2'   | 10:CJ:54:PHE:HD2  | 2.00                     | 0.43              |
| 1:CA:1247:U:H3    | 1:CA:1290:G:H1    | 1.65                     | 0.43              |
| 1:CA:1302:U:H5''  | 1:CA:1303:C:OP2   | 2.18                     | 0.43              |
| 2:CB:98:LEU:HB2   | 2:CB:101:MET:HG3  | 2.00                     | 0.43              |
| 2:CB:238:LEU:O    | 2:CB:239:VAL:C    | 2.60                     | 0.43              |
| 4:CD:133:VAL:CG1  | 4:CD:138:TYR:CD1  | 3.01                     | 0.43              |
| 4:CD:188:LEU:O    | 4:CD:189:PRO:C    | 2.61                     | 0.43              |
| 5:CE:43:LEU:HD12  | 5:CE:44:GLY:N     | 2.34                     | 0.43              |
| 5:CE:101:ILE:O    | 5:CE:120:THR:HB   | 2.18                     | 0.43              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 10:CJ:62:HIS:CD2  | 10:CJ:62:HIS:H     | 2.37                     | 0.43              |
| 11:CK:61:ALA:O    | 11:CK:64:ALA:N     | 2.51                     | 0.43              |
| 12:CL:36:VAL:O    | 12:CL:58:VAL:HA    | 2.19                     | 0.43              |
| 20:CT:53:LEU:HD21 | 20:CT:100:ILE:CG1  | 2.48                     | 0.43              |
| 21:CU:6:ARG:NE    | 21:CU:15:ARG:NH1   | 2.66                     | 0.43              |
| 22:CV:24:C:H2'    | 22:CV:25:U:H5'     | 1.97                     | 0.43              |
| 22:CV:29:C:O2'    | 22:CV:30:G:H5''    | 2.15                     | 0.43              |
| 25:DA:1111:A:O2'  | 25:DA:1112:G:H4'   | 2.18                     | 0.43              |
| 25:DA:1331:A:C6   | 25:DA:1333:C:C2    | 3.06                     | 0.43              |
| 25:DA:1641:A:H2'  | 25:DA:1642:G:O4'   | 2.18                     | 0.43              |
| 25:DA:2014:A:O2'  | 52:D5:2:ALA:HB2    | 2.18                     | 0.43              |
| 25:DA:2170:A:H8   | 25:DA:2170:A:O5'   | 2.01                     | 0.43              |
| 25:DA:2646:C:H2'  | 25:DA:2647:U:O4'   | 2.17                     | 0.43              |
| 25:DA:2725:A:N3   | 25:DA:2726:U:C5    | 2.86                     | 0.43              |
| 30:DF:9:ILE:HD12  | 30:DF:123:LEU:HD21 | 2.00                     | 0.43              |
| 30:DF:32:LEU:CD2  | 30:DF:108:LYS:HB3  | 2.48                     | 0.43              |
| 30:DF:57:VAL:HG13 | 30:DF:58:ALA:N     | 2.33                     | 0.43              |
| 31:DG:106:LEU:O   | 31:DG:110:ALA:HB3  | 2.18                     | 0.43              |
| 31:DG:146:TYR:O   | 31:DG:148:MET:N    | 2.52                     | 0.43              |
| 32:DH:6:ARG:HA    | 32:DH:66:GLY:HA2   | 2.00                     | 0.43              |
| 33:DI:60:GLU:CG   | 33:DI:61:ARG:HH22  | 2.27                     | 0.43              |
| 33:DI:79:ILE:HD13 | 33:DI:79:ILE:HA    | 1.87                     | 0.43              |
| 34:DN:57:ALA:C    | 34:DN:58:ASP:O     | 2.61                     | 0.43              |
| 35:DO:87:ILE:HG23 | 35:DO:91:LEU:HA    | 2.01                     | 0.43              |
| 36:DP:2:LYS:O     | 36:DP:3:LEU:C      | 2.62                     | 0.43              |
| 37:DQ:38:GLU:HG3  | 37:DQ:127:ILE:HB   | 2.00                     | 0.43              |
| 37:DQ:64:ILE:HG23 | 37:DQ:106:VAL:HG12 | 2.00                     | 0.43              |
| 40:DT:61:PHE:CD2  | 40:DT:61:PHE:N     | 2.86                     | 0.43              |
| 40:DT:78:LEU:HB3  | 40:DT:79:HIS:ND1   | 2.34                     | 0.43              |
| 41:DU:21:ALA:HB1  | 41:DU:24:TYR:CE1   | 2.53                     | 0.43              |
| 42:DV:72:VAL:O    | 42:DV:72:VAL:HG13  | 2.19                     | 0.43              |
| 43:DW:9:TYR:N     | 43:DW:9:TYR:CD2    | 2.83                     | 0.43              |
| 46:DZ:128:VAL:HB  | 46:DZ:161:VAL:HG13 | 1.99                     | 0.43              |
| 48:D1:52:ARG:CG   | 48:D1:53:VAL:H     | 2.21                     | 0.43              |
| 49:D2:22:GLU:O    | 49:D2:26:ARG:HG3   | 2.19                     | 0.43              |
| 52:D5:31:VAL:HG13 | 52:D5:42:PRO:HD3   | 2.00                     | 0.43              |
| 55:D8:32:LEU:HB3  | 55:D8:36:LYS:NZ    | 2.32                     | 0.43              |
| 1:AA:542:G:OP1    | 4:AD:10:ARG:NH2    | 2.52                     | 0.43              |
| 1:AA:752:G:O2'    | 1:AA:753:A:OP2     | 2.30                     | 0.43              |
| 1:AA:798:G:OP1    | 11:AK:122:LYS:NZ   | 2.52                     | 0.43              |
| 1:AA:981:U:C4     | 1:AA:982:U:C2      | 3.06                     | 0.43              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AA:1274:G:N2    | 1:AA:1275:A:H62    | 2.16                     | 0.43              |
| 1:AA:1286:A:C2    | 21:AU:22:ARG:NH2   | 2.87                     | 0.43              |
| 1:AA:1305:G:H5''  | 21:AU:4:GLY:C      | 2.43                     | 0.43              |
| 3:AC:6:HIS:HD2    | 3:AC:7:PRO:CD      | 2.31                     | 0.43              |
| 3:AC:76:VAL:CG2   | 3:AC:77:ILE:N      | 2.81                     | 0.43              |
| 4:AD:176:LEU:HD12 | 4:AD:177:ASP:N     | 2.34                     | 0.43              |
| 5:AE:100:VAL:HA   | 5:AE:118:ILE:HG22  | 1.99                     | 0.43              |
| 6:AF:17:SER:O     | 6:AF:20:ALA:HB3    | 2.18                     | 0.43              |
| 8:AH:9:MET:SD     | 8:AH:32:LYS:HD3    | 2.58                     | 0.43              |
| 14:AN:59:ALA:HB1  | 14:AN:61:TRP:HZ3   | 1.82                     | 0.43              |
| 18:AR:37:VAL:O    | 18:AR:38:GLU:C     | 2.62                     | 0.43              |
| 20:AT:81:LYS:H    | 20:AT:81:LYS:HG3   | 1.58                     | 0.43              |
| 22:AV:50:G:H1     | 22:AV:66:C:H42     | 1.64                     | 0.43              |
| 23:AW:9:A:C8      | 23:AW:46:G:N2      | 2.87                     | 0.43              |
| 23:AW:34:G:N7     | 24:AX:14:A:N1      | 2.67                     | 0.43              |
| 23:AW:75:C:H6     | 23:AW:75:C:O5'     | 2.02                     | 0.43              |
| 25:BA:17:G:H4'    | 41:BU:25:TRP:CZ2   | 2.52                     | 0.43              |
| 25:BA:30:G:O2'    | 25:BA:1214:A:N3    | 2.38                     | 0.43              |
| 25:BA:1204:A:H2   | 25:BA:1241:A:N1    | 2.16                     | 0.43              |
| 25:BA:1385:G:H1'  | 25:BA:1386:C:C6    | 2.54                     | 0.43              |
| 25:BA:1600:C:OP1  | 44:BX:58:HIS:NE2   | 2.36                     | 0.43              |
| 25:BA:1638:C:O2   | 25:BA:2698:U:O2'   | 2.36                     | 0.43              |
| 25:BA:2300:G:H1   | 25:BA:2316:C:H42   | 1.66                     | 0.43              |
| 25:BA:2675:A:H61  | 25:BA:2732:G:H1    | 1.66                     | 0.43              |
| 28:BD:44:ASN:HB2  | 28:BD:45:ASN:H     | 1.66                     | 0.43              |
| 29:BE:39:PRO:C    | 29:BE:43:GLY:HA2   | 2.33                     | 0.43              |
| 29:BE:154:LYS:O   | 29:BE:155:LYS:C    | 2.60                     | 0.43              |
| 30:BF:18:ARG:HG3  | 30:BF:19:GLU:H     | 1.84                     | 0.43              |
| 30:BF:69:HIS:ND1  | 30:BF:69:HIS:N     | 2.66                     | 0.43              |
| 30:BF:135:LYS:HB3 | 30:BF:138:GLU:HG3  | 1.99                     | 0.43              |
| 33:BI:6:LEU:O     | 33:BI:7:GLU:C      | 2.59                     | 0.43              |
| 33:BI:92:VAL:HG13 | 33:BI:120:ILE:HG13 | 2.01                     | 0.43              |
| 34:BN:10:GLU:O    | 34:BN:11:PRO:C     | 2.62                     | 0.43              |
| 42:BV:40:LEU:CD2  | 42:BV:40:LEU:N     | 2.82                     | 0.43              |
| 55:B8:41:ILE:HD12 | 55:B8:41:ILE:N     | 2.32                     | 0.43              |
| 1:CA:128:G:H22    | 1:CA:130:A:N6      | 2.16                     | 0.43              |
| 1:CA:407:G:C5'    | 4:CD:3:ARG:HH12    | 2.31                     | 0.43              |
| 1:CA:953:G:H2'    | 1:CA:954:G:O4'     | 2.18                     | 0.43              |
| 2:CB:216:SER:O    | 2:CB:218:ALA:N     | 2.52                     | 0.43              |
| 3:CC:29:TYR:C     | 3:CC:29:TYR:CD2    | 2.97                     | 0.43              |
| 3:CC:113:ALA:HB3  | 3:CC:114:PRO:CD    | 2.45                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:CD:108:LEU:HB2   | 4:CD:110:PHE:HD1   | 1.66                     | 0.43              |
| 5:CE:98:THR:HG22   | 5:CE:99:GLY:C      | 2.41                     | 0.43              |
| 5:CE:107:ARG:O     | 5:CE:108:ALA:C     | 2.61                     | 0.43              |
| 6:CF:10:LEU:HD12   | 6:CF:10:LEU:N      | 2.34                     | 0.43              |
| 7:CG:27:ILE:O      | 7:CG:30:ILE:N      | 2.47                     | 0.43              |
| 7:CG:111:ARG:HH11  | 7:CG:113:GLU:CD    | 2.25                     | 0.43              |
| 9:CI:11:LYS:C      | 9:CI:13:ALA:N      | 2.76                     | 0.43              |
| 12:CL:119:LYS:C    | 12:CL:121:GLY:H    | 2.26                     | 0.43              |
| 13:CM:108:ARG:O    | 13:CM:109:THR:C    | 2.59                     | 0.43              |
| 13:CM:115:LYS:C    | 13:CM:116:THR:O    | 2.59                     | 0.43              |
| 15:CO:66:LEU:HD12  | 15:CO:66:LEU:N     | 2.32                     | 0.43              |
| 23:CW:4:C:H2'      | 23:CW:5:G:H8       | 1.84                     | 0.43              |
| 23:CW:34:G:C5      | 24:CX:14:A:C6      | 3.06                     | 0.43              |
| 23:CY:28:G:C5      | 23:CY:29:G:N7      | 2.87                     | 0.43              |
| 25:DA:297:C:O2'    | 25:DA:298:G:OP1    | 2.32                     | 0.43              |
| 25:DA:527:C:H1'    | 25:DA:528:A:C6     | 2.52                     | 0.43              |
| 25:DA:644:A:H4'    | 25:DA:645:C:C4     | 2.49                     | 0.43              |
| 25:DA:755:C:H2'    | 25:DA:756:C:C6     | 2.54                     | 0.43              |
| 25:DA:887:A:C1'    | 25:DA:889:C:H41    | 2.11                     | 0.43              |
| 25:DA:913:U:O2'    | 25:DA:914:C:C6     | 2.70                     | 0.43              |
| 25:DA:1218:C:H5''  | 41:DU:19:LYS:NZ    | 2.33                     | 0.43              |
| 25:DA:1558:A:H1'   | 25:DA:1560:G:OP2   | 2.18                     | 0.43              |
| 25:DA:1827:C:O2'   | 25:DA:1970:A:N3    | 2.46                     | 0.43              |
| 25:DA:2090:G:C6    | 25:DA:2091:U:C4    | 3.06                     | 0.43              |
| 25:DA:2437:U:O2'   | 25:DA:2438:U:H5'   | 2.19                     | 0.43              |
| 27:DC:55:ASP:CG    | 27:DC:56:GLN:N     | 2.77                     | 0.43              |
| 28:DD:264:LYS:HD3  | 28:DD:266:SER:CB   | 2.45                     | 0.43              |
| 30:DF:23:ASP:O     | 30:DF:24:LEU:C     | 2.62                     | 0.43              |
| 30:DF:37:VAL:HG12  | 30:DF:41:LEU:HD12  | 2.00                     | 0.43              |
| 31:DG:34:LEU:HD22  | 31:DG:35:GLU:N     | 2.33                     | 0.43              |
| 31:DG:83:ARG:HG2   | 31:DG:83:ARG:NH1   | 2.34                     | 0.43              |
| 33:DI:93:THR:HG22  | 33:DI:119:PRO:CB   | 2.39                     | 0.43              |
| 33:DI:124:GLY:N    | 33:DI:142:VAL:HG21 | 2.33                     | 0.43              |
| 35:DO:27:GLY:C     | 35:DO:29:ASN:H     | 2.26                     | 0.43              |
| 37:DQ:25:ASP:OD1   | 37:DQ:25:ASP:N     | 2.52                     | 0.43              |
| 41:DU:92:ARG:NH2   | 42:DV:11:GLN:O     | 2.51                     | 0.43              |
| 41:DU:109:LEU:HD23 | 41:DU:109:LEU:HA   | 1.82                     | 0.43              |
| 42:DV:37:VAL:CG2   | 42:DV:37:VAL:O     | 2.66                     | 0.43              |
| 44:DX:57:LEU:HD21  | 44:DX:78:LYS:HE2   | 2.01                     | 0.43              |
| 46:DZ:56:VAL:HG12  | 46:DZ:57:ILE:N     | 2.32                     | 0.43              |
| 48:D1:83:GLU:O     | 48:D1:84:GLY:O     | 2.36                     | 0.43              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 50:D3:23:LEU:HB3   | 50:D3:28:LEU:HB2  | 2.00                     | 0.43              |
| 50:D3:26:LEU:O     | 50:D3:35:ARG:HD3  | 2.18                     | 0.43              |
| 50:D3:26:LEU:O     | 50:D3:27:GLY:C    | 2.61                     | 0.43              |
| 56:D9:19:ARG:HG2   | 56:D9:24:TYR:CD1  | 2.54                     | 0.43              |
| 1:AA:1125:U:H2'    | 1:AA:1126:U:OP2   | 2.19                     | 0.43              |
| 2:AB:102:LEU:HD12  | 2:AB:102:LEU:N    | 2.34                     | 0.43              |
| 3:AC:91:LEU:O      | 3:AC:99:VAL:HG11  | 2.18                     | 0.43              |
| 4:AD:175:SER:HB3   | 4:AD:186:LEU:HD11 | 1.99                     | 0.43              |
| 7:AG:94:ARG:HE     | 7:AG:94:ARG:HB2   | 1.70                     | 0.43              |
| 7:AG:153:HIS:CE1   | 11:AK:57:THR:HG23 | 2.52                     | 0.43              |
| 8:AH:75:ARG:O      | 8:AH:76:PRO:C     | 2.62                     | 0.43              |
| 10:AJ:50:ILE:HA    | 10:AJ:60:ARG:HG2  | 2.00                     | 0.43              |
| 12:AL:45:PRO:HG2   | 12:AL:50:SER:HA   | 2.01                     | 0.43              |
| 12:AL:126:LYS:CE   | 12:AL:127:GLU:H   | 2.21                     | 0.43              |
| 14:AN:27:CYS:SG    | 14:AN:40:CYS:SG   | 3.16                     | 0.43              |
| 15:AO:80:ALA:O     | 15:AO:83:GLU:OE1  | 2.36                     | 0.43              |
| 17:AQ:57:VAL:HG12  | 17:AQ:76:LEU:HD12 | 2.00                     | 0.43              |
| 17:AQ:81:ARG:C     | 17:AQ:83:ASP:H    | 2.27                     | 0.43              |
| 18:AR:38:GLU:O     | 18:AR:39:VAL:C    | 2.61                     | 0.43              |
| 19:AS:16:LEU:HD11  | 19:AS:41:VAL:HG21 | 2.00                     | 0.43              |
| 19:AS:35:SER:C     | 19:AS:37:ARG:H    | 2.27                     | 0.43              |
| 25:BA:90:U:HO2'    | 25:BA:92:A:H8     | 1.62                     | 0.43              |
| 25:BA:127:A:H5''   | 25:BA:128:C:C6    | 2.53                     | 0.43              |
| 25:BA:305:U:H2'    | 25:BA:306:U:C6    | 2.53                     | 0.43              |
| 25:BA:320:A:H4'    | 25:BA:322:A:N7    | 2.33                     | 0.43              |
| 25:BA:747:U:C4     | 52:B5:2:ALA:N     | 2.87                     | 0.43              |
| 25:BA:752:A:O2'    | 25:BA:753:C:OP2   | 2.30                     | 0.43              |
| 25:BA:1397:U:C4    | 25:BA:1602:U:O2   | 2.72                     | 0.43              |
| 25:BA:1426:G:O2'   | 25:BA:1572:A:N6   | 2.45                     | 0.43              |
| 25:BA:1901:A:OP2   | 28:BD:255:LYS:NZ  | 2.38                     | 0.43              |
| 25:BA:1943:U:C1'   | 25:BA:1945:G:H5'  | 2.49                     | 0.43              |
| 25:BA:1991:U:H2'   | 25:BA:1992:G:H5'' | 2.00                     | 0.43              |
| 25:BA:2051:A:H8    | 25:BA:2051:A:OP2  | 2.02                     | 0.43              |
| 25:BA:2127:G:C6    | 25:BA:2162:G:N3   | 2.87                     | 0.43              |
| 28:BD:48:ARG:NH1   | 28:BD:48:ARG:HG3  | 2.33                     | 0.43              |
| 28:BD:80:ALA:HB1   | 28:BD:96:HIS:NE2  | 2.30                     | 0.43              |
| 28:BD:180:GLY:O    | 28:BD:181:GLU:O   | 2.36                     | 0.43              |
| 29:BE:113:PHE:CD2  | 29:BE:113:PHE:C   | 2.97                     | 0.43              |
| 29:BE:167:VAL:HG22 | 29:BE:168:MET:H   | 1.84                     | 0.43              |
| 30:BF:31:HIS:O     | 30:BF:32:LEU:C    | 2.60                     | 0.43              |
| 30:BF:144:LYS:C    | 30:BF:146:ALA:H   | 2.26                     | 0.43              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 32:BH:98:LEU:HB2   | 32:BH:125:VAL:CG2 | 2.35                     | 0.43              |
| 32:BH:111:HIS:HA   | 32:BH:112:PRO:HD2 | 1.73                     | 0.43              |
| 32:BH:138:LYS:O    | 32:BH:141:VAL:N   | 2.49                     | 0.43              |
| 34:BN:62:VAL:CG1   | 34:BN:66:LYS:HB3  | 2.49                     | 0.43              |
| 34:BN:99:LEU:HD22  | 34:BN:99:LEU:O    | 2.18                     | 0.43              |
| 34:BN:123:TYR:CZ   | 34:BN:130:HIS:NE2 | 2.86                     | 0.43              |
| 35:BO:17:ARG:HA    | 35:BO:17:ARG:HD2  | 1.77                     | 0.43              |
| 44:BX:12:VAL:HG23  | 44:BX:13:LEU:N    | 2.34                     | 0.43              |
| 45:BY:81:LYS:HB3   | 45:BY:96:ILE:HG22 | 2.01                     | 0.43              |
| 48:B1:19:GLN:O     | 48:B1:35:THR:HG22 | 2.18                     | 0.43              |
| 48:B1:46:LEU:H     | 48:B1:46:LEU:CD2  | 2.32                     | 0.43              |
| 49:B2:61:LEU:HA    | 49:B2:64:LEU:HB3  | 2.00                     | 0.43              |
| 1:CA:253:U:O2      | 1:CA:275:G:H1'    | 2.18                     | 0.43              |
| 1:CA:710:G:C5'     | 6:CF:54:LYS:HE2   | 2.44                     | 0.43              |
| 1:CA:1002:G:N2     | 1:CA:1003:G:H1'   | 2.34                     | 0.43              |
| 2:CB:41:ILE:HG22   | 2:CB:41:ILE:O     | 2.19                     | 0.43              |
| 2:CB:136:VAL:O     | 2:CB:140:HIS:HB2  | 2.18                     | 0.43              |
| 3:CC:17:ASP:O      | 3:CC:18:TRP:C     | 2.60                     | 0.43              |
| 3:CC:70:VAL:O      | 3:CC:106:VAL:HG23 | 2.19                     | 0.43              |
| 7:CG:25:ALA:O      | 7:CG:28:ASN:N     | 2.51                     | 0.43              |
| 8:CH:116:LYS:HD3   | 8:CH:127:LEU:HD12 | 2.00                     | 0.43              |
| 9:CI:55:ALA:HB1    | 9:CI:58:HIS:CG    | 2.53                     | 0.43              |
| 10:CJ:44:VAL:HG13  | 10:CJ:45:ARG:N    | 2.32                     | 0.43              |
| 12:CL:27:LEU:O     | 12:CL:29:GLY:N    | 2.52                     | 0.43              |
| 13:CM:29:ARG:HD3   | 13:CM:64:TRP:CE2  | 2.54                     | 0.43              |
| 13:CM:65:LYS:HB2   | 13:CM:69:GLU:HB2  | 2.01                     | 0.43              |
| 13:CM:88:ARG:HD3   | 13:CM:98:VAL:HG11 | 1.99                     | 0.43              |
| 16:CP:57:ARG:O     | 16:CP:60:LEU:HB2  | 2.19                     | 0.43              |
| 18:CR:59:SER:HB3   | 18:CR:62:GLU:HG3  | 2.00                     | 0.43              |
| 23:CW:38:A:H2'     | 23:CW:39:U:C5'    | 2.49                     | 0.43              |
| 25:DA:265:A:N6     | 25:DA:428:A:H1'   | 2.34                     | 0.43              |
| 25:DA:528:A:H2     | 25:DA:2043:C:C5'  | 2.31                     | 0.43              |
| 25:DA:706:A:H2'    | 25:DA:707:G:O4'   | 2.19                     | 0.43              |
| 25:DA:869:G:O2'    | 37:DQ:8:LYS:HG3   | 2.19                     | 0.43              |
| 25:DA:876:C:H2'    | 25:DA:877:U:O4'   | 2.19                     | 0.43              |
| 25:DA:943:U:OP2    | 36:DP:36:LYS:CD   | 2.67                     | 0.43              |
| 25:DA:1264:G:H5'   | 52:D5:11:THR:OG1  | 2.19                     | 0.43              |
| 25:DA:1340:U:H1'   | 25:DA:1603:A:H5'  | 2.01                     | 0.43              |
| 25:DA:2208:A:N3    | 25:DA:2219:G:N2   | 2.66                     | 0.43              |
| 30:DF:119:ARG:HH11 | 30:DF:119:ARG:HG2 | 1.83                     | 0.43              |
| 31:DG:9:ARG:C      | 31:DG:11:TYR:N    | 2.75                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:DG:67:LYS:HG3   | 51:D4:6:HIS:ND1    | 2.32                     | 0.43              |
| 32:DH:43:VAL:O     | 32:DH:43:VAL:HG23  | 2.19                     | 0.43              |
| 32:DH:147:ASN:ND2  | 32:DH:147:ASN:H    | 2.15                     | 0.43              |
| 34:DN:3:THR:HG22   | 34:DN:5:VAL:HG12   | 2.00                     | 0.43              |
| 34:DN:97:ARG:O     | 34:DN:98:VAL:C     | 2.61                     | 0.43              |
| 34:DN:120:LEU:C    | 34:DN:120:LEU:HD13 | 2.43                     | 0.43              |
| 37:DQ:2:LEU:O      | 37:DQ:2:LEU:HG     | 2.18                     | 0.43              |
| 41:DU:8:VAL:HG11   | 41:DU:12:ARG:NE    | 2.34                     | 0.43              |
| 41:DU:57:PHE:O     | 41:DU:58:ARG:C     | 2.60                     | 0.43              |
| 42:DV:1:MET:HE2    | 42:DV:43:GLU:HG2   | 1.97                     | 0.43              |
| 46:DZ:112:ARG:HH11 | 46:DZ:112:ARG:HG2  | 1.84                     | 0.43              |
| 46:DZ:116:VAL:O    | 46:DZ:118:GLN:N    | 2.51                     | 0.43              |
| 48:D1:44:PRO:HB2   | 48:D1:46:LEU:HD13  | 2.00                     | 0.43              |
| 52:D5:58:LEU:C     | 52:D5:59:GLU:CG    | 2.92                     | 0.43              |
| 55:D8:57:ARG:C     | 55:D8:59:LYS:N     | 2.77                     | 0.43              |
| 1:AA:299:A:H2'     | 1:AA:300:A:C8      | 2.54                     | 0.43              |
| 1:AA:1067:A:N6     | 1:AA:1109:C:H4'    | 2.33                     | 0.43              |
| 1:AA:1281:U:O2'    | 1:AA:1282:C:H5'    | 2.19                     | 0.43              |
| 2:AB:67:THR:O      | 2:AB:68:ILE:HD13   | 2.19                     | 0.43              |
| 7:AG:41:ARG:O      | 7:AG:43:PHE:N      | 2.52                     | 0.43              |
| 9:AI:27:THR:HG23   | 9:AI:31:GLN:H      | 1.84                     | 0.43              |
| 11:AK:54:ARG:HH12  | 23:AW:40:C:P       | 2.41                     | 0.43              |
| 12:AL:55:VAL:CG1   | 12:AL:56:ALA:N     | 2.82                     | 0.43              |
| 14:AN:22:THR:OG1   | 14:AN:33:VAL:HG21  | 2.18                     | 0.43              |
| 17:AQ:64:PRO:HA    | 17:AQ:70:ARG:HG3   | 2.01                     | 0.43              |
| 18:AR:66:LEU:HD11  | 18:AR:70:ILE:HD11  | 2.00                     | 0.43              |
| 20:AT:33:ILE:O     | 20:AT:37:SER:OG    | 2.36                     | 0.43              |
| 25:BA:139(A):G:N2  | 44:BX:44:GLU:OE1   | 2.42                     | 0.43              |
| 25:BA:1512:U:H2'   | 25:BA:1513:C:C6    | 2.54                     | 0.43              |
| 25:BA:1795:C:C4    | 25:BA:1796:U:C4    | 3.07                     | 0.43              |
| 25:BA:1889:A:H2'   | 25:BA:1890:A:C8    | 2.54                     | 0.43              |
| 26:BB:65:C:C5      | 26:BB:109:C:C4     | 3.06                     | 0.43              |
| 26:BB:90:A:C5      | 26:BB:91:C:H1'     | 2.54                     | 0.43              |
| 27:BC:62:VAL:O     | 27:BC:63:SER:C     | 2.61                     | 0.43              |
| 29:BE:24:THR:HG21  | 29:BE:188:VAL:HB   | 2.00                     | 0.43              |
| 29:BE:137:HIS:CB   | 29:BE:138:PRO:HD2  | 2.43                     | 0.43              |
| 31:BG:9:ARG:O      | 31:BG:10:LYS:C     | 2.62                     | 0.43              |
| 31:BG:85:GLY:O     | 31:BG:86:MET:C     | 2.61                     | 0.43              |
| 33:BI:72:LEU:HD13  | 33:BI:73:GLU:HA    | 2.01                     | 0.43              |
| 33:BI:93:THR:O     | 33:BI:96:ASP:HB2   | 2.19                     | 0.43              |
| 33:BI:97:ILE:HD12  | 33:BI:114:LEU:CD1  | 2.41                     | 0.43              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 34:BN:53:VAL:HG11 | 34:BN:128:HIS:HB2  | 2.01                     | 0.43              |
| 34:BN:128:HIS:O   | 34:BN:128:HIS:CG   | 2.71                     | 0.43              |
| 35:BO:7:TYR:HE1   | 35:BO:20:MET:HB2   | 1.82                     | 0.43              |
| 35:BO:86:ILE:HD12 | 35:BO:86:ILE:H     | 1.82                     | 0.43              |
| 36:BP:24:GLY:O    | 36:BP:25:SER:HB3   | 2.18                     | 0.43              |
| 36:BP:96:THR:C    | 36:BP:97:PRO:O     | 2.59                     | 0.43              |
| 38:BR:4:LEU:HD21  | 38:BR:8:ARG:HH21   | 1.83                     | 0.43              |
| 38:BR:34:ILE:HB   | 38:BR:114:VAL:HG12 | 2.01                     | 0.43              |
| 40:BT:51:ARG:O    | 40:BT:61:PHE:HA    | 2.19                     | 0.43              |
| 40:BT:102:ILE:O   | 40:BT:106:SER:HB3  | 2.18                     | 0.43              |
| 42:BV:21:ARG:CB   | 42:BV:91:TYR:HB2   | 2.48                     | 0.43              |
| 48:B1:64:ALA:HA   | 48:B1:67:ILE:HG13  | 1.99                     | 0.43              |
| 48:B1:83:GLU:HB3  | 48:B1:84:GLY:H     | 1.43                     | 0.43              |
| 50:B3:51:ALA:O    | 50:B3:53:LEU:N     | 2.51                     | 0.43              |
| 53:B6:40:CYS:SG   | 53:B6:45:LYS:HB3   | 2.58                     | 0.43              |
| 54:B7:30:VAL:O    | 54:B7:32:LYS:N     | 2.52                     | 0.43              |
| 55:B8:37:SER:OG   | 55:B8:40:GLU:HG3   | 2.19                     | 0.43              |
| 1:CA:61:G:C5      | 1:CA:107:G:N2      | 2.87                     | 0.43              |
| 1:CA:689:C:OP1    | 11:CK:27:ASN:ND2   | 2.50                     | 0.43              |
| 1:CA:1287:A:H2'   | 1:CA:1288:A:C8     | 2.53                     | 0.43              |
| 1:CA:1306:A:H61   | 1:CA:1331:G:H1'    | 1.84                     | 0.43              |
| 3:CC:155:GLY:HA2  | 3:CC:164:ARG:O     | 2.18                     | 0.43              |
| 4:CD:31:CYS:C     | 4:CD:33:MET:N      | 2.65                     | 0.43              |
| 4:CD:61:LYS:HD3   | 4:CD:62:GLN:N      | 2.34                     | 0.43              |
| 4:CD:62:GLN:HA    | 4:CD:62:GLN:OE1    | 2.19                     | 0.43              |
| 4:CD:99:SER:O     | 4:CD:100:ARG:C     | 2.60                     | 0.43              |
| 5:CE:120:THR:CG2  | 5:CE:121:LYS:N     | 2.81                     | 0.43              |
| 5:CE:145:LYS:O    | 5:CE:149:GLU:HG2   | 2.19                     | 0.43              |
| 9:CI:97:LYS:HB3   | 9:CI:98:PRO:HD3    | 2.01                     | 0.43              |
| 10:CJ:47:PHE:HZ   | 14:CN:37:PHE:HZ    | 1.67                     | 0.43              |
| 10:CJ:48:THR:OG1  | 10:CJ:62:HIS:HB3   | 2.19                     | 0.43              |
| 11:CK:32:ILE:HD11 | 11:CK:68:ALA:C     | 2.43                     | 0.43              |
| 11:CK:33:THR:HG21 | 11:CK:37:GLY:O     | 2.19                     | 0.43              |
| 11:CK:97:ALA:O    | 11:CK:101:SER:HB3  | 2.18                     | 0.43              |
| 12:CL:31:PRO:C    | 12:CL:32:PHE:CG    | 2.97                     | 0.43              |
| 12:CL:82:VAL:HG12 | 12:CL:83:VAL:H     | 1.83                     | 0.43              |
| 16:CP:39:TYR:CZ   | 16:CP:41:PRO:HA    | 2.52                     | 0.43              |
| 16:CP:70:ALA:O    | 16:CP:74:LEU:CD1   | 2.66                     | 0.43              |
| 17:CQ:16:GLN:O    | 17:CQ:17:LYS:HB2   | 2.18                     | 0.43              |
| 19:CS:70:LYS:O    | 19:CS:71:LEU:C     | 2.61                     | 0.43              |
| 23:CY:36:A:C5     | 23:CY:37:A:N7      | 2.87                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:DA:443:A:OP2   | 25:DA:614(B):G:N2 | 2.27                     | 0.43              |
| 25:DA:1011:G:H5'' | 41:DU:77:SER:HB3  | 2.01                     | 0.43              |
| 25:DA:1301:A:O2'  | 25:DA:1302:A:O5'  | 2.37                     | 0.43              |
| 25:DA:1694:C:H5'  | 25:DA:1695:G:C5   | 2.54                     | 0.43              |
| 25:DA:1799:G:C5   | 25:DA:1819:A:N6   | 2.86                     | 0.43              |
| 25:DA:2015:A:C1'  | 52:D5:2:ALA:HA    | 2.46                     | 0.43              |
| 25:DA:2043:C:H1'  | 25:DA:2779:U:O4   | 2.19                     | 0.43              |
| 25:DA:2330:G:H21  | 47:D0:42:GLY:HA2  | 1.84                     | 0.43              |
| 25:DA:2712:U:H2'  | 25:DA:2713:A:H5'' | 2.00                     | 0.43              |
| 29:DE:9:VAL:CG1   | 29:DE:25:VAL:O    | 2.67                     | 0.43              |
| 29:DE:52:LEU:CD2  | 29:DE:76:ARG:HB2  | 2.47                     | 0.43              |
| 29:DE:72:VAL:O    | 29:DE:73:GLU:O    | 2.35                     | 0.43              |
| 29:DE:111:ARG:HB3 | 38:DR:1:MET:HE1   | 2.00                     | 0.43              |
| 30:DF:183:VAL:O   | 30:DF:184:TYR:C   | 2.62                     | 0.43              |
| 35:DO:104:ARG:NH1 | 40:DT:35:LYS:CE   | 2.47                     | 0.43              |
| 40:DT:7:ILE:O     | 40:DT:10:VAL:HB   | 2.18                     | 0.43              |
| 41:DU:83:LEU:HD12 | 41:DU:113:ALA:CB  | 2.47                     | 0.43              |
| 47:D0:45:PHE:CD1  | 47:D0:45:PHE:N    | 2.85                     | 0.43              |
| 47:D0:63:VAL:O    | 47:D0:63:VAL:HG23 | 2.17                     | 0.43              |
| 51:D4:13:ARG:O    | 51:D4:31:ILE:HB   | 2.18                     | 0.43              |
| 1:AA:778:G:H2'    | 1:AA:779:C:O4'    | 2.19                     | 0.43              |
| 1:AA:1100:C:O2'   | 1:AA:1102:A:OP1   | 2.28                     | 0.43              |
| 1:AA:1143:G:H2'   | 1:AA:1144:G:H8    | 1.84                     | 0.43              |
| 1:AA:1179:A:O3'   | 9:AI:103:THR:HG23 | 2.19                     | 0.43              |
| 1:AA:1250:A:H2    | 1:AA:1353:G:H21   | 1.66                     | 0.43              |
| 1:AA:1329:A:H4'   | 13:AM:24:GLY:HA2  | 1.99                     | 0.43              |
| 2:AB:15:VAL:N     | 2:AB:16:HIS:CE1   | 2.87                     | 0.43              |
| 2:AB:127:ILE:O    | 2:AB:128:GLU:C    | 2.61                     | 0.43              |
| 3:AC:22:TRP:HH2   | 3:AC:32:LEU:C     | 2.27                     | 0.43              |
| 4:AD:101:LEU:HA   | 4:AD:101:LEU:HD12 | 1.81                     | 0.43              |
| 5:AE:71:LEU:HD22  | 5:AE:115:VAL:HG22 | 2.01                     | 0.43              |
| 7:AG:87:VAL:CG1   | 7:AG:88:PRO:HD2   | 2.49                     | 0.43              |
| 7:AG:122:HIS:O    | 7:AG:123:GLU:C    | 2.61                     | 0.43              |
| 10:AJ:33:GLN:N    | 10:AJ:75:ILE:HD11 | 2.34                     | 0.43              |
| 12:AL:77:LEU:CD1  | 12:AL:83:VAL:HG21 | 2.49                     | 0.43              |
| 13:AM:112:GLY:O   | 13:AM:113:PRO:C   | 2.61                     | 0.43              |
| 15:AO:21:ASP:OD2  | 15:AO:24:SER:HB3  | 2.19                     | 0.43              |
| 17:AQ:57:VAL:HG12 | 17:AQ:76:LEU:CD1  | 2.49                     | 0.43              |
| 20:AT:53:LEU:CD1  | 20:AT:102:GLY:C   | 2.91                     | 0.43              |
| 20:AT:64:ASP:HA   | 20:AT:67:ALA:HB2  | 2.00                     | 0.43              |
| 20:AT:69:GLY:O    | 20:AT:73:HIS:CD2  | 2.72                     | 0.43              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 22:AV:20:G:H21    | 22:AV:58:A:H1'     | 1.84                     | 0.43              |
| 22:AV:60:A:C2'    | 22:AV:61:U:H5'     | 2.49                     | 0.43              |
| 23:AW:9:A:N6      | 23:AW:22:G:C5      | 2.87                     | 0.43              |
| 23:AW:39:U:O2     | 23:AW:39:U:C3'     | 2.67                     | 0.43              |
| 25:BA:519:U:H2'   | 25:BA:520:G:C8     | 2.54                     | 0.43              |
| 25:BA:619:G:H3'   | 25:BA:620:G:H21    | 1.83                     | 0.43              |
| 25:BA:668:G:C8    | 25:BA:670:A:C8     | 3.07                     | 0.43              |
| 25:BA:952:G:P     | 37:BQ:16:ARG:NH2   | 2.92                     | 0.43              |
| 25:BA:1224:C:H4'  | 42:BV:86:GLY:O     | 2.19                     | 0.43              |
| 25:BA:1434:A:H61  | 25:BA:1558:A:H62   | 1.65                     | 0.43              |
| 25:BA:1567:A:H2   | 28:BD:28:GLU:HB3   | 1.84                     | 0.43              |
| 25:BA:2631:G:N2   | 29:BE:61:ARG:HH12  | 2.16                     | 0.43              |
| 25:BA:2870:C:H2'  | 25:BA:2871:C:O4'   | 2.19                     | 0.43              |
| 30:BF:81:PRO:C    | 30:BF:83:PHE:H     | 2.26                     | 0.43              |
| 32:BH:85:LYS:HD3  | 32:BH:133:VAL:CB   | 2.43                     | 0.43              |
| 32:BH:100:GLY:C   | 32:BH:102:ALA:N    | 2.76                     | 0.43              |
| 34:BN:123:TYR:HH  | 34:BN:130:HIS:CD2  | 2.37                     | 0.43              |
| 35:BO:2:ILE:HD13  | 35:BO:2:ILE:HA     | 1.87                     | 0.43              |
| 36:BP:96:THR:O    | 36:BP:100:LEU:HD23 | 2.19                     | 0.43              |
| 37:BQ:55:VAL:HG12 | 37:BQ:64:ILE:CD1   | 2.49                     | 0.43              |
| 40:BT:102:ILE:O   | 40:BT:103:ARG:C    | 2.61                     | 0.43              |
| 41:BU:39:LEU:HD23 | 41:BU:39:LEU:HA    | 1.77                     | 0.43              |
| 47:B0:53:MET:HE1  | 47:B0:57:PHE:CD1   | 2.54                     | 0.43              |
| 48:B1:86:SER:O    | 48:B1:90:ILE:HG12  | 2.18                     | 0.43              |
| 2:CB:215:LEU:HA   | 2:CB:215:LEU:HD23  | 1.79                     | 0.43              |
| 5:CE:60:TYR:CE1   | 5:CE:64:ARG:HD3    | 2.51                     | 0.43              |
| 7:CG:125:MET:O    | 7:CG:126:ASP:C     | 2.61                     | 0.43              |
| 11:CK:69:ALA:HB1  | 11:CK:73:MET:HE2   | 2.00                     | 0.43              |
| 15:CO:82:ILE:CD1  | 15:CO:87:ILE:HB    | 2.49                     | 0.43              |
| 17:CQ:86:GLU:O    | 17:CQ:90:ILE:HG12  | 2.18                     | 0.43              |
| 20:CT:72:LEU:HD22 | 20:CT:73:HIS:N     | 2.34                     | 0.43              |
| 23:CW:13:C:N3     | 23:CW:23:A:N1      | 2.67                     | 0.43              |
| 25:DA:483:A:O2'   | 45:DY:59:GLY:HA2   | 2.19                     | 0.43              |
| 25:DA:724:U:H2'   | 25:DA:725:G:O4'    | 2.19                     | 0.43              |
| 25:DA:753:C:OP2   | 25:DA:753:C:H6     | 1.99                     | 0.43              |
| 25:DA:995:C:N3    | 34:DN:1:MET:CG     | 2.76                     | 0.43              |
| 25:DA:1287:A:N6   | 25:DA:1288:U:C4    | 2.86                     | 0.43              |
| 25:DA:1453:U:O2'  | 25:DA:1455:G:C8    | 2.65                     | 0.43              |
| 25:DA:2208:A:H1'  | 25:DA:2219:G:C2    | 2.53                     | 0.43              |
| 25:DA:2824:C:H2'  | 25:DA:2825:C:O4'   | 2.19                     | 0.43              |
| 27:DC:191:ALA:O   | 27:DC:195:ALA:HB3  | 2.18                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 28:DD:26:LYS:NZ    | 28:DD:82:ILE:O     | 2.44                     | 0.43              |
| 28:DD:35:LYS:HD3   | 28:DD:35:LYS:HA    | 1.89                     | 0.43              |
| 30:DF:40:GLN:HE22  | 30:DF:184:TYR:HB3  | 1.84                     | 0.43              |
| 31:DG:68:PRO:HG2   | 31:DG:90:LEU:CD1   | 2.49                     | 0.43              |
| 31:DG:137:GLU:HB2  | 31:DG:152:LEU:HD22 | 2.00                     | 0.43              |
| 33:DI:78:THR:HG22  | 33:DI:141:LYS:HD2  | 2.00                     | 0.43              |
| 33:DI:112:LYS:H    | 33:DI:112:LYS:HG2  | 1.67                     | 0.43              |
| 34:DN:34:LEU:HD12  | 34:DN:34:LEU:HA    | 1.79                     | 0.43              |
| 39:DS:69:VAL:HG13  | 39:DS:101:LEU:CD2  | 2.49                     | 0.43              |
| 41:DU:65:ILE:HD11  | 41:DU:96:ALA:HB3   | 2.00                     | 0.43              |
| 45:DY:75:ILE:HB    | 45:DY:80:GLY:HA2   | 2.00                     | 0.43              |
| 46:DZ:8:TYR:HB2    | 46:DZ:38:TYR:CZ    | 2.54                     | 0.43              |
| 49:D2:10:LEU:HD23  | 49:D2:10:LEU:HA    | 1.83                     | 0.43              |
| 1:AA:246:A:N6      | 1:AA:279:A:C4      | 2.87                     | 0.43              |
| 1:AA:323:U:H5'     | 20:AT:23:ARG:HB2   | 2.00                     | 0.43              |
| 1:AA:668:G:O2'     | 15:AO:46:HIS:HD2   | 2.01                     | 0.43              |
| 1:AA:939:G:H5''    | 7:AG:102:ARG:CZ    | 2.47                     | 0.43              |
| 1:AA:1276:G:C2'    | 1:AA:1277:C:H5'    | 2.49                     | 0.43              |
| 1:AA:1342:C:H1'    | 9:AI:124:GLN:OE1   | 2.19                     | 0.43              |
| 2:AB:15:VAL:H      | 2:AB:16:HIS:CE1    | 2.37                     | 0.43              |
| 2:AB:70:PHE:CE2    | 2:AB:163:PHE:HD1   | 2.37                     | 0.43              |
| 3:AC:196:LEU:HB3   | 3:AC:197:GLY:H     | 1.66                     | 0.43              |
| 4:AD:80:GLU:OE2    | 4:AD:80:GLU:HA     | 2.18                     | 0.43              |
| 5:AE:105:VAL:N     | 5:AE:106:PRO:CD    | 2.82                     | 0.43              |
| 9:AI:50:LEU:O      | 9:AI:54:ASP:N      | 2.50                     | 0.43              |
| 9:AI:97:LYS:HE2    | 9:AI:97:LYS:HB2    | 1.77                     | 0.43              |
| 12:AL:6:THR:O      | 12:AL:10:LEU:HD12  | 2.18                     | 0.43              |
| 12:AL:10:LEU:HB3   | 17:AQ:32:TYR:CE1   | 2.54                     | 0.43              |
| 12:AL:112:ASP:C    | 12:AL:113:ARG:O    | 2.57                     | 0.43              |
| 19:AS:14:HIS:CD2   | 19:AS:15:LEU:HD22  | 2.53                     | 0.43              |
| 23:AW:53:G:N1      | 23:AW:54:U:C4      | 2.87                     | 0.43              |
| 25:BA:1273:U:H5'   | 25:BA:1274:A:OP1   | 2.19                     | 0.43              |
| 25:BA:1654:A:OP2   | 38:BR:3:HIS:ND1    | 2.52                     | 0.43              |
| 25:BA:2847:U:C4    | 25:BA:2848:G:C2    | 3.07                     | 0.43              |
| 27:BC:54:SER:O     | 27:BC:55:ASP:HB3   | 2.18                     | 0.43              |
| 28:BD:264:LYS:HG2  | 28:BD:265:PRO:N    | 2.33                     | 0.43              |
| 30:BF:107:LYS:O    | 30:BF:108:LYS:C    | 2.60                     | 0.43              |
| 31:BG:75:LYS:HB2   | 31:BG:77:ILE:HD11  | 2.00                     | 0.43              |
| 34:BN:15:LEU:HD12  | 34:BN:16:ILE:H     | 1.82                     | 0.43              |
| 35:BO:3:GLN:CB     | 35:BO:4:PRO:HD2    | 2.42                     | 0.43              |
| 35:BO:104:ARG:HH22 | 40:BT:35:LYS:HZ1   | 1.65                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 39:BS:17:ARG:C    | 39:BS:19:LYS:N    | 2.77                     | 0.43              |
| 39:BS:98:VAL:HG22 | 39:BS:100:ALA:N   | 2.33                     | 0.43              |
| 40:BT:29:ARG:HD2  | 40:BT:85:LYS:C    | 2.44                     | 0.43              |
| 40:BT:88:ILE:HG22 | 40:BT:89:VAL:CG2  | 2.34                     | 0.43              |
| 41:BU:74:LEU:HD11 | 41:BU:79:PHE:HB2  | 2.01                     | 0.43              |
| 42:BV:35:LEU:O    | 42:BV:36:PRO:C    | 2.62                     | 0.43              |
| 42:BV:57:VAL:HG23 | 42:BV:98:GLU:O    | 2.18                     | 0.43              |
| 43:BW:51:LEU:HD13 | 43:BW:52:GLU:HA   | 2.01                     | 0.43              |
| 43:BW:64:MET:HE3  | 43:BW:109:GLU:HG2 | 2.01                     | 0.43              |
| 50:B3:39:ASP:OD1  | 50:B3:44:ARG:CG   | 2.65                     | 0.43              |
| 55:B8:4:MET:HB2   | 55:B8:4:MET:HE2   | 1.61                     | 0.43              |
| 55:B8:16:ILE:CG2  | 55:B8:64:TYR:HD2  | 2.32                     | 0.43              |
| 55:B8:64:TYR:N    | 55:B8:64:TYR:CD1  | 2.86                     | 0.43              |
| 1:CA:244:U:O4     | 1:CA:906:G:H1'    | 2.18                     | 0.43              |
| 1:CA:511:C:C2     | 1:CA:512:U:C4     | 3.07                     | 0.43              |
| 1:CA:815:A:H4'    | 1:CA:817:C:C4     | 2.54                     | 0.43              |
| 1:CA:859:A:H2'    | 1:CA:860:A:O4'    | 2.19                     | 0.43              |
| 1:CA:881:G:OP2    | 12:CL:12:ARG:NH2  | 2.52                     | 0.43              |
| 1:CA:950:U:H2'    | 1:CA:951:G:C8     | 2.54                     | 0.43              |
| 1:CA:1151:A:H2'   | 1:CA:1152:A:C8    | 2.54                     | 0.43              |
| 3:CC:63:ASN:C     | 3:CC:64:VAL:CG2   | 2.90                     | 0.43              |
| 3:CC:103:VAL:O    | 3:CC:104:GLN:C    | 2.62                     | 0.43              |
| 3:CC:134:ILE:N    | 3:CC:134:ILE:HD13 | 2.33                     | 0.43              |
| 4:CD:19:LEU:CB    | 4:CD:21:LEU:HD11  | 2.48                     | 0.43              |
| 4:CD:122:ARG:HD2  | 4:CD:122:ARG:HA   | 1.71                     | 0.43              |
| 5:CE:65:ASN:OD1   | 5:CE:65:ASN:C     | 2.61                     | 0.43              |
| 7:CG:54:THR:C     | 7:CG:56:GLN:H     | 2.27                     | 0.43              |
| 9:CI:84:ALA:O     | 9:CI:87:GLN:HB3   | 2.19                     | 0.43              |
| 9:CI:127:LYS:NZ   | 22:CV:35:C:OP2    | 2.43                     | 0.43              |
| 11:CK:62:GLN:C    | 11:CK:64:ALA:N    | 2.77                     | 0.43              |
| 12:CL:46:LYS:CG   | 12:CL:47:LYS:N    | 2.54                     | 0.43              |
| 12:CL:115:LYS:O   | 12:CL:117:ARG:N   | 2.52                     | 0.43              |
| 18:CR:56:THR:CB   | 18:CR:58:LEU:CD1  | 2.97                     | 0.43              |
| 23:CW:21:A:C6     | 23:CW:46:G:C4     | 3.07                     | 0.43              |
| 25:DA:197:A:N6    | 25:DA:2430:A:H2'  | 2.34                     | 0.43              |
| 25:DA:286:C:C2'   | 25:DA:287:C:H5'   | 2.49                     | 0.43              |
| 25:DA:670:A:H4'   | 25:DA:671:C:O5'   | 2.18                     | 0.43              |
| 25:DA:1288:U:O2'  | 25:DA:1647:G:N2   | 2.52                     | 0.43              |
| 25:DA:2111:C:O4'  | 25:DA:2118:U:H1'  | 2.18                     | 0.43              |
| 25:DA:2457:U:O4   | 25:DA:2458:G:C6   | 2.72                     | 0.43              |
| 25:DA:2820:A:O4'  | 38:DR:4:LEU:HD23  | 2.18                     | 0.43              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 28:DD:81:ALA:HA    | 28:DD:113:VAL:CG1 | 2.49                     | 0.43              |
| 28:DD:231:HIS:CG   | 28:DD:232:PRO:HD2 | 2.54                     | 0.43              |
| 29:DE:64:LYS:C     | 29:DE:66:HIS:H    | 2.27                     | 0.43              |
| 30:DF:9:ILE:CD1    | 30:DF:125:LEU:HG  | 2.37                     | 0.43              |
| 30:DF:34:TRP:HD1   | 36:DP:6:LEU:HB3   | 1.84                     | 0.43              |
| 31:DG:14:GLU:O     | 31:DG:17:PRO:HG2  | 2.19                     | 0.43              |
| 32:DH:12:PRO:HD3   | 32:DH:48:GLY:O    | 2.19                     | 0.43              |
| 32:DH:41:MET:CE    | 32:DH:64:LEU:HB2  | 2.49                     | 0.43              |
| 32:DH:154:PRO:HG2  | 32:DH:162:ILE:C   | 2.42                     | 0.43              |
| 33:DI:65:ALA:O     | 33:DI:66:GLU:C    | 2.62                     | 0.43              |
| 36:DP:114:ILE:HG23 | 36:DP:127:ALA:HB2 | 2.01                     | 0.43              |
| 37:DQ:16:ARG:HG2   | 37:DQ:17:LEU:H    | 1.83                     | 0.43              |
| 37:DQ:66:ILE:HG22  | 37:DQ:104:PHE:CD2 | 2.54                     | 0.43              |
| 38:DR:52:ILE:HD13  | 38:DR:79:LEU:HD21 | 2.01                     | 0.43              |
| 39:DS:18:ILE:HD12  | 39:DS:88:ASP:HA   | 2.00                     | 0.43              |
| 40:DT:134:GLU:O    | 40:DT:135:ALA:HB3 | 2.19                     | 0.43              |
| 42:DV:47:VAL:O     | 42:DV:48:GLY:C    | 2.62                     | 0.43              |
| 44:DX:47:PHE:CE1   | 49:D2:33:MET:HE1  | 2.54                     | 0.43              |
| 45:DY:19:LYS:O     | 45:DY:20:TYR:CD1  | 2.72                     | 0.43              |
| 46:DZ:58:VAL:HG13  | 46:DZ:67:LEU:N    | 2.34                     | 0.43              |
| 46:DZ:70:LEU:HD23  | 46:DZ:70:LEU:HA   | 1.87                     | 0.43              |
| 49:D2:56:GLN:HE21  | 49:D2:56:GLN:HA   | 1.84                     | 0.43              |
| 55:D8:23:VAL:HG11  | 55:D8:46:ARG:HH11 | 1.81                     | 0.43              |
| 1:AA:533:A:O2'     | 1:AA:534:U:O5'    | 2.37                     | 0.42              |
| 1:AA:1135:U:H2'    | 1:AA:1137:C:H1'   | 2.01                     | 0.42              |
| 1:AA:1214:C:H4'    | 1:AA:1215:G:OP1   | 2.19                     | 0.42              |
| 2:AB:19:HIS:CE1    | 2:AB:205:ASP:OD1  | 2.72                     | 0.42              |
| 2:AB:174:VAL:HG13  | 2:AB:184:VAL:HG11 | 2.01                     | 0.42              |
| 3:AC:172:ARG:C     | 3:AC:173:VAL:HG23 | 2.44                     | 0.42              |
| 4:AD:12:CYS:O      | 4:AD:17:VAL:O     | 2.37                     | 0.42              |
| 4:AD:111:ALA:HB2   | 4:AD:120:LEU:HD12 | 2.01                     | 0.42              |
| 4:AD:202:LEU:O     | 4:AD:205:GLU:HB2  | 2.19                     | 0.42              |
| 5:AE:116:THR:C     | 5:AE:117:ASP:CG   | 2.87                     | 0.42              |
| 8:AH:19:VAL:O      | 8:AH:19:VAL:HG23  | 2.18                     | 0.42              |
| 9:AI:111:ARG:HG2   | 9:AI:112:LYS:N    | 2.33                     | 0.42              |
| 12:AL:92:ASP:O     | 12:AL:93:LEU:HD23 | 2.19                     | 0.42              |
| 14:AN:15:LYS:HD2   | 14:AN:16:PHE:CZ   | 2.54                     | 0.42              |
| 17:AQ:74:LEU:O     | 17:AQ:75:ARG:HB3  | 2.19                     | 0.42              |
| 25:BA:844:C:H2'    | 25:BA:845:G:O4'   | 2.19                     | 0.42              |
| 25:BA:958:U:H5     | 37:BQ:41:TRP:CE3  | 2.36                     | 0.42              |
| 25:BA:1379:A:O2'   | 25:BA:1380:G:OP1  | 2.34                     | 0.42              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 25:BA:1385:G:O6    | 25:BA:1403:C:N3   | 2.51                     | 0.42              |
| 25:BA:1652:A:N6    | 25:BA:1653:G:C2   | 2.87                     | 0.42              |
| 25:BA:2660:A:H2'   | 25:BA:2661:G:O4'  | 2.19                     | 0.42              |
| 26:BB:83:G:H4'     | 50:B3:52:HIS:CD2  | 2.53                     | 0.42              |
| 28:BD:33:LEU:CD2   | 28:BD:102:LYS:HE3 | 2.49                     | 0.42              |
| 29:BE:48:GLN:HG2   | 29:BE:48:GLN:O    | 2.18                     | 0.42              |
| 30:BF:182:ASN:C    | 30:BF:184:TYR:H   | 2.27                     | 0.42              |
| 31:BG:115:ARG:HH22 | 31:BG:136:ARG:NH1 | 2.16                     | 0.42              |
| 33:BI:30:LEU:O     | 33:BI:31:LEU:C    | 2.62                     | 0.42              |
| 34:BN:93:THR:O     | 34:BN:94:HIS:CB   | 2.67                     | 0.42              |
| 34:BN:134:ARG:O    | 34:BN:136:GLU:N   | 2.52                     | 0.42              |
| 37:BQ:3:MET:O      | 37:BQ:3:MET:HG2   | 2.16                     | 0.42              |
| 37:BQ:35:VAL:HG22  | 37:BQ:36:ALA:O    | 2.19                     | 0.42              |
| 38:BR:38:VAL:HB    | 38:BR:39:PRO:HD3  | 2.01                     | 0.42              |
| 39:BS:14:VAL:HG12  | 39:BS:17:ARG:HG2  | 2.00                     | 0.42              |
| 40:BT:31:SER:C     | 40:BT:32:TYR:CG   | 2.93                     | 0.42              |
| 40:BT:50:ILE:O     | 40:BT:99:LEU:HD12 | 2.19                     | 0.42              |
| 40:BT:128:GLU:H    | 40:BT:128:GLU:HG3 | 1.66                     | 0.42              |
| 43:BW:31:GLU:O     | 43:BW:34:ASN:HB2  | 2.19                     | 0.42              |
| 43:BW:44:ALA:C     | 43:BW:46:PHE:N    | 2.77                     | 0.42              |
| 45:BY:27:VAL:HG12  | 45:BY:29:GLU:H    | 1.84                     | 0.42              |
| 47:B0:27:GLU:HB2   | 47:B0:69:PHE:CD1  | 2.42                     | 0.42              |
| 53:B6:33:LYS:HE2   | 53:B6:33:LYS:HA   | 2.00                     | 0.42              |
| 53:B6:41:PRO:HB2   | 53:B6:42:TRP:H    | 1.52                     | 0.42              |
| 1:CA:60:A:C2       | 1:CA:378:G:H1'    | 2.54                     | 0.42              |
| 1:CA:129:U:O2'     | 1:CA:130:A:OP1    | 2.30                     | 0.42              |
| 1:CA:381:C:H2'     | 1:CA:382:A:O4'    | 2.19                     | 0.42              |
| 1:CA:1031:G:H2'    | 1:CA:1032:G:C8    | 2.54                     | 0.42              |
| 1:CA:1032:G:H2'    | 1:CA:1033:G:C8    | 2.54                     | 0.42              |
| 2:CB:14:GLY:C      | 2:CB:15:VAL:HG22  | 2.44                     | 0.42              |
| 2:CB:19:HIS:CG     | 2:CB:20:GLU:N     | 2.86                     | 0.42              |
| 3:CC:107:GLN:N     | 3:CC:107:GLN:OE1  | 2.49                     | 0.42              |
| 4:CD:11:LEU:C      | 4:CD:13:ARG:H     | 2.26                     | 0.42              |
| 4:CD:72:GLU:O      | 4:CD:73:ARG:C     | 2.61                     | 0.42              |
| 10:CJ:26:ALA:HA    | 10:CJ:29:ARG:HH21 | 1.84                     | 0.42              |
| 16:CP:71:ARG:HA    | 16:CP:74:LEU:HD12 | 2.00                     | 0.42              |
| 17:CQ:33:GLY:O     | 17:CQ:34:LYS:O    | 2.36                     | 0.42              |
| 19:CS:63:THR:HG22  | 19:CS:66:MET:HG3  | 1.86                     | 0.42              |
| 22:CV:35:C:N4      | 24:CX:18:G:H1     | 2.16                     | 0.42              |
| 24:CX:16:A:C2      | 24:CX:17:U:C6     | 3.06                     | 0.42              |
| 23:CY:36:A:C8      | 23:CY:36:A:C5'    | 2.99                     | 0.42              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 25:DA:127:A:H5''   | 25:DA:128:C:C6    | 2.54                     | 0.42              |
| 25:DA:1236:G:O2'   | 25:DA:1237:A:H8   | 2.02                     | 0.42              |
| 25:DA:1342:A:O4'   | 25:DA:1397:U:C4'  | 2.68                     | 0.42              |
| 25:DA:1542:A:HO2'  | 25:DA:1543:C:P    | 2.41                     | 0.42              |
| 25:DA:2124:G:H1    | 25:DA:2174:C:H42  | 1.67                     | 0.42              |
| 25:DA:2517:C:C4    | 25:DA:2542:A:C6   | 3.07                     | 0.42              |
| 28:DD:118:VAL:HG22 | 28:DD:119:ALA:H   | 1.81                     | 0.42              |
| 31:DG:47:LYS:NZ    | 31:DG:81:LYS:HG2  | 2.34                     | 0.42              |
| 32:DH:143:GLN:C    | 32:DH:143:GLN:NE2 | 2.75                     | 0.42              |
| 35:DO:26:LYS:O     | 35:DO:27:GLY:O    | 2.37                     | 0.42              |
| 36:DP:34:GLY:O     | 36:DP:36:LYS:HB2  | 2.19                     | 0.42              |
| 36:DP:46:LYS:HG2   | 36:DP:51:PHE:CE1  | 2.54                     | 0.42              |
| 37:DQ:56:ARG:CZ    | 37:DQ:56:ARG:HA   | 2.49                     | 0.42              |
| 41:DU:8:VAL:HG12   | 41:DU:12:ARG:HG3  | 2.00                     | 0.42              |
| 46:DZ:28:MET:HA    | 46:DZ:88:PHE:O    | 2.18                     | 0.42              |
| 46:DZ:103:ARG:C    | 46:DZ:105:VAL:H   | 2.27                     | 0.42              |
| 48:D1:66:HIS:C     | 48:D1:68:PRO:CD   | 2.91                     | 0.42              |
| 1:AA:397:A:H3'     | 1:AA:397:A:N3     | 2.33                     | 0.42              |
| 1:AA:963:G:N2      | 1:AA:972:C:O2     | 2.52                     | 0.42              |
| 1:AA:1104:G:H4'    | 2:AB:111:ARG:NH1  | 2.34                     | 0.42              |
| 3:AC:8:ILE:C       | 3:AC:10:PHE:H     | 2.27                     | 0.42              |
| 3:AC:139:GLN:C     | 3:AC:141:VAL:H    | 2.27                     | 0.42              |
| 5:AE:100:VAL:C     | 5:AE:101:ILE:HD13 | 2.44                     | 0.42              |
| 5:AE:109:ILE:HD12  | 5:AE:135:THR:HB   | 2.01                     | 0.42              |
| 6:AF:61:LEU:HB3    | 6:AF:62:TRP:H     | 1.51                     | 0.42              |
| 6:AF:82:ARG:HA     | 6:AF:82:ARG:HD2   | 1.46                     | 0.42              |
| 6:AF:96:PRO:HB3    | 18:AR:30:ASP:CG   | 2.43                     | 0.42              |
| 7:AG:3:ARG:NH1     | 7:AG:3:ARG:HG3    | 2.33                     | 0.42              |
| 7:AG:62:PHE:HA     | 7:AG:124:LEU:HD21 | 2.01                     | 0.42              |
| 7:AG:69:VAL:HG21   | 7:AG:104:LEU:HD21 | 2.01                     | 0.42              |
| 8:AH:26:VAL:HG22   | 8:AH:27:PRO:O     | 2.19                     | 0.42              |
| 8:AH:42:GLU:HG3    | 8:AH:109:ILE:CD1  | 2.48                     | 0.42              |
| 10:AJ:55:LYS:O     | 10:AJ:56:HIS:CG   | 2.72                     | 0.42              |
| 10:AJ:62:HIS:O     | 14:AN:59:ALA:CB   | 2.62                     | 0.42              |
| 11:AK:21:ILE:HG13  | 11:AK:30:VAL:CG1  | 2.49                     | 0.42              |
| 12:AL:64:TYR:HB3   | 12:AL:65:GLU:H    | 1.15                     | 0.42              |
| 15:AO:74:ASP:C     | 15:AO:76:GLU:H    | 2.27                     | 0.42              |
| 17:AQ:21:VAL:HG12  | 17:AQ:23:VAL:HG23 | 2.00                     | 0.42              |
| 19:AS:28:LYS:C     | 19:AS:29:ARG:HG3  | 2.44                     | 0.42              |
| 20:AT:10:LEU:HD22  | 20:AT:12:ALA:HB2  | 2.01                     | 0.42              |
| 20:AT:43:LEU:HB3   | 20:AT:48:LYS:HB2  | 2.01                     | 0.42              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 20:AT:53:LEU:HD22   | 20:AT:53:LEU:HA    | 1.76                     | 0.42              |
| 22:AV:73:A:N6       | 22:AV:74:A:C6      | 2.88                     | 0.42              |
| 23:AW:70:G:H2'      | 23:AW:70:G:N3      | 2.34                     | 0.42              |
| 23:AY:37:A:O2'      | 25:BA:1913:A:N1    | 2.50                     | 0.42              |
| 25:BA:197:A:H62     | 25:BA:2430:A:H2'   | 1.84                     | 0.42              |
| 25:BA:271(F):C:H2'  | 25:BA:271(G):C:H6  | 1.83                     | 0.42              |
| 25:BA:663:G:H5''    | 36:BP:18:ARG:HG3   | 2.00                     | 0.42              |
| 25:BA:1385:G:C6     | 25:BA:1403:C:N3    | 2.87                     | 0.42              |
| 25:BA:1386:C:O2'    | 25:BA:1387:C:H5'   | 2.19                     | 0.42              |
| 25:BA:1747(A):G:C2' | 25:BA:1748:G:H5''  | 2.47                     | 0.42              |
| 25:BA:1846:G:H5'    | 25:BA:1847:A:OP2   | 2.19                     | 0.42              |
| 25:BA:2344:U:O2'    | 25:BA:2345:G:O5'   | 2.32                     | 0.42              |
| 25:BA:2481:G:O2'    | 25:BA:2482:G:O5'   | 2.37                     | 0.42              |
| 28:BD:61:LEU:O      | 28:BD:63:ARG:NH1   | 2.52                     | 0.42              |
| 28:BD:181:GLU:HG2   | 28:BD:182:LEU:N    | 2.33                     | 0.42              |
| 29:BE:7:VAL:CG2     | 29:BE:27:LEU:HB3   | 2.49                     | 0.42              |
| 29:BE:39:PRO:O      | 29:BE:43:GLY:N     | 2.52                     | 0.42              |
| 29:BE:72:VAL:O      | 29:BE:73:GLU:O     | 2.38                     | 0.42              |
| 29:BE:119:ARG:HG2   | 29:BE:160:TYR:HB2  | 2.01                     | 0.42              |
| 31:BG:9:ARG:C       | 31:BG:11:TYR:N     | 2.74                     | 0.42              |
| 32:BH:144:VAL:O     | 32:BH:148:ILE:HG12 | 2.18                     | 0.42              |
| 33:BI:92:VAL:HG13   | 33:BI:120:ILE:HB   | 2.01                     | 0.42              |
| 34:BN:18:ALA:CB     | 34:BN:21:LYS:HB3   | 2.48                     | 0.42              |
| 37:BQ:59:ARG:H      | 37:BQ:59:ARG:HG2   | 1.67                     | 0.42              |
| 39:BS:61:ASN:CG     | 39:BS:62:LYS:N     | 2.77                     | 0.42              |
| 40:BT:1:MET:H1      | 40:BT:7:ILE:CG1    | 2.32                     | 0.42              |
| 45:BY:44:ILE:O      | 45:BY:62:GLU:HG2   | 2.19                     | 0.42              |
| 46:BZ:23:LYS:HB3    | 46:BZ:38:TYR:CD1   | 2.54                     | 0.42              |
| 46:BZ:29:TYR:CD1    | 46:BZ:29:TYR:C     | 2.97                     | 0.42              |
| 49:B2:61:LEU:HA     | 49:B2:61:LEU:HD23  | 1.71                     | 0.42              |
| 54:B7:11:LYS:O      | 54:B7:15:THR:HB    | 2.19                     | 0.42              |
| 2:CB:103:THR:OG1    | 2:CB:176:GLU:CG    | 2.68                     | 0.42              |
| 2:CB:223:ILE:HA     | 2:CB:226:ARG:CG    | 2.46                     | 0.42              |
| 3:CC:102:ASN:O      | 3:CC:103:VAL:CG2   | 2.67                     | 0.42              |
| 3:CC:188:LEU:HD12   | 3:CC:195:VAL:HG13  | 2.02                     | 0.42              |
| 5:CE:118:ILE:HG13   | 5:CE:119:LEU:H     | 1.84                     | 0.42              |
| 9:CI:121:ARG:NH1    | 9:CI:122:ALA:O     | 2.48                     | 0.42              |
| 12:CL:117:ARG:O     | 12:CL:119:LYS:O    | 2.38                     | 0.42              |
| 17:CQ:5:VAL:HG22    | 17:CQ:60:ILE:HG13  | 2.02                     | 0.42              |
| 18:CR:63:GLN:O      | 18:CR:66:LEU:HB3   | 2.18                     | 0.42              |
| 19:CS:10:PHE:HZ     | 19:CS:70:LYS:NZ    | 2.17                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:DA:221:A:O2'   | 25:DA:222:A:OP2   | 2.30                     | 0.42              |
| 25:DA:459:U:H4'   | 54:D7:40:TRP:CZ3  | 2.54                     | 0.42              |
| 25:DA:526:A:O2'   | 25:DA:2043:C:O2   | 2.31                     | 0.42              |
| 25:DA:1022:G:O2'  | 25:DA:1024:G:N7   | 2.52                     | 0.42              |
| 25:DA:1455:G:C2   | 25:DA:1456:G:C8   | 3.07                     | 0.42              |
| 25:DA:1818:U:C5   | 28:DD:157:ARG:CZ  | 3.02                     | 0.42              |
| 25:DA:2449:U:O2'  | 25:DA:2450:A:C8   | 2.72                     | 0.42              |
| 25:DA:2449:U:O2'  | 25:DA:2450:A:H8   | 2.02                     | 0.42              |
| 27:DC:83:ILE:HA   | 27:DC:94:VAL:CG2  | 2.50                     | 0.42              |
| 27:DC:86:ALA:O    | 27:DC:91:ALA:HB3  | 2.19                     | 0.42              |
| 28:DD:211:ARG:HA  | 28:DD:214:TRP:CG  | 2.54                     | 0.42              |
| 29:DE:38:THR:HA   | 29:DE:39:PRO:HD3  | 1.86                     | 0.42              |
| 29:DE:95:ILE:N    | 29:DE:95:ILE:CD1  | 2.82                     | 0.42              |
| 31:DG:81:LYS:N    | 31:DG:81:LYS:CD   | 2.78                     | 0.42              |
| 32:DH:66:GLY:O    | 32:DH:67:LEU:C    | 2.62                     | 0.42              |
| 34:DN:10:GLU:OE2  | 34:DN:11:PRO:HD2  | 2.19                     | 0.42              |
| 34:DN:26:LEU:HG   | 34:DN:30:ILE:CD1  | 2.49                     | 0.42              |
| 36:DP:38:GLN:HG2  | 36:DP:45:LEU:CD1  | 2.49                     | 0.42              |
| 36:DP:96:THR:C    | 36:DP:97:PRO:O    | 2.59                     | 0.42              |
| 37:DQ:20:ALA:H    | 46:DZ:79:ARG:HD2  | 1.84                     | 0.42              |
| 37:DQ:76:LYS:HB3  | 37:DQ:91:GLU:HG3  | 2.01                     | 0.42              |
| 38:DR:70:LEU:HD13 | 38:DR:75:LEU:HD12 | 2.01                     | 0.42              |
| 43:DW:62:HIS:O    | 43:DW:63:ASP:C    | 2.61                     | 0.42              |
| 48:D1:84:GLY:O    | 48:D1:85:LEU:C    | 2.62                     | 0.42              |
| 49:D2:34:GLU:O    | 49:D2:38:GLN:CG   | 2.67                     | 0.42              |
| 50:D3:29:ARG:HG3  | 50:D3:29:ARG:NH1  | 2.33                     | 0.42              |
| 50:D3:31:LEU:C    | 50:D3:33:GLN:N    | 2.77                     | 0.42              |
| 52:D5:56:LYS:HB3  | 52:D5:56:LYS:HZ2  | 1.82                     | 0.42              |
| 1:AA:664:G:OP1    | 18:AR:64:ARG:NE   | 2.49                     | 0.42              |
| 1:AA:687:A:O2'    | 1:AA:688:G:P      | 2.78                     | 0.42              |
| 1:AA:791:G:H5''   | 1:AA:792:A:OP2    | 2.19                     | 0.42              |
| 1:AA:1060:C:H5''  | 10:AJ:51:ARG:HD2  | 2.01                     | 0.42              |
| 1:AA:1316:G:N2    | 1:AA:1319:A:OP2   | 2.51                     | 0.42              |
| 2:AB:114:ARG:HA   | 2:AB:117:GLU:HB2  | 2.01                     | 0.42              |
| 2:AB:168:THR:HG23 | 2:AB:192:SER:CB   | 2.49                     | 0.42              |
| 3:AC:122:GLU:O    | 3:AC:126:ARG:HG3  | 2.19                     | 0.42              |
| 4:AD:20:TYR:CE2   | 4:AD:27:TYR:CE2   | 3.02                     | 0.42              |
| 8:AH:118:VAL:C    | 8:AH:119:LEU:HD23 | 2.44                     | 0.42              |
| 8:AH:138:TRP:OXT  | 8:AH:138:TRP:HE3  | 2.02                     | 0.42              |
| 9:AI:22:GLY:O     | 9:AI:23:ASN:C     | 2.63                     | 0.42              |
| 9:AI:87:GLN:O     | 9:AI:90:PRO:HD3   | 2.20                     | 0.42              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 9:AI:95:LYS:NZ      | 9:AI:96:LEU:HD13   | 2.33                     | 0.42              |
| 11:AK:82:VAL:HG12   | 11:AK:82:VAL:O     | 2.18                     | 0.42              |
| 16:AP:4:ILE:HB      | 16:AP:66:PRO:HB3   | 2.01                     | 0.42              |
| 19:AS:17:GLU:O      | 19:AS:21:GLU:HG3   | 2.20                     | 0.42              |
| 19:AS:72:GLY:C      | 19:AS:74:PHE:H     | 2.27                     | 0.42              |
| 23:AY:39:U:H2'      | 23:AY:40:C:C6      | 2.49                     | 0.42              |
| 25:BA:34:C:C6       | 25:BA:34:C:C3'     | 3.02                     | 0.42              |
| 25:BA:171:G:H2'     | 25:BA:172:C:C6     | 2.54                     | 0.42              |
| 25:BA:591:C:H1'     | 55:B8:2:PRO:HA     | 1.99                     | 0.42              |
| 25:BA:995:C:OP2     | 41:BU:54:LYS:NZ    | 2.41                     | 0.42              |
| 25:BA:1300:U:O4'    | 25:BA:1626:G:C2    | 2.73                     | 0.42              |
| 25:BA:1390:U:C2     | 25:BA:1395:A:N6    | 2.88                     | 0.42              |
| 25:BA:2122:U:H2'    | 25:BA:2123:G:C8    | 2.54                     | 0.42              |
| 25:BA:2712(A):A:H4' | 38:BR:13:HIS:CB    | 2.49                     | 0.42              |
| 25:BA:2853:C:H2'    | 25:BA:2854:G:C8    | 2.53                     | 0.42              |
| 25:BA:2876:G:H4'    | 40:BT:2:ASN:O      | 2.19                     | 0.42              |
| 27:BC:73:ARG:HG2    | 27:BC:92:ASP:OD1   | 2.19                     | 0.42              |
| 27:BC:77:ILE:HD11   | 27:BC:100:ILE:HD11 | 2.02                     | 0.42              |
| 28:BD:24:ILE:O      | 28:BD:25:THR:C     | 2.62                     | 0.42              |
| 28:BD:30:GLU:CD     | 28:BD:63:ARG:HH21  | 2.26                     | 0.42              |
| 28:BD:31:LYS:HD3    | 28:BD:94:LEU:HD11  | 2.01                     | 0.42              |
| 28:BD:49:ILE:HD11   | 28:BD:51:VAL:C     | 2.43                     | 0.42              |
| 28:BD:165:ILE:HG22  | 28:BD:166:GLN:N    | 2.34                     | 0.42              |
| 28:BD:172:TYR:CD2   | 28:BD:184:LYS:HD2  | 2.53                     | 0.42              |
| 28:BD:233:HIS:NE2   | 28:BD:247:ALA:N    | 2.65                     | 0.42              |
| 29:BE:120:TRP:O     | 29:BE:121:ASN:C    | 2.62                     | 0.42              |
| 29:BE:176:ILE:N     | 29:BE:176:ILE:CD1  | 2.82                     | 0.42              |
| 29:BE:177:PRO:HG2   | 29:BE:178:GLU:H    | 1.84                     | 0.42              |
| 30:BF:192:LEU:C     | 30:BF:193:VAL:HG23 | 2.44                     | 0.42              |
| 31:BG:7:LEU:HD12    | 31:BG:104:GLU:N    | 2.34                     | 0.42              |
| 34:BN:49:GLY:O      | 34:BN:50:ASP:C     | 2.62                     | 0.42              |
| 41:BU:111:GLU:O     | 41:BU:113:ALA:N    | 2.52                     | 0.42              |
| 42:BV:1:MET:HE2     | 42:BV:1:MET:HA     | 2.01                     | 0.42              |
| 44:BX:12:VAL:HA     | 44:BX:27:THR:OG1   | 2.20                     | 0.42              |
| 44:BX:35:THR:O      | 44:BX:37:THR:N     | 2.52                     | 0.42              |
| 45:BY:67:LEU:CD1    | 45:BY:71:LYS:CG    | 2.92                     | 0.42              |
| 45:BY:77:PRO:O      | 45:BY:78:ALA:HB2   | 2.19                     | 0.42              |
| 46:BZ:132:ASN:HB3   | 46:BZ:159:PRO:O    | 2.19                     | 0.42              |
| 50:B3:4:LEU:HD23    | 50:B3:57:GLU:O     | 2.18                     | 0.42              |
| 55:B8:23:VAL:HA     | 55:B8:47:LYS:O     | 2.17                     | 0.42              |
| 1:CA:246:A:C4       | 1:CA:282:A:N6      | 2.87                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:251:G:C4      | 1:CA:252:U:H5      | 2.37                     | 0.42              |
| 1:CA:261:U:OP2     | 20:CT:79:ARG:NH2   | 2.51                     | 0.42              |
| 1:CA:371:G:O2'     | 1:CA:373:A:N7      | 2.49                     | 0.42              |
| 1:CA:473:G:H5''    | 16:CP:81:ARG:HH21  | 1.84                     | 0.42              |
| 1:CA:855:G:O5'     | 1:CA:871:U:O4      | 2.37                     | 0.42              |
| 1:CA:1504:G:P      | 1:CA:1504:G:C3'    | 3.05                     | 0.42              |
| 4:CD:198:VAL:CG1   | 4:CD:199:ASN:H     | 2.28                     | 0.42              |
| 5:CE:90:VAL:HG23   | 5:CE:121:LYS:N     | 2.33                     | 0.42              |
| 6:CF:48:LEU:HD13   | 6:CF:52:ILE:HG12   | 2.01                     | 0.42              |
| 9:CI:10:ARG:CD     | 9:CI:75:ASP:HB3    | 2.48                     | 0.42              |
| 9:CI:59:PHE:C      | 9:CI:61:ALA:H      | 2.28                     | 0.42              |
| 9:CI:102:LEU:HD22  | 9:CI:102:LEU:HA    | 1.85                     | 0.42              |
| 10:CJ:22:LYS:O     | 10:CJ:24:VAL:N     | 2.44                     | 0.42              |
| 10:CJ:47:PHE:CE2   | 14:CN:37:PHE:CE2   | 3.08                     | 0.42              |
| 11:CK:32:ILE:HD12  | 11:CK:72:ALA:HB2   | 2.00                     | 0.42              |
| 13:CM:117:VAL:O    | 13:CM:118:ALA:C    | 2.62                     | 0.42              |
| 15:CO:39:LEU:O     | 15:CO:40:SER:C     | 2.62                     | 0.42              |
| 18:CR:23:LYS:HB3   | 18:CR:56:THR:O     | 2.18                     | 0.42              |
| 19:CS:53:ASN:O     | 19:CS:77:THR:HG22  | 2.20                     | 0.42              |
| 25:DA:517:C:OP1    | 52:D5:16:ARG:NH2   | 2.52                     | 0.42              |
| 25:DA:784:A:C5     | 28:DD:229:VAL:HG21 | 2.53                     | 0.42              |
| 25:DA:890:A:C5     | 25:DA:892:G:C5     | 3.07                     | 0.42              |
| 25:DA:1022:G:H4'   | 25:DA:1023:U:O5'   | 2.20                     | 0.42              |
| 25:DA:1191:G:P     | 36:DP:32:THR:HB    | 2.60                     | 0.42              |
| 25:DA:1363:C:H2'   | 25:DA:1364:G:H8    | 1.85                     | 0.42              |
| 25:DA:1711:C:H2'   | 25:DA:1712:C:C6    | 2.54                     | 0.42              |
| 25:DA:2198:A:H1'   | 33:DI:28:ASN:O     | 2.20                     | 0.42              |
| 26:DB:42:C:O2'     | 31:DG:67:LYS:HD2   | 2.20                     | 0.42              |
| 26:DB:66:A:C2      | 26:DB:109:C:C2     | 3.07                     | 0.42              |
| 27:DC:36:LYS:O     | 27:DC:37:PHE:C     | 2.62                     | 0.42              |
| 28:DD:69:ARG:NH2   | 28:DD:192:THR:HB   | 2.34                     | 0.42              |
| 28:DD:158:ALA:O    | 28:DD:159:ALA:C    | 2.62                     | 0.42              |
| 30:DF:178:PRO:HB3  | 30:DF:198:ALA:HB1  | 2.01                     | 0.42              |
| 31:DG:35:GLU:O     | 31:DG:36:LYS:HB3   | 2.18                     | 0.42              |
| 32:DH:45:VAL:O     | 32:DH:45:VAL:HG13  | 2.19                     | 0.42              |
| 33:DI:52:ARG:HB3   | 33:DI:52:ARG:CZ    | 2.49                     | 0.42              |
| 33:DI:92:VAL:O     | 33:DI:92:VAL:CG2   | 2.67                     | 0.42              |
| 34:DN:23:LEU:HB3   | 34:DN:60:ILE:CG2   | 2.44                     | 0.42              |
| 36:DP:61:ARG:NH1   | 55:D8:13:ARG:CD    | 2.82                     | 0.42              |
| 40:DT:3:ARG:O      | 40:DT:7:ILE:HG12   | 2.19                     | 0.42              |
| 40:DT:129:ARG:HH11 | 40:DT:130:ALA:C    | 2.27                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 46:DZ:99:TYR:HB3   | 46:DZ:123:ASP:OD1  | 2.20                     | 0.42              |
| 49:D2:20:GLU:O     | 49:D2:23:LYS:HB2   | 2.19                     | 0.42              |
| 1:AA:35:G:H2'      | 1:AA:36:C:C6       | 2.55                     | 0.42              |
| 1:AA:198:G:H2'     | 1:AA:199:G:H8      | 1.83                     | 0.42              |
| 1:AA:324:G:N2      | 1:AA:327:A:C8      | 2.87                     | 0.42              |
| 1:AA:806:C:H2'     | 1:AA:807:A:C8      | 2.54                     | 0.42              |
| 1:AA:885:G:HO2'    | 1:AA:914:A:H2      | 1.67                     | 0.42              |
| 1:AA:1189:C:H5''   | 3:AC:5:ILE:CG2     | 2.49                     | 0.42              |
| 1:AA:1343:G:C4'    | 9:AI:122:ALA:HB3   | 2.47                     | 0.42              |
| 2:AB:137:ARG:C     | 2:AB:137:ARG:HD3   | 2.45                     | 0.42              |
| 2:AB:188:ALA:O     | 2:AB:189:ASP:HB3   | 2.20                     | 0.42              |
| 3:AC:39:ILE:C      | 3:AC:41:GLY:N      | 2.76                     | 0.42              |
| 3:AC:135:LYS:O     | 3:AC:139:GLN:HB2   | 2.20                     | 0.42              |
| 3:AC:178:LEU:C     | 3:AC:180:ALA:H     | 2.27                     | 0.42              |
| 4:AD:120:LEU:HD23  | 4:AD:120:LEU:HA    | 1.74                     | 0.42              |
| 10:AJ:8:LEU:HD21   | 10:AJ:96:ILE:HG22  | 2.00                     | 0.42              |
| 11:AK:44:SER:C     | 11:AK:46:GLY:N     | 2.77                     | 0.42              |
| 14:AN:25:VAL:HG12  | 14:AN:26:ARG:N     | 2.34                     | 0.42              |
| 18:AR:25:THR:O     | 18:AR:25:THR:HG22  | 2.19                     | 0.42              |
| 18:AR:37:VAL:HG12  | 18:AR:79:LEU:HD23  | 2.02                     | 0.42              |
| 19:AS:28:LYS:HD3   | 19:AS:28:LYS:HA    | 1.78                     | 0.42              |
| 23:AW:51:U:C4      | 23:AW:52:G:N7      | 2.87                     | 0.42              |
| 24:AX:13:A:N1      | 24:AX:14:A:C8      | 2.86                     | 0.42              |
| 25:BA:35:G:C5      | 25:BA:454:A:C2     | 3.07                     | 0.42              |
| 25:BA:1212:G:O2'   | 25:BA:1236:G:N2    | 2.53                     | 0.42              |
| 25:BA:2208:A:H1'   | 25:BA:2219:G:C4    | 2.55                     | 0.42              |
| 25:BA:2320:A:H1'   | 25:BA:2321:G:C6    | 2.54                     | 0.42              |
| 28:BD:165:ILE:HA   | 28:BD:175:LEU:HD23 | 2.01                     | 0.42              |
| 29:BE:13:ARG:NH2   | 40:BT:77:PRO:HB3   | 2.35                     | 0.42              |
| 29:BE:56:PRO:O     | 29:BE:57:LYS:HB2   | 2.18                     | 0.42              |
| 29:BE:150:VAL:HG12 | 29:BE:151:TYR:N    | 2.32                     | 0.42              |
| 29:BE:179:GLU:HA   | 29:BE:179:GLU:OE1  | 2.20                     | 0.42              |
| 30:BF:64:ILE:N     | 30:BF:76:GLY:O     | 2.44                     | 0.42              |
| 32:BH:75:ALA:O     | 32:BH:79:VAL:HG13  | 2.18                     | 0.42              |
| 33:BI:66:GLU:HA    | 33:BI:69:LYS:HB3   | 2.01                     | 0.42              |
| 33:BI:78:THR:HG23  | 33:BI:141:LYS:HB2  | 2.00                     | 0.42              |
| 33:BI:132:PRO:HD2  | 33:BI:133:HIS:CE1  | 2.54                     | 0.42              |
| 34:BN:26:LEU:CG    | 34:BN:30:ILE:HD11  | 2.50                     | 0.42              |
| 35:BO:63:VAL:CG1   | 35:BO:106:LEU:HD11 | 2.49                     | 0.42              |
| 35:BO:98:VAL:HG12  | 35:BO:117:LEU:CD2  | 2.45                     | 0.42              |
| 36:BP:124:LYS:HE3  | 36:BP:145:PRO:HD3  | 2.02                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 40:BT:57:PHE:O    | 40:BT:59:THR:HG22 | 2.18                     | 0.42              |
| 46:BZ:3:TYR:O     | 46:BZ:57:ILE:HA   | 2.18                     | 0.42              |
| 46:BZ:29:TYR:O    | 46:BZ:29:TYR:HD1  | 2.02                     | 0.42              |
| 49:B2:63:VAL:HA   | 49:B2:66:GLU:CG   | 2.49                     | 0.42              |
| 50:B3:23:LEU:HD23 | 50:B3:28:LEU:HB2  | 2.01                     | 0.42              |
| 52:B5:16:ARG:NH1  | 52:B5:17:ASP:OD1  | 2.52                     | 0.42              |
| 52:B5:36:CYS:HB2  | 52:B5:49:CYS:HG   | 1.80                     | 0.42              |
| 55:B8:61:LEU:N    | 55:B8:63:PRO:HD2  | 2.35                     | 0.42              |
| 1:CA:31:G:N7      | 1:CA:48:C:C2      | 2.88                     | 0.42              |
| 1:CA:765:G:N2     | 1:CA:812:C:HO2'   | 2.17                     | 0.42              |
| 1:CA:1226:C:O2'   | 1:CA:1227:A:O5'   | 2.30                     | 0.42              |
| 1:CA:1446:U:O2    | 1:CA:1457:G:C6    | 2.72                     | 0.42              |
| 1:CA:1456:G:N3    | 1:CA:1456:G:C5'   | 2.77                     | 0.42              |
| 1:CA:1468:A:H2'   | 1:CA:1469:G:O4'   | 2.20                     | 0.42              |
| 2:CB:21:ARG:C     | 2:CB:23:ARG:H     | 2.27                     | 0.42              |
| 5:CE:112:LEU:HD23 | 5:CE:112:LEU:N    | 2.34                     | 0.42              |
| 6:CF:82:ARG:HD2   | 6:CF:82:ARG:HA    | 1.81                     | 0.42              |
| 7:CG:146:GLU:O    | 7:CG:149:ARG:CB   | 2.67                     | 0.42              |
| 10:CJ:63:PHE:HD1  | 14:CN:58:LYS:HG2  | 1.85                     | 0.42              |
| 10:CJ:71:LEU:O    | 10:CJ:72:VAL:HG23 | 2.20                     | 0.42              |
| 12:CL:78:GLN:O    | 12:CL:81:SER:OG   | 2.31                     | 0.42              |
| 14:CN:23:ARG:O    | 14:CN:24:CYS:C    | 2.62                     | 0.42              |
| 16:CP:4:ILE:HB    | 16:CP:66:PRO:CB   | 2.45                     | 0.42              |
| 19:CS:25:LYS:O    | 19:CS:27:GLU:OE1  | 2.37                     | 0.42              |
| 23:CW:50:U:C4     | 23:CW:65:G:N2     | 2.87                     | 0.42              |
| 25:DA:51:G:H1'    | 25:DA:118:A:N6    | 2.34                     | 0.42              |
| 25:DA:195:A:OP1   | 36:DP:46:LYS:HE2  | 2.19                     | 0.42              |
| 25:DA:9271:G:H2'  | 25:DA:9272:G:C8   | 2.54                     | 0.42              |
| 25:DA:307:G:N2    | 25:DA:310:A:OP2   | 2.52                     | 0.42              |
| 25:DA:752:A:C4'   | 25:DA:753:C:O5'   | 2.58                     | 0.42              |
| 25:DA:1042:G:H1   | 25:DA:1113:U:H3   | 1.67                     | 0.42              |
| 25:DA:1408:C:H2'  | 25:DA:1409:C:C6   | 2.54                     | 0.42              |
| 25:DA:1637:A:H4'  | 25:DA:2711:A:O2'  | 2.19                     | 0.42              |
| 25:DA:2116:G:O2'  | 25:DA:2117:A:OP1  | 2.36                     | 0.42              |
| 25:DA:2438:U:O5'  | 25:DA:2438:U:H6   | 2.03                     | 0.42              |
| 25:DA:2867:G:C5   | 40:DT:23:ARG:NH1  | 2.87                     | 0.42              |
| 28:DD:149:PRO:O   | 28:DD:150:LYS:HB2 | 2.18                     | 0.42              |
| 28:DD:218:ARG:HG3 | 28:DD:218:ARG:NH1 | 2.31                     | 0.42              |
| 29:DE:1:MET:HE3   | 29:DE:83:ASP:HB2  | 2.02                     | 0.42              |
| 29:DE:39:PRO:HA   | 29:DE:43:GLY:CA   | 2.49                     | 0.42              |
| 29:DE:47:VAL:HG21 | 29:DE:86:PRO:HD3  | 2.00                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 30:DF:59:TYR:HD1   | 30:DF:78:ILE:HB    | 1.83                     | 0.42              |
| 30:DF:133:ASN:O    | 30:DF:135:LYS:HB2  | 2.20                     | 0.42              |
| 31:DG:53:LEU:HD23  | 31:DG:53:LEU:C     | 2.44                     | 0.42              |
| 34:DN:10:GLU:HA    | 34:DN:11:PRO:HD2   | 1.79                     | 0.42              |
| 34:DN:42:TRP:CZ3   | 34:DN:48:MET:HE1   | 2.55                     | 0.42              |
| 34:DN:76:SER:C     | 34:DN:78:TYR:H     | 2.26                     | 0.42              |
| 37:DQ:18:LYS:O     | 37:DQ:98:LYS:HD3   | 2.19                     | 0.42              |
| 39:DS:26:LEU:HD22  | 39:DS:87:PHE:CD1   | 2.54                     | 0.42              |
| 39:DS:49:VAL:CG1   | 39:DS:76:LYS:HB2   | 2.49                     | 0.42              |
| 46:DZ:18:LEU:O     | 46:DZ:19:ARG:C     | 2.63                     | 0.42              |
| 46:DZ:38:TYR:HD1   | 46:DZ:39:VAL:O     | 2.03                     | 0.42              |
| 50:D3:1:MET:CE     | 50:D3:41:PRO:HD3   | 2.49                     | 0.42              |
| 1:AA:189(F):U:H2'  | 17:AQ:63:ARG:NH2   | 2.30                     | 0.42              |
| 1:AA:591:U:OP2     | 8:AH:30:ARG:NH1    | 2.52                     | 0.42              |
| 1:AA:607:A:C2      | 16:AP:31:LYS:HB2   | 2.54                     | 0.42              |
| 1:AA:828:A:H62     | 1:AA:858:G:H21     | 1.68                     | 0.42              |
| 1:AA:1240:U:C5     | 7:AG:109:ASN:OD1   | 2.73                     | 0.42              |
| 1:AA:1277:C:O2'    | 1:AA:1278:U:C5'    | 2.68                     | 0.42              |
| 1:AA:1442(A):G:H22 | 40:BT:119:LYS:HB2  | 1.85                     | 0.42              |
| 3:AC:142:MET:C     | 3:AC:144:SER:N     | 2.75                     | 0.42              |
| 3:AC:154:SER:OG    | 3:AC:155:GLY:N     | 2.51                     | 0.42              |
| 7:AG:69:VAL:HG12   | 7:AG:69:VAL:O      | 2.19                     | 0.42              |
| 8:AH:104:ARG:CZ    | 8:AH:138:TRP:CZ2   | 3.02                     | 0.42              |
| 9:AI:118:LYS:HB2   | 9:AI:121:ARG:CB    | 2.50                     | 0.42              |
| 10:AJ:38:ILE:CG1   | 10:AJ:71:LEU:O     | 2.67                     | 0.42              |
| 11:AK:12:ARG:CG    | 11:AK:13:GLN:N     | 2.82                     | 0.42              |
| 11:AK:33:THR:HA    | 11:AK:40:ILE:HG12  | 2.01                     | 0.42              |
| 12:AL:26:ALA:C     | 12:AL:27:LEU:CD2   | 2.90                     | 0.42              |
| 13:AM:3:ARG:HD3    | 31:BG:113:ARG:HH21 | 1.85                     | 0.42              |
| 14:AN:18:VAL:C     | 14:AN:20:ALA:H     | 2.27                     | 0.42              |
| 14:AN:25:VAL:HB    | 14:AN:39:LEU:HD21  | 2.02                     | 0.42              |
| 20:AT:58:LYS:O     | 20:AT:58:LYS:HG3   | 2.19                     | 0.42              |
| 25:BA:181:A:C2     | 25:BA:434:U:O2'    | 2.72                     | 0.42              |
| 25:BA:320:A:H3'    | 30:BF:136:THR:CG2  | 2.50                     | 0.42              |
| 25:BA:589:C:H2'    | 25:BA:590:A:H8     | 1.84                     | 0.42              |
| 25:BA:1568:G:C5'   | 28:BD:61:LEU:HB2   | 2.48                     | 0.42              |
| 25:BA:1854:A:H3'   | 25:BA:1855:G:H8    | 1.84                     | 0.42              |
| 25:BA:1902:C:H5'   | 28:BD:246:PRO:HD3  | 2.01                     | 0.42              |
| 25:BA:2262:U:H2'   | 25:BA:2263:C:C6    | 2.55                     | 0.42              |
| 25:BA:2415:G:H4'   | 36:BP:66:GLY:HA3   | 2.01                     | 0.42              |
| 25:BA:2638:G:P     | 29:BE:82:ARG:HH22  | 2.42                     | 0.42              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 25:BA:2712:U:O2'   | 25:BA:2712(A):A:H3' | 2.19                     | 0.42              |
| 25:BA:2848:G:C5'   | 25:BA:2849:U:OP1    | 2.67                     | 0.42              |
| 26:BB:20:C:C2'     | 26:BB:21:G:H5'      | 2.50                     | 0.42              |
| 26:BB:20:C:H2'     | 26:BB:21:G:H5'      | 2.01                     | 0.42              |
| 28:BD:12:SER:HB2   | 28:BD:208:LYS:CB    | 2.49                     | 0.42              |
| 28:BD:175:LEU:HD12 | 28:BD:185:VAL:HG21  | 2.01                     | 0.42              |
| 29:BE:18:ASP:O     | 29:BE:19:ARG:HB3    | 2.20                     | 0.42              |
| 31:BG:66:GLN:C     | 31:BG:67:LYS:O      | 2.60                     | 0.42              |
| 32:BH:89:ILE:O     | 32:BH:161:GLY:O     | 2.37                     | 0.42              |
| 33:BI:79:ILE:HA    | 33:BI:80:PRO:HD2    | 1.84                     | 0.42              |
| 34:BN:34:LEU:HD12  | 34:BN:34:LEU:HA     | 1.63                     | 0.42              |
| 34:BN:65:LYS:H     | 34:BN:65:LYS:HD2    | 1.84                     | 0.42              |
| 37:BQ:26:TYR:CE1   | 37:BQ:28:ALA:HB2    | 2.54                     | 0.42              |
| 38:BR:79:LEU:HD22  | 38:BR:79:LEU:C      | 2.45                     | 0.42              |
| 43:BW:12:ILE:O     | 43:BW:12:ILE:CG2    | 2.66                     | 0.42              |
| 43:BW:48:ALA:O     | 43:BW:51:LEU:N      | 2.52                     | 0.42              |
| 43:BW:75:TYR:C     | 43:BW:75:TYR:HD2    | 2.27                     | 0.42              |
| 45:BY:20:TYR:CE1   | 45:BY:42:VAL:CA     | 3.01                     | 0.42              |
| 46:BZ:56:VAL:HG12  | 46:BZ:57:ILE:N      | 2.34                     | 0.42              |
| 46:BZ:63:ASP:C     | 46:BZ:65:GLN:N      | 2.78                     | 0.42              |
| 47:B0:84:LEU:H     | 47:B0:84:LEU:HD12   | 1.84                     | 0.42              |
| 49:B2:48:HIS:O     | 49:B2:49:LYS:C      | 2.62                     | 0.42              |
| 52:B5:32:PRO:O     | 52:B5:33:CYS:CB     | 2.63                     | 0.42              |
| 1:CA:280:C:H1'     | 17:CQ:38:ARG:CD     | 2.49                     | 0.42              |
| 1:CA:337:C:H2'     | 1:CA:338:A:C8       | 2.55                     | 0.42              |
| 1:CA:1286:A:H5''   | 21:CU:25:LYS:HZ1    | 1.84                     | 0.42              |
| 2:CB:8:LYS:HD3     | 2:CB:217:ARG:NH2    | 2.34                     | 0.42              |
| 2:CB:155:LEU:HD11  | 2:CB:159:PRO:HD3    | 2.02                     | 0.42              |
| 3:CC:95:THR:HG22   | 3:CC:97:LYS:HB2     | 2.01                     | 0.42              |
| 4:CD:120:LEU:HD23  | 4:CD:120:LEU:HA     | 1.78                     | 0.42              |
| 5:CE:107:ARG:HG2   | 5:CE:111:GLU:CD     | 2.44                     | 0.42              |
| 9:CI:35:GLU:O      | 9:CI:38:GLN:HB2     | 2.19                     | 0.42              |
| 10:CJ:30:SER:HB3   | 10:CJ:80:LYS:CE     | 2.49                     | 0.42              |
| 13:CM:108:ARG:HH11 | 13:CM:108:ARG:HG3   | 1.85                     | 0.42              |
| 14:CN:4:LYS:C      | 14:CN:6:LEU:N       | 2.76                     | 0.42              |
| 14:CN:9:LYS:O      | 14:CN:10:ALA:C      | 2.62                     | 0.42              |
| 16:CP:9:PHE:HB3    | 16:CP:10:GLY:H      | 1.56                     | 0.42              |
| 20:CT:12:ALA:C     | 20:CT:14:LYS:N      | 2.77                     | 0.42              |
| 22:CV:4:G:O2'      | 22:CV:5:G:H8        | 2.02                     | 0.42              |
| 22:CV:19:G:C1'     | 22:CV:59:A:C2       | 3.03                     | 0.42              |
| 23:CY:36:A:C6      | 23:CY:37:A:N7       | 2.88                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:DA:74:A:O2'     | 25:DA:75:G:OP2     | 2.33                     | 0.42              |
| 25:DA:265:A:H5'    | 25:DA:265:A:N3     | 2.35                     | 0.42              |
| 25:DA:352:G:H2'    | 25:DA:352:G:N3     | 2.35                     | 0.42              |
| 25:DA:1022:G:O2'   | 25:DA:1023:U:OP2   | 2.32                     | 0.42              |
| 25:DA:1230:C:H2'   | 25:DA:1231:G:H8    | 1.83                     | 0.42              |
| 25:DA:1301:A:O2'   | 25:DA:1302:A:H3'   | 2.20                     | 0.42              |
| 25:DA:2197:U:O2'   | 25:DA:2198:A:O5'   | 2.38                     | 0.42              |
| 25:DA:2466:C:H5''  | 56:D9:6:SER:HB2    | 2.01                     | 0.42              |
| 25:DA:2489:G:O6    | 25:DA:2490:G:N1    | 2.52                     | 0.42              |
| 25:DA:2507:C:H5'   | 25:DA:2573:C:N4    | 2.35                     | 0.42              |
| 25:DA:2577:A:H5''  | 25:DA:2578:G:C5'   | 2.47                     | 0.42              |
| 25:DA:2811:G:N2    | 25:DA:2891:G:H1'   | 2.35                     | 0.42              |
| 28:DD:65:ILE:H     | 28:DD:65:ILE:HD13  | 1.84                     | 0.42              |
| 28:DD:165:ILE:HD13 | 28:DD:175:LEU:CD2  | 2.49                     | 0.42              |
| 28:DD:263:ARG:NH1  | 28:DD:263:ARG:HB2  | 2.34                     | 0.42              |
| 30:DF:203:GLN:HE21 | 30:DF:203:GLN:HB2  | 1.66                     | 0.42              |
| 31:DG:7:LEU:CD2    | 31:DG:176:LEU:HD22 | 2.36                     | 0.42              |
| 31:DG:53:LEU:CD2   | 31:DG:54:GLU:N     | 2.77                     | 0.42              |
| 31:DG:122:PRO:HG3  | 31:DG:182:LYS:OXT  | 2.20                     | 0.42              |
| 31:DG:142:PRO:C    | 31:DG:144:ILE:H    | 2.28                     | 0.42              |
| 32:DH:24:VAL:CG2   | 32:DH:35:VAL:HB    | 2.49                     | 0.42              |
| 32:DH:143:GLN:O    | 32:DH:146:ALA:HB3  | 2.20                     | 0.42              |
| 33:DI:81:VAL:O     | 33:DI:83:ALA:N     | 2.52                     | 0.42              |
| 34:DN:125:GLY:HA3  | 34:DN:126:PRO:C    | 2.45                     | 0.42              |
| 37:DQ:110:THR:HG1  | 37:DQ:112:GLU:HG2  | 1.84                     | 0.42              |
| 38:DR:44:LEU:HD11  | 38:DR:48:VAL:HG21  | 2.02                     | 0.42              |
| 39:DS:52:SER:O     | 39:DS:56:LEU:HD22  | 2.19                     | 0.42              |
| 1:AA:818:G:H3'     | 1:AA:819:A:C5'     | 2.50                     | 0.42              |
| 1:AA:967:C:H2'     | 1:AA:968:A:N7      | 2.34                     | 0.42              |
| 1:AA:1134:G:N2     | 1:AA:1141:C:O2     | 2.52                     | 0.42              |
| 1:AA:1424:C:H2'    | 1:AA:1425:U:O4'    | 2.19                     | 0.42              |
| 2:AB:19:HIS:HD1    | 2:AB:20:GLU:HG2    | 1.83                     | 0.42              |
| 2:AB:30:ARG:H      | 2:AB:30:ARG:HG2    | 1.52                     | 0.42              |
| 3:AC:91:LEU:HD12   | 3:AC:101:LEU:HD12  | 2.02                     | 0.42              |
| 3:AC:109:PRO:HA    | 3:AC:115:LEU:HD12  | 2.01                     | 0.42              |
| 3:AC:124:ILE:C     | 3:AC:126:ARG:N     | 2.78                     | 0.42              |
| 3:AC:147:LYS:CB    | 3:AC:203:PHE:CD2   | 3.03                     | 0.42              |
| 4:AD:24:GLU:O      | 4:AD:27:TYR:HB2    | 2.20                     | 0.42              |
| 7:AG:85:TYR:CD1    | 7:AG:154:TYR:CE1   | 3.08                     | 0.42              |
| 10:AJ:9:ARG:HG2    | 10:AJ:69:ASN:OD1   | 2.19                     | 0.42              |
| 10:AJ:63:PHE:HB3   | 14:AN:59:ALA:N     | 2.35                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:AO:54:ARG:O    | 15:AO:58:MET:HG3  | 2.20                     | 0.42              |
| 16:AP:67:THR:HG22 | 16:AP:68:ASP:H    | 1.84                     | 0.42              |
| 18:AR:30:ASP:C    | 18:AR:32:ARG:H    | 2.28                     | 0.42              |
| 22:AV:7:G:H3'     | 22:AV:8:U:C5'     | 2.50                     | 0.42              |
| 23:AW:15:G:N2     | 23:AW:59:U:H1'    | 2.33                     | 0.42              |
| 24:AX:20:U:O4     | 24:AX:21:C:N4     | 2.52                     | 0.42              |
| 25:BA:746:A:C5    | 25:BA:2611:U:H5'' | 2.54                     | 0.42              |
| 25:BA:857:C:OP2   | 47:B0:77:ARG:NH2  | 2.53                     | 0.42              |
| 25:BA:969:U:OP1   | 50:B3:17:LYS:N    | 2.51                     | 0.42              |
| 25:BA:991:C:C5    | 25:BA:1185:C:C4   | 3.07                     | 0.42              |
| 25:BA:1618:A:H5'' | 25:BA:1619:G:OP2  | 2.19                     | 0.42              |
| 25:BA:1668:A:OP1  | 35:BO:5:GLN:HG3   | 2.19                     | 0.42              |
| 25:BA:1937:A:N7   | 25:BA:1939:U:H2'  | 2.35                     | 0.42              |
| 25:BA:2140:C:H2'  | 25:BA:2141:G:H8   | 1.85                     | 0.42              |
| 25:BA:2345:G:N3   | 25:BA:2345:G:C2'  | 2.83                     | 0.42              |
| 25:BA:2725:A:O2'  | 25:BA:2726:U:O5'  | 2.36                     | 0.42              |
| 27:BC:41:VAL:HA   | 27:BC:213:TYR:HA  | 2.02                     | 0.42              |
| 29:BE:81:ILE:O    | 29:BE:81:ILE:CG2  | 2.63                     | 0.42              |
| 30:BF:10:PRO:HG2  | 30:BF:11:VAL:HG23 | 2.01                     | 0.42              |
| 33:BI:99:GLU:O    | 33:BI:103:ARG:HG3 | 2.20                     | 0.42              |
| 37:BQ:2:LEU:O     | 37:BQ:70:PRO:CG   | 2.67                     | 0.42              |
| 39:BS:74:ALA:O    | 39:BS:77:ALA:HB3  | 2.19                     | 0.42              |
| 40:BT:12:SER:O    | 40:BT:15:VAL:HG12 | 2.19                     | 0.42              |
| 41:BU:95:LEU:HD13 | 42:BV:4:ILE:HG12  | 1.97                     | 0.42              |
| 44:BX:34:ALA:HA   | 44:BX:38:GLU:OE1  | 2.18                     | 0.42              |
| 46:BZ:76:LEU:CD2  | 46:BZ:76:LEU:H    | 2.33                     | 0.42              |
| 49:B2:65:ASN:CB   | 49:B2:69:ARG:HH22 | 2.33                     | 0.42              |
| 51:B4:59:VAL:HG12 | 51:B4:61:VAL:N    | 2.34                     | 0.42              |
| 1:CA:61:G:C6      | 1:CA:107:G:C6     | 3.08                     | 0.42              |
| 1:CA:193:C:H5'    | 20:CT:57:ARG:HG2  | 2.01                     | 0.42              |
| 1:CA:298:A:H2'    | 1:CA:299:A:O4'    | 2.19                     | 0.42              |
| 1:CA:687:A:N6     | 1:CA:703:G:H1'    | 2.35                     | 0.42              |
| 1:CA:1065:U:C5'   | 1:CA:1066:C:H5''  | 2.37                     | 0.42              |
| 1:CA:1412:C:H2'   | 1:CA:1413:A:H8    | 1.84                     | 0.42              |
| 2:CB:77:ALA:CB    | 2:CB:211:ILE:HD13 | 2.44                     | 0.42              |
| 3:CC:129:ALA:HB3  | 3:CC:132:ARG:HB2  | 2.01                     | 0.42              |
| 5:CE:30:ALA:O     | 5:CE:45:PHE:HD1   | 2.02                     | 0.42              |
| 7:CG:6:ARG:O      | 7:CG:6:ARG:CG     | 2.68                     | 0.42              |
| 7:CG:69:VAL:CG2   | 7:CG:135:VAL:HG22 | 2.50                     | 0.42              |
| 9:CI:25:LYS:HG2   | 9:CI:60:ASP:OD1   | 2.20                     | 0.42              |
| 10:CJ:3:LYS:O     | 10:CJ:100:THR:HA  | 2.20                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:CJ:9:ARG:HB3    | 10:CJ:10:GLY:H     | 1.71                     | 0.42              |
| 13:CM:87:TYR:HA    | 13:CM:90:LEU:CG    | 2.48                     | 0.42              |
| 14:CN:27:CYS:O     | 14:CN:28:GLY:C     | 2.62                     | 0.42              |
| 18:CR:54:ARG:H     | 18:CR:54:ARG:HG3   | 1.60                     | 0.42              |
| 19:CS:10:PHE:CZ    | 19:CS:70:LYS:CE    | 3.02                     | 0.42              |
| 19:CS:58:VAL:O     | 19:CS:58:VAL:HG22  | 2.20                     | 0.42              |
| 19:CS:58:VAL:HA    | 19:CS:59:PRO:HD2   | 1.89                     | 0.42              |
| 20:CT:29:LYS:HD3   | 20:CT:66:ALA:CA    | 2.50                     | 0.42              |
| 25:DA:184:C:O2'    | 25:DA:217:G:N3     | 2.53                     | 0.42              |
| 25:DA:1204:A:C4    | 25:DA:1206:G:C6    | 3.07                     | 0.42              |
| 25:DA:1676:A:H2'   | 25:DA:1677:A:O4'   | 2.20                     | 0.42              |
| 25:DA:2116:G:O2'   | 25:DA:2117:A:P     | 2.78                     | 0.42              |
| 25:DA:2158:A:O2'   | 25:DA:2159:G:C8    | 2.72                     | 0.42              |
| 25:DA:2593:U:H2'   | 25:DA:2594:C:H6    | 1.84                     | 0.42              |
| 27:DC:47:LEU:HB2   | 27:DC:207:THR:CB   | 2.50                     | 0.42              |
| 27:DC:55:ASP:CG    | 27:DC:56:GLN:H     | 2.26                     | 0.42              |
| 28:DD:147:LEU:CD1  | 28:DD:155:LEU:HD21 | 2.49                     | 0.42              |
| 28:DD:241:PRO:O    | 28:DD:242:ARG:HB2  | 2.20                     | 0.42              |
| 30:DF:89:VAL:O     | 30:DF:91:GLY:N     | 2.49                     | 0.42              |
| 30:DF:117:ARG:HH11 | 30:DF:117:ARG:HG3  | 1.83                     | 0.42              |
| 30:DF:129:PHE:O    | 30:DF:142:TRP:CD1  | 2.73                     | 0.42              |
| 30:DF:149:ASP:OD1  | 30:DF:149:ASP:N    | 2.49                     | 0.42              |
| 31:DG:61:ALA:HA    | 31:DG:64:THR:HG23  | 2.02                     | 0.42              |
| 32:DH:58:GLU:O     | 32:DH:59:ARG:C     | 2.63                     | 0.42              |
| 33:DI:81:VAL:HG22  | 33:DI:143:SER:O    | 2.19                     | 0.42              |
| 34:DN:24:GLY:H     | 34:DN:27:ALA:H     | 1.67                     | 0.42              |
| 38:DR:118:GLU:HA   | 38:DR:118:GLU:OE1  | 2.20                     | 0.42              |
| 41:DU:78:THR:HG22  | 41:DU:79:PHE:N     | 2.33                     | 0.42              |
| 42:DV:44:LYS:O     | 42:DV:46:VAL:HG12  | 2.20                     | 0.42              |
| 42:DV:47:VAL:HG13  | 42:DV:48:GLY:H     | 1.85                     | 0.42              |
| 45:DY:48:ALA:CB    | 45:DY:61:ILE:HD13  | 2.49                     | 0.42              |
| 45:DY:50:ARG:CA    | 45:DY:53:PRO:HD2   | 2.49                     | 0.42              |
| 47:D0:72:ARG:NE    | 47:D0:75:LEU:HD13  | 2.35                     | 0.42              |
| 50:D3:1:MET:HE1    | 50:D3:41:PRO:HD3   | 2.02                     | 0.42              |
| 51:D4:19:GLY:O     | 51:D4:20:ASN:C     | 2.62                     | 0.42              |
| 53:D6:17:LYS:O     | 53:D6:18:ARG:HD3   | 2.19                     | 0.42              |
| 55:D8:16:ILE:HG22  | 55:D8:64:TYR:CD2   | 2.55                     | 0.42              |
| 1:AA:254:G:O3'     | 17:AQ:69:LYS:NZ    | 2.49                     | 0.42              |
| 1:AA:327:A:C4      | 1:AA:329:A:N7      | 2.88                     | 0.42              |
| 1:AA:1066:C:H2'    | 1:AA:1067:A:O5'    | 2.20                     | 0.42              |
| 1:AA:1213:A:N6     | 1:AA:1215:G:N3     | 2.68                     | 0.42              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AA:1223:C:H5''  | 1:AA:1224:G:H5''   | 2.02                     | 0.42              |
| 1:AA:1226:C:H42   | 13:AM:104:ARG:HB2  | 1.81                     | 0.42              |
| 1:AA:1513:A:H2'   | 1:AA:1514:C:C6     | 2.54                     | 0.42              |
| 5:AE:41:VAL:O     | 5:AE:67:VAL:HG12   | 2.19                     | 0.42              |
| 6:AF:48:LEU:HD21  | 6:AF:58:GLY:HA3    | 2.02                     | 0.42              |
| 7:AG:141:VAL:O    | 7:AG:144:MET:HB2   | 2.20                     | 0.42              |
| 8:AH:20:TYR:HA    | 8:AH:65:TYR:CZ     | 2.55                     | 0.42              |
| 13:AM:94:ARG:CG   | 19:AS:82:GLY:N     | 2.81                     | 0.42              |
| 14:AN:4:LYS:O     | 14:AN:5:ALA:C      | 2.61                     | 0.42              |
| 17:AQ:31:LEU:HG   | 17:AQ:32:TYR:CE2   | 2.55                     | 0.42              |
| 18:AR:33:ASP:OD1  | 18:AR:33:ASP:C     | 2.63                     | 0.42              |
| 25:BA:500:G:N1    | 25:BA:503:A:OP2    | 2.52                     | 0.42              |
| 25:BA:571:A:O4'   | 25:BA:2030:A:N6    | 2.53                     | 0.42              |
| 25:BA:636:G:N3    | 36:BP:115:LEU:HD11 | 2.34                     | 0.42              |
| 25:BA:973:A:O2'   | 25:BA:1186:G:N2    | 2.52                     | 0.42              |
| 25:BA:1820:U:C2   | 28:BD:202:LYS:HB3  | 2.55                     | 0.42              |
| 25:BA:2443:C:H2'  | 25:BA:2444:G:C8    | 2.54                     | 0.42              |
| 26:BB:80:U:H2'    | 26:BB:81:G:C8      | 2.55                     | 0.42              |
| 27:BC:62:VAL:HG11 | 27:BC:193:ILE:O    | 2.19                     | 0.42              |
| 28:BD:44:ASN:CB   | 28:BD:48:ARG:O     | 2.68                     | 0.42              |
| 28:BD:63:ARG:NH2  | 28:BD:86:PRO:HD3   | 2.34                     | 0.42              |
| 31:BG:83:ARG:HD3  | 31:BG:84:LYS:HB2   | 2.01                     | 0.42              |
| 32:BH:102:ALA:HB2 | 32:BH:116:GLU:HA   | 2.00                     | 0.42              |
| 33:BI:12:LEU:O    | 33:BI:12:LEU:HG    | 2.19                     | 0.42              |
| 34:BN:97:ARG:O    | 34:BN:98:VAL:C     | 2.63                     | 0.42              |
| 35:BO:31:LYS:HD3  | 35:BO:31:LYS:HA    | 1.90                     | 0.42              |
| 36:BP:46:LYS:HG2  | 36:BP:51:PHE:CD1   | 2.54                     | 0.42              |
| 39:BS:27:SER:C    | 39:BS:28:VAL:HG23  | 2.45                     | 0.42              |
| 40:BT:92:GLY:HA2  | 40:BT:114:LEU:CB   | 2.42                     | 0.42              |
| 41:BU:17:ILE:HD13 | 41:BU:17:ILE:HA    | 1.74                     | 0.42              |
| 45:BY:16:ALA:O    | 45:BY:17:SER:O     | 2.37                     | 0.42              |
| 45:BY:26:LYS:O    | 45:BY:27:VAL:C     | 2.62                     | 0.42              |
| 50:B3:40:THR:HB   | 50:B3:41:PRO:CD    | 2.50                     | 0.42              |
| 53:B6:17:LYS:HD3  | 53:B6:17:LYS:HA    | 1.90                     | 0.42              |
| 55:B8:63:PRO:HB2  | 55:B8:64:TYR:CD1   | 2.51                     | 0.42              |
| 1:CA:279:A:OP2    | 17:CQ:95:TYR:OH    | 2.37                     | 0.42              |
| 1:CA:355:C:O4'    | 1:CA:388:G:O2'     | 2.36                     | 0.42              |
| 1:CA:691:G:O5'    | 11:CK:26:ASN:ND2   | 2.52                     | 0.42              |
| 1:CA:950:U:C1'    | 1:CA:971:G:C5      | 3.02                     | 0.42              |
| 1:CA:1051:C:O2'   | 1:CA:1052:U:H5'    | 2.19                     | 0.42              |
| 3:CC:113:ALA:O    | 3:CC:114:PRO:C     | 2.61                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:CC:117:ALA:O     | 3:CC:120:VAL:HB    | 2.20                     | 0.42              |
| 7:CG:50:ILE:O      | 7:CG:54:THR:O      | 2.37                     | 0.42              |
| 7:CG:104:LEU:HD13  | 7:CG:104:LEU:HA    | 1.50                     | 0.42              |
| 8:CH:85:ARG:HD2    | 8:CH:88:LYS:HG3    | 2.02                     | 0.42              |
| 10:CJ:4:ILE:HG12   | 10:CJ:100:THR:CG2  | 2.50                     | 0.42              |
| 10:CJ:16:LEU:HA    | 10:CJ:16:LEU:HD23  | 1.70                     | 0.42              |
| 10:CJ:30:SER:HB3   | 10:CJ:80:LYS:HE3   | 2.00                     | 0.42              |
| 12:CL:53:ARG:HB2   | 12:CL:93:LEU:HD11  | 2.00                     | 0.42              |
| 16:CP:60:LEU:HA    | 16:CP:60:LEU:HD23  | 1.66                     | 0.42              |
| 16:CP:71:ARG:O     | 16:CP:72:ARG:C     | 2.61                     | 0.42              |
| 19:CS:45:VAL:C     | 19:CS:62:ILE:HG23  | 2.44                     | 0.42              |
| 21:CU:6:ARG:NE     | 21:CU:15:ARG:HH22  | 1.95                     | 0.42              |
| 22:CV:19:G:N3      | 22:CV:59:A:C4      | 2.87                     | 0.42              |
| 23:CW:37:A:C6      | 23:CW:38:A:N1      | 2.87                     | 0.42              |
| 23:CW:55:U:H6      | 23:CW:58:A:N7      | 2.18                     | 0.42              |
| 25:DA:413:C:H2'    | 25:DA:414:C:H6     | 1.84                     | 0.42              |
| 25:DA:604:G:C5     | 25:DA:605:C:N4     | 2.88                     | 0.42              |
| 25:DA:740:U:H2'    | 25:DA:741:G:C8     | 2.55                     | 0.42              |
| 25:DA:839:U:H2'    | 25:DA:840:C:C6     | 2.54                     | 0.42              |
| 25:DA:849:A:C2     | 50:D3:24:LYS:HG2   | 2.55                     | 0.42              |
| 25:DA:1204:A:C1'   | 25:DA:1206:G:C5    | 3.00                     | 0.42              |
| 25:DA:1455:G:N7    | 38:DR:64:ARG:NH1   | 2.67                     | 0.42              |
| 25:DA:1778:U:O4    | 25:DA:1784:A:H1'   | 2.19                     | 0.42              |
| 25:DA:1987:G:H5''  | 25:DA:1987:G:H8    | 1.84                     | 0.42              |
| 25:DA:2287:A:H62   | 25:DA:2344:U:H3    | 1.67                     | 0.42              |
| 25:DA:2320:A:H61   | 25:DA:2333:A:H2'   | 1.85                     | 0.42              |
| 25:DA:2632:A:N3    | 29:DE:61:ARG:HD3   | 2.35                     | 0.42              |
| 27:DC:23:ASP:C     | 27:DC:25:ALA:N     | 2.75                     | 0.42              |
| 30:DF:124:LEU:HG   | 30:DF:126:VAL:HG13 | 2.00                     | 0.42              |
| 30:DF:181:LEU:HA   | 30:DF:181:LEU:HD22 | 1.80                     | 0.42              |
| 31:DG:55:LYS:HZ2   | 31:DG:148:MET:CG   | 2.32                     | 0.42              |
| 32:DH:111:HIS:CE1  | 32:DH:112:PRO:O    | 2.73                     | 0.42              |
| 33:DI:29:TYR:CE1   | 33:DI:33:ARG:NE    | 2.88                     | 0.42              |
| 33:DI:98:ALA:O     | 33:DI:99:GLU:C     | 2.61                     | 0.42              |
| 33:DI:99:GLU:HG2   | 33:DI:103:ARG:HH21 | 1.80                     | 0.42              |
| 33:DI:145:VAL:HG23 | 33:DI:146:ALA:H    | 1.85                     | 0.42              |
| 34:DN:90:MET:O     | 34:DN:91:LEU:C     | 2.62                     | 0.42              |
| 34:DN:96:GLU:OE2   | 34:DN:96:GLU:N     | 2.39                     | 0.42              |
| 36:DP:14:LYS:O     | 36:DP:16:ARG:N     | 2.52                     | 0.42              |
| 36:DP:46:LYS:HG2   | 36:DP:51:PHE:CD1   | 2.54                     | 0.42              |
| 38:DR:1:MET:SD     | 38:DR:1:MET:N      | 2.79                     | 0.42              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 39:DS:68:GLN:C    | 39:DS:70:GLY:N     | 2.77                     | 0.42              |
| 43:DW:71:VAL:O    | 43:DW:71:VAL:HG12  | 2.19                     | 0.42              |
| 46:DZ:52:SER:C    | 46:DZ:53:ILE:CG1   | 2.92                     | 0.42              |
| 47:D0:51:VAL:HG22 | 47:D0:81:VAL:HG23  | 2.01                     | 0.42              |
| 48:D1:5:CYS:SG    | 48:D1:62:VAL:CG2   | 3.07                     | 0.42              |
| 48:D1:67:ILE:HG13 | 48:D1:67:ILE:H     | 1.62                     | 0.42              |
| 51:D4:11:PRO:O    | 51:D4:29:PRO:HG3   | 2.19                     | 0.42              |
| 53:D6:10:LEU:N    | 53:D6:10:LEU:HD22  | 2.34                     | 0.42              |
| 1:AA:1059:C:O2'   | 10:AJ:52:GLY:HA2   | 2.20                     | 0.42              |
| 3:AC:8:ILE:C      | 3:AC:10:PHE:N      | 2.76                     | 0.42              |
| 3:AC:22:TRP:CD2   | 3:AC:59:ARG:HD2    | 2.55                     | 0.42              |
| 3:AC:73:PRO:O     | 3:AC:74:GLY:C      | 2.62                     | 0.42              |
| 5:AE:41:VAL:HG11  | 5:AE:113:ALA:N     | 2.34                     | 0.42              |
| 6:AF:23:LYS:HE2   | 6:AF:23:LYS:HB3    | 1.77                     | 0.42              |
| 7:AG:52:GLU:C     | 7:AG:54:THR:H      | 2.27                     | 0.42              |
| 8:AH:7:ALA:HB2    | 8:AH:85:ARG:HG3    | 2.01                     | 0.42              |
| 12:AL:58:VAL:O    | 12:AL:65:GLU:HA    | 2.20                     | 0.42              |
| 12:AL:68:ALA:HA   | 12:AL:98:TYR:O     | 2.20                     | 0.42              |
| 18:AR:86:VAL:O    | 18:AR:87:ARG:O     | 2.37                     | 0.42              |
| 25:BA:74:A:O2'    | 25:BA:75:G:OP2     | 2.30                     | 0.42              |
| 25:BA:92:A:H2'    | 25:BA:93:G:C8      | 2.55                     | 0.42              |
| 25:BA:1966:A:H8   | 25:BA:1966:A:O5'   | 2.03                     | 0.42              |
| 25:BA:2145:C:HO2' | 25:BA:2146:C:P     | 2.41                     | 0.42              |
| 28:BD:17:THR:HG1  | 28:BD:205:VAL:H    | 1.62                     | 0.42              |
| 28:BD:69:ARG:HD2  | 28:BD:119:ALA:HB2  | 2.02                     | 0.42              |
| 28:BD:132:PRO:O   | 28:BD:133:LEU:C    | 2.63                     | 0.42              |
| 29:BE:82:ARG:HD3  | 29:BE:82:ARG:HA    | 1.78                     | 0.42              |
| 30:BF:22:ALA:O    | 30:BF:26:ALA:CB    | 2.54                     | 0.42              |
| 30:BF:33:LEU:HD12 | 30:BF:33:LEU:HA    | 1.78                     | 0.42              |
| 31:BG:38:VAL:O    | 31:BG:38:VAL:HG12  | 2.19                     | 0.42              |
| 31:BG:47:LYS:HE3  | 31:BG:81:LYS:HD2   | 2.02                     | 0.42              |
| 32:BH:80:SER:O    | 32:BH:81:GLU:HB2   | 2.20                     | 0.42              |
| 33:BI:77:LEU:HD12 | 33:BI:77:LEU:HA    | 1.86                     | 0.42              |
| 33:BI:93:THR:HG22 | 33:BI:94:ALA:H     | 1.85                     | 0.42              |
| 35:BO:9:GLU:O     | 35:BO:83:ALA:HA    | 2.19                     | 0.42              |
| 35:BO:34:THR:HG23 | 35:BO:35:VAL:N     | 2.35                     | 0.42              |
| 36:BP:46:LYS:HG2  | 36:BP:51:PHE:CE1   | 2.54                     | 0.42              |
| 38:BR:78:LYS:O    | 38:BR:83:ILE:HG13  | 2.20                     | 0.42              |
| 41:BU:62:ILE:HD12 | 41:BU:93:LYS:HG2   | 2.02                     | 0.42              |
| 41:BU:95:LEU:HD11 | 42:BV:4:ILE:HG23   | 1.99                     | 0.42              |
| 43:BW:70:TYR:O    | 43:BW:107:LEU:HD12 | 2.20                     | 0.42              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 44:BX:5:TYR:CE2   | 49:B2:30:ARG:HB2   | 2.55                     | 0.42              |
| 1:CA:13:U:H5'     | 1:CA:14:U:OP2      | 2.20                     | 0.42              |
| 1:CA:128:G:O2'    | 1:CA:129:U:H5'     | 2.20                     | 0.42              |
| 1:CA:234:C:H2'    | 1:CA:235:C:C6      | 2.55                     | 0.42              |
| 1:CA:279:A:C5'    | 1:CA:281:G:H5'     | 2.50                     | 0.42              |
| 1:CA:473:G:H2'    | 1:CA:474:G:C8      | 2.55                     | 0.42              |
| 1:CA:1249:C:O2'   | 9:CI:73:GLN:NE2    | 2.53                     | 0.42              |
| 1:CA:1256:A:H5'   | 1:CA:1258:G:O4'    | 2.19                     | 0.42              |
| 1:CA:1309:G:N7    | 13:CM:99:ARG:NH2   | 2.68                     | 0.42              |
| 2:CB:178:ARG:HH21 | 8:CH:74:PRO:HB3    | 1.85                     | 0.42              |
| 3:CC:16:ARG:HA    | 3:CC:16:ARG:HH11   | 1.84                     | 0.42              |
| 3:CC:129:ALA:HB1  | 3:CC:132:ARG:HB2   | 2.02                     | 0.42              |
| 5:CE:42:GLY:C     | 5:CE:136:MET:HE2   | 2.45                     | 0.42              |
| 10:CJ:97:GLU:HA   | 10:CJ:97:GLU:OE2   | 2.20                     | 0.42              |
| 14:CN:4:LYS:CD    | 14:CN:7:ILE:HD11   | 2.41                     | 0.42              |
| 14:CN:51:GLY:C    | 14:CN:53:LEU:N     | 2.77                     | 0.42              |
| 18:CR:45:SER:C    | 18:CR:47:THR:H     | 2.27                     | 0.42              |
| 22:CV:15:G:N1     | 22:CV:49:C:C5      | 2.60                     | 0.42              |
| 25:DA:82:G:O6     | 25:DA:83:G:O6      | 2.38                     | 0.42              |
| 25:DA:383:U:H2'   | 25:DA:385:C:H5     | 1.84                     | 0.42              |
| 25:DA:481:G:O2'   | 25:DA:482:A:P      | 2.77                     | 0.42              |
| 25:DA:971:C:H2'   | 25:DA:972:G:O4'    | 2.19                     | 0.42              |
| 25:DA:1155:A:H4'  | 41:DU:55:ARG:HH12  | 1.85                     | 0.42              |
| 25:DA:1419:A:N6   | 25:DA:1494:A:N1    | 2.56                     | 0.42              |
| 25:DA:1508:A:H4'  | 25:DA:1509(A):A:C4 | 2.55                     | 0.42              |
| 25:DA:1952:A:C6   | 25:DA:1953:A:N1    | 2.87                     | 0.42              |
| 25:DA:2282:G:O2'  | 25:DA:2390:U:O4    | 2.37                     | 0.42              |
| 25:DA:2489:G:C6   | 25:DA:2490:G:C2    | 3.08                     | 0.42              |
| 25:DA:2638:G:O2'  | 25:DA:2639:A:C8    | 2.73                     | 0.42              |
| 25:DA:2645:G:H4'  | 25:DA:2732:G:O2'   | 2.20                     | 0.42              |
| 28:DD:12:SER:O    | 28:DD:16:MET:HE3   | 2.19                     | 0.42              |
| 28:DD:267:SER:C   | 28:DD:269:PHE:N    | 2.78                     | 0.42              |
| 29:DE:119:ARG:HD2 | 29:DE:120:TRP:CD1  | 2.55                     | 0.42              |
| 30:DF:117:ARG:NH2 | 30:DF:189:THR:O    | 2.53                     | 0.42              |
| 30:DF:127:GLU:OE1 | 30:DF:127:GLU:CA   | 2.68                     | 0.42              |
| 30:DF:134:GLY:H   | 30:DF:162:LEU:CD2  | 2.31                     | 0.42              |
| 32:DH:10:PRO:C    | 32:DH:11:VAL:HG13  | 2.44                     | 0.42              |
| 32:DH:88:LEU:O    | 32:DH:163:TYR:N    | 2.43                     | 0.42              |
| 32:DH:94:TYR:N    | 32:DH:94:TYR:CD1   | 2.88                     | 0.42              |
| 33:DI:29:TYR:CD1  | 33:DI:33:ARG:NE    | 2.86                     | 0.42              |
| 33:DI:74:ASN:CG   | 33:DI:75:LEU:N     | 2.78                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 33:DI:111:PRO:O   | 33:DI:112:LYS:C   | 2.61                     | 0.42              |
| 34:DN:48:MET:HE3  | 34:DN:48:MET:N    | 2.35                     | 0.42              |
| 36:DP:10:PRO:HB2  | 36:DP:11:GLY:H    | 1.69                     | 0.42              |
| 37:DQ:42:ILE:HD12 | 37:DQ:42:ILE:N    | 2.35                     | 0.42              |
| 37:DQ:133:ARG:O   | 37:DQ:134:ARG:CB  | 2.65                     | 0.42              |
| 38:DR:77:ARG:C    | 38:DR:79:LEU:H    | 2.28                     | 0.42              |
| 41:DU:76:TYR:C    | 41:DU:78:THR:H    | 2.28                     | 0.42              |
| 41:DU:95:LEU:O    | 41:DU:98:LEU:HG   | 2.20                     | 0.42              |
| 42:DV:24:LYS:HA   | 42:DV:92:THR:HG23 | 2.01                     | 0.42              |
| 42:DV:35:LEU:N    | 42:DV:35:LEU:CD2  | 2.81                     | 0.42              |
| 45:DY:33:LYS:HG3  | 45:DY:34:LYS:N    | 2.33                     | 0.42              |
| 46:DZ:24:LEU:O    | 46:DZ:24:LEU:HD23 | 2.19                     | 0.42              |
| 49:D2:14:ARG:HD3  | 49:D2:66:GLU:OE2  | 2.19                     | 0.42              |
| 49:D2:28:LYS:HB3  | 49:D2:57:ILE:CD1  | 2.50                     | 0.42              |
| 49:D2:60:LEU:HD23 | 49:D2:60:LEU:HA   | 1.82                     | 0.42              |
| 54:D7:42:LEU:HA   | 54:D7:42:LEU:HD23 | 1.84                     | 0.42              |
| 1:AA:406:G:C4     | 1:AA:495:A:C6     | 3.08                     | 0.42              |
| 1:AA:833:U:H2'    | 1:AA:834:C:H6     | 1.85                     | 0.42              |
| 1:AA:1181:G:C2    | 1:AA:1182:G:N2    | 2.88                     | 0.42              |
| 1:AA:1239:A:H4'   | 1:AA:1240:U:O5'   | 2.20                     | 0.42              |
| 1:AA:1347:G:HO2'  | 1:AA:1348:U:P     | 2.39                     | 0.42              |
| 2:AB:96:ARG:HH12  | 2:AB:147:LYS:NZ   | 2.17                     | 0.42              |
| 2:AB:143:GLU:O    | 2:AB:147:LYS:N    | 2.53                     | 0.42              |
| 3:AC:141:VAL:CG1  | 3:AC:149:ALA:HB2  | 2.48                     | 0.42              |
| 3:AC:182:ILE:HG12 | 3:AC:203:PHE:CD1  | 2.54                     | 0.42              |
| 4:AD:149:ALA:HB3  | 4:AD:152:SER:CB   | 2.49                     | 0.42              |
| 4:AD:196:LEU:HB3  | 4:AD:197:PRO:HD2  | 2.01                     | 0.42              |
| 5:AE:112:LEU:O    | 5:AE:113:ALA:C    | 2.62                     | 0.42              |
| 7:AG:150:ALA:O    | 7:AG:153:HIS:HE1  | 2.02                     | 0.42              |
| 9:AI:27:THR:CG2   | 9:AI:31:GLN:H     | 2.32                     | 0.42              |
| 11:AK:29:ILE:HA   | 11:AK:44:SER:HA   | 2.01                     | 0.42              |
| 11:AK:58:PRO:O    | 11:AK:59:TYR:C    | 2.62                     | 0.42              |
| 14:AN:16:PHE:CD2  | 14:AN:16:PHE:N    | 2.86                     | 0.42              |
| 16:AP:8:ARG:HH21  | 16:AP:15:PRO:HG3  | 1.84                     | 0.42              |
| 17:AQ:45:HIS:O    | 17:AQ:73:VAL:HG23 | 2.19                     | 0.42              |
| 20:AT:63:ILE:HG22 | 20:AT:77:ALA:HB1  | 2.01                     | 0.42              |
| 20:AT:80:ARG:H    | 20:AT:80:ARG:HG2  | 1.68                     | 0.42              |
| 25:BA:481:G:O2'   | 25:BA:482:A:P     | 2.78                     | 0.42              |
| 25:BA:1301:A:HO2' | 25:BA:1302:A:P    | 2.41                     | 0.42              |
| 25:BA:1602:U:H4'  | 25:BA:1603:A:OP2  | 2.20                     | 0.42              |
| 25:BA:1637:A:H4'  | 25:BA:2711:A:O2'  | 2.20                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:BA:1658:C:OP1   | 29:BE:132:HIS:O    | 2.38                     | 0.42              |
| 25:BA:2012:G:OP1   | 43:BW:11:ARG:NH2   | 2.39                     | 0.42              |
| 25:BA:2150:U:H2'   | 25:BA:2151:G:H8    | 1.85                     | 0.42              |
| 25:BA:2814:C:O2'   | 52:B5:29:THR:HG21  | 2.20                     | 0.42              |
| 25:BA:2849:U:O4    | 40:BT:23:ARG:NH2   | 2.52                     | 0.42              |
| 27:BC:24:GLU:C     | 27:BC:26:ALA:N     | 2.77                     | 0.42              |
| 27:BC:187:ASP:C    | 27:BC:189:ILE:N    | 2.75                     | 0.42              |
| 28:BD:58:HIS:ND1   | 28:BD:59:LYS:O     | 2.52                     | 0.42              |
| 28:BD:231:HIS:O    | 28:BD:232:PRO:C    | 2.62                     | 0.42              |
| 29:BE:34:VAL:HG22  | 29:BE:48:GLN:NE2   | 2.35                     | 0.42              |
| 29:BE:78:LEU:O     | 29:BE:78:LEU:HD12  | 2.20                     | 0.42              |
| 29:BE:119:ARG:C    | 29:BE:120:TRP:CG   | 2.98                     | 0.42              |
| 29:BE:167:VAL:HG22 | 29:BE:168:MET:N    | 2.35                     | 0.42              |
| 31:BG:56:ALA:HA    | 31:BG:59:GLU:HG2   | 2.02                     | 0.42              |
| 33:BI:72:LEU:CD1   | 33:BI:72:LEU:C     | 2.92                     | 0.42              |
| 33:BI:120:ILE:HG22 | 33:BI:121:LYS:N    | 2.34                     | 0.42              |
| 34:BN:42:TRP:CD1   | 41:BU:63:VAL:HG11  | 2.55                     | 0.42              |
| 35:BO:104:ARG:NH1  | 35:BO:104:ARG:HB2  | 2.34                     | 0.42              |
| 35:BO:115:VAL:HG12 | 35:BO:116:SER:N    | 2.34                     | 0.42              |
| 36:BP:101:VAL:CG1  | 36:BP:102:ARG:N    | 2.83                     | 0.42              |
| 37:BQ:42:ILE:N     | 37:BQ:42:ILE:CD1   | 2.82                     | 0.42              |
| 38:BR:97:VAL:HG22  | 38:BR:114:VAL:HG23 | 2.01                     | 0.42              |
| 39:BS:28:VAL:HB    | 39:BS:89:ARG:HA    | 2.01                     | 0.42              |
| 44:BX:52:VAL:HG23  | 44:BX:82:GLN:O     | 2.20                     | 0.42              |
| 46:BZ:22:GLY:C     | 46:BZ:41:LEU:HD12  | 2.45                     | 0.42              |
| 46:BZ:48:PHE:O     | 46:BZ:49:ARG:C     | 2.63                     | 0.42              |
| 49:B2:59:ARG:O     | 49:B2:62:THR:HB    | 2.19                     | 0.42              |
| 53:B6:13:CYS:HB3   | 53:B6:14:THR:H     | 1.74                     | 0.42              |
| 53:B6:19:ARG:O     | 53:B6:20:ASN:O     | 2.37                     | 0.42              |
| 55:B8:41:ILE:N     | 55:B8:41:ILE:CD1   | 2.83                     | 0.42              |
| 1:CA:329:A:C6      | 1:CA:332:G:C2      | 3.08                     | 0.42              |
| 1:CA:674:G:H2'     | 1:CA:675:A:C8      | 2.54                     | 0.42              |
| 1:CA:1238:A:C8     | 1:CA:1301:U:O4     | 2.73                     | 0.42              |
| 1:CA:1240:U:O2'    | 1:CA:1241:G:OP1    | 2.36                     | 0.42              |
| 1:CA:1301:U:C4     | 1:CA:1303:C:H1'    | 2.55                     | 0.42              |
| 2:CB:178:ARG:HG3   | 8:CH:71:GLY:C      | 2.45                     | 0.42              |
| 2:CB:211:ILE:O     | 2:CB:212:GLN:C     | 2.63                     | 0.42              |
| 3:CC:8:ILE:C       | 3:CC:10:PHE:N      | 2.74                     | 0.42              |
| 4:CD:79:PHE:CE2    | 4:CD:207:TYR:HD1   | 2.36                     | 0.42              |
| 8:CH:1:MET:HG2     | 8:CH:2:LEU:N       | 2.35                     | 0.42              |
| 8:CH:14:ARG:O      | 8:CH:18:ARG:HD3    | 2.20                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:CH:23:SER:HA     | 8:CH:61:VAL:O      | 2.20                     | 0.42              |
| 8:CH:48:TYR:HA     | 8:CH:60:ARG:O      | 2.19                     | 0.42              |
| 11:CK:61:ALA:C     | 11:CK:64:ALA:H     | 2.28                     | 0.42              |
| 13:CM:49:THR:C     | 13:CM:51:ALA:H     | 2.27                     | 0.42              |
| 15:CO:82:ILE:HD13  | 15:CO:87:ILE:HB    | 2.01                     | 0.42              |
| 19:CS:16:LEU:HD13  | 19:CS:16:LEU:N     | 2.35                     | 0.42              |
| 19:CS:25:LYS:O     | 19:CS:26:GLY:C     | 2.62                     | 0.42              |
| 20:CT:38:LYS:O     | 20:CT:40:ALA:N     | 2.53                     | 0.42              |
| 25:DA:271(Q):G:H2' | 25:DA:271(R):G:C8  | 2.55                     | 0.42              |
| 25:DA:635:C:O2'    | 25:DA:639:U:OP1    | 2.38                     | 0.42              |
| 25:DA:931:G:O2'    | 50:D3:24:LYS:HD3   | 2.19                     | 0.42              |
| 25:DA:1331:A:HO2'  | 25:DA:1332:G:H8    | 1.68                     | 0.42              |
| 25:DA:1902:C:H4'   | 28:DD:244:ARG:HA   | 2.02                     | 0.42              |
| 26:DB:89:G:H2'     | 26:DB:90:A:O4'     | 2.20                     | 0.42              |
| 28:DD:82:ILE:O     | 28:DD:82:ILE:HG22  | 2.20                     | 0.42              |
| 28:DD:154:LYS:HB2  | 28:DD:155:LEU:HD12 | 2.01                     | 0.42              |
| 30:DF:51:THR:OG1   | 30:DF:91:GLY:C     | 2.62                     | 0.42              |
| 30:DF:59:TYR:N     | 30:DF:59:TYR:CD2   | 2.85                     | 0.42              |
| 30:DF:153:SER:OG   | 30:DF:190:GLU:N    | 2.53                     | 0.42              |
| 31:DG:63:ILE:HG22  | 31:DG:144:ILE:HD11 | 2.02                     | 0.42              |
| 31:DG:126:ASP:OD2  | 31:DG:130:ASN:HB2  | 2.20                     | 0.42              |
| 32:DH:105:LEU:CD2  | 32:DH:113:VAL:HB   | 2.50                     | 0.42              |
| 32:DH:139:GLN:HG3  | 32:DH:140:LYS:N    | 2.35                     | 0.42              |
| 34:DN:18:ALA:HB1   | 34:DN:21:LYS:HB3   | 1.99                     | 0.42              |
| 35:DO:10:VAL:HG13  | 35:DO:17:ARG:O     | 2.19                     | 0.42              |
| 37:DQ:50:ALA:O     | 37:DQ:53:ALA:HB3   | 2.20                     | 0.42              |
| 38:DR:42:LYS:O     | 38:DR:45:ARG:HG2   | 2.20                     | 0.42              |
| 43:DW:6:ILE:O      | 43:DW:6:ILE:HG22   | 2.17                     | 0.42              |
| 43:DW:84:ARG:HB2   | 43:DW:96:ILE:CG2   | 2.44                     | 0.42              |
| 45:DY:14:LEU:HD23  | 45:DY:15:VAL:C     | 2.44                     | 0.42              |
| 46:DZ:29:TYR:CE2   | 46:DZ:87:ASP:HB2   | 2.54                     | 0.42              |
| 46:DZ:105:VAL:O    | 46:DZ:140:ASP:HB3  | 2.19                     | 0.42              |
| 52:D5:34:PRO:HB2   | 52:D5:35:GLU:H     | 1.65                     | 0.42              |
| 53:D6:12:GLU:HA    | 53:D6:23:THR:HA    | 2.00                     | 0.42              |
| 55:D8:31:HIS:O     | 55:D8:32:LEU:C     | 2.62                     | 0.42              |
| 1:AA:34:C:H2'      | 1:AA:35:G:C8       | 2.55                     | 0.42              |
| 1:AA:154:C:O2'     | 1:AA:155:C:OP1     | 2.36                     | 0.42              |
| 1:AA:176:C:H2'     | 1:AA:177:C:C6      | 2.55                     | 0.42              |
| 1:AA:540:G:C6      | 1:AA:541:G:C5      | 3.08                     | 0.42              |
| 1:AA:806:C:H2'     | 1:AA:807:A:H8      | 1.84                     | 0.42              |
| 1:AA:919:A:H2'     | 1:AA:920:U:H5'     | 2.01                     | 0.42              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:AA:927:G:H1      | 1:AA:1390:U:H3    | 1.68                     | 0.42              |
| 1:AA:979:C:H3'     | 1:AA:980:C:C5'    | 2.47                     | 0.42              |
| 2:AB:165:VAL:HG23  | 2:AB:166:ASP:N    | 2.24                     | 0.42              |
| 3:AC:133:ALA:O     | 3:AC:136:GLN:HB2  | 2.20                     | 0.42              |
| 4:AD:32:ALA:HA     | 4:AD:35:ARG:HD3   | 2.01                     | 0.42              |
| 4:AD:94:LEU:H      | 4:AD:94:LEU:HG    | 1.34                     | 0.42              |
| 4:AD:109:GLY:C     | 4:AD:111:ALA:H    | 2.27                     | 0.42              |
| 9:AI:36:TYR:CE2    | 9:AI:37:PHE:CE2   | 3.07                     | 0.42              |
| 10:AJ:33:GLN:HB2   | 10:AJ:75:ILE:HD11 | 2.01                     | 0.42              |
| 11:AK:70:LYS:HA    | 11:AK:73:MET:HE2  | 2.02                     | 0.42              |
| 23:AW:18:G:N2      | 23:AW:55:U:H6     | 2.17                     | 0.42              |
| 23:AW:50:U:C4      | 23:AW:51:U:C4     | 3.07                     | 0.42              |
| 25:BA:120:U:H1'    | 25:BA:149:A:C4    | 2.55                     | 0.42              |
| 25:BA:181:A:C2     | 25:BA:435:C:H5    | 2.34                     | 0.42              |
| 25:BA:467:G:OP1    | 54:B7:33:ARG:HD2  | 2.20                     | 0.42              |
| 25:BA:605:C:O2     | 25:BA:657:U:O2'   | 2.37                     | 0.42              |
| 25:BA:958:U:O4     | 37:BQ:41:TRP:CG   | 2.73                     | 0.42              |
| 25:BA:1251:C:C2'   | 25:BA:1252:G:H5'' | 2.49                     | 0.42              |
| 25:BA:1310:G:OP2   | 54:B7:9:ARG:NH1   | 2.53                     | 0.42              |
| 25:BA:1328:G:H8    | 25:BA:1328:G:O5'  | 2.03                     | 0.42              |
| 25:BA:1750:G:O2'   | 25:BA:2860:A:N1   | 2.49                     | 0.42              |
| 25:BA:2021:C:H4'   | 25:BA:2022:U:OP1  | 2.17                     | 0.42              |
| 31:BG:72:ARG:CD    | 31:BG:86:MET:CA   | 2.94                     | 0.42              |
| 31:BG:110:ALA:CA   | 31:BG:140:ILE:CG2 | 2.98                     | 0.42              |
| 35:BO:8:LEU:N      | 35:BO:8:LEU:CD2   | 2.83                     | 0.42              |
| 35:BO:49:ARG:N     | 35:BO:49:ARG:HD3  | 2.35                     | 0.42              |
| 36:BP:2:LYS:O      | 36:BP:3:LEU:C     | 2.62                     | 0.42              |
| 36:BP:114:ILE:HG23 | 36:BP:127:ALA:HB2 | 2.01                     | 0.42              |
| 37:BQ:104:PHE:O    | 37:BQ:105:GLU:HB3 | 2.19                     | 0.42              |
| 38:BR:13:HIS:O     | 38:BR:14:SER:CB   | 2.45                     | 0.42              |
| 40:BT:3:ARG:HG3    | 40:BT:6:LEU:CB    | 2.38                     | 0.42              |
| 40:BT:53:ARG:HG2   | 40:BT:53:ARG:HH11 | 1.84                     | 0.42              |
| 40:BT:126:ALA:C    | 40:BT:128:GLU:H   | 2.28                     | 0.42              |
| 41:BU:12:ARG:HA    | 41:BU:15:LYS:HD2  | 2.02                     | 0.42              |
| 1:CA:8:A:H1'       | 5:CE:103:GLY:N    | 2.34                     | 0.42              |
| 1:CA:429:U:C4'     | 1:CA:430:A:H8     | 2.32                     | 0.42              |
| 1:CA:484:G:C1'     | 1:CA:486:U:C6     | 3.02                     | 0.42              |
| 1:CA:484:G:C4      | 1:CA:486:U:C4     | 3.08                     | 0.42              |
| 1:CA:820:U:HO2'    | 1:CA:821:G:P      | 2.43                     | 0.42              |
| 1:CA:1068:G:O2'    | 1:CA:1069:C:H5'   | 2.20                     | 0.42              |
| 1:CA:1084:G:C5     | 1:CA:1085:U:C4    | 3.08                     | 0.42              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:CA:1457:G:C8     | 1:CA:1457:G:O5'   | 2.66                     | 0.42              |
| 4:CD:58:LEU:C      | 4:CD:58:LEU:HD22  | 2.44                     | 0.42              |
| 5:CE:122:GLU:HG2   | 5:CE:131:ILE:HD11 | 2.01                     | 0.42              |
| 7:CG:31:MET:HE2    | 7:CG:31:MET:HB3   | 1.89                     | 0.42              |
| 8:CH:114:THR:HG21  | 8:CH:129:VAL:HG23 | 2.02                     | 0.42              |
| 11:CK:88:GLY:C     | 11:CK:90:GLY:N    | 2.77                     | 0.42              |
| 13:CM:2:ALA:O      | 13:CM:4:ILE:HG12  | 2.20                     | 0.42              |
| 13:CM:12:ASN:C     | 13:CM:13:LYS:HG3  | 2.45                     | 0.42              |
| 13:CM:15:VAL:CG1   | 13:CM:19:LEU:HD21 | 2.50                     | 0.42              |
| 15:CO:70:LEU:HD12  | 15:CO:70:LEU:HA   | 1.81                     | 0.42              |
| 16:CP:6:LEU:HB3    | 16:CP:17:TYR:HD2  | 1.84                     | 0.42              |
| 16:CP:17:TYR:HD1   | 16:CP:41:PRO:HD3  | 1.84                     | 0.42              |
| 18:CR:44:LEU:HD23  | 18:CR:44:LEU:HA   | 1.84                     | 0.42              |
| 19:CS:47:HIS:N     | 19:CS:62:ILE:HG21 | 2.35                     | 0.42              |
| 20:CT:74:LYS:C     | 20:CT:76:ALA:H    | 2.26                     | 0.42              |
| 23:CW:12:U:H6      | 23:CW:12:U:O5'    | 2.02                     | 0.42              |
| 23:CW:30:G:C2      | 23:CW:41:C:N3     | 2.88                     | 0.42              |
| 25:DA:572:A:N3     | 25:DA:573:G:H1'   | 2.35                     | 0.42              |
| 25:DA:614(A):U:C3' | 25:DA:614(A):U:C6 | 3.03                     | 0.42              |
| 25:DA:729:G:C6     | 28:DD:208:LYS:HB2 | 2.55                     | 0.42              |
| 25:DA:996:A:O2'    | 41:DU:92:ARG:HB3  | 2.19                     | 0.42              |
| 25:DA:1301:A:H4'   | 25:DA:1302:A:OP1  | 2.20                     | 0.42              |
| 25:DA:1453:U:O4    | 25:DA:2702:U:O4   | 2.37                     | 0.42              |
| 25:DA:1458:C:H5''  | 25:DA:1459:G:OP1  | 2.20                     | 0.42              |
| 25:DA:1819:A:O2'   | 25:DA:1820:U:OP2  | 2.30                     | 0.42              |
| 25:DA:1826:G:O2'   | 28:DD:242:ARG:NH2 | 2.52                     | 0.42              |
| 25:DA:2114:A:H2'   | 25:DA:2115:G:O4'  | 2.20                     | 0.42              |
| 25:DA:2615:U:H6    | 25:DA:2615:U:O5'  | 2.03                     | 0.42              |
| 25:DA:2695:C:H2'   | 25:DA:2696:U:C6   | 2.55                     | 0.42              |
| 25:DA:2749:A:H4'   | 32:DH:62:LYS:HB3  | 2.02                     | 0.42              |
| 28:DD:6:PHE:HE1    | 28:DD:18:VAL:CG2  | 2.33                     | 0.42              |
| 28:DD:13:ARG:O     | 28:DD:13:ARG:CG   | 2.67                     | 0.42              |
| 28:DD:26:LYS:HZ3   | 28:DD:27:THR:HG22 | 1.84                     | 0.42              |
| 29:DE:169:ASN:OD1  | 29:DE:203:LYS:HB3 | 2.19                     | 0.42              |
| 31:DG:115:ARG:HG2  | 31:DG:115:ARG:NH1 | 2.34                     | 0.42              |
| 32:DH:84:SER:O     | 32:DH:133:VAL:O   | 2.38                     | 0.42              |
| 32:DH:147:ASN:O    | 32:DH:148:ILE:C   | 2.62                     | 0.42              |
| 34:DN:46:VAL:O     | 34:DN:47:ALA:CB   | 2.62                     | 0.42              |
| 35:DO:1:MET:CE     | 35:DO:67:LYS:HG2  | 2.46                     | 0.42              |
| 35:DO:68:GLU:OE2   | 35:DO:78:ARG:NH1  | 2.52                     | 0.42              |
| 37:DQ:1:MET:O      | 37:DQ:2:LEU:HB2   | 2.20                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 40:DT:19:LEU:CD2  | 40:DT:85:LYS:HD3  | 2.49                     | 0.42              |
| 41:DU:31:SER:HB3  | 41:DU:34:LYS:HB2  | 2.00                     | 0.42              |
| 42:DV:22:VAL:O    | 42:DV:23:GLU:C    | 2.63                     | 0.42              |
| 42:DV:65:GLY:HA3  | 42:DV:91:TYR:CZ   | 2.55                     | 0.42              |
| 45:DY:6:HIS:O     | 45:DY:7:VAL:HG13  | 2.19                     | 0.42              |
| 45:DY:42:VAL:HG12 | 45:DY:65:ALA:H    | 1.83                     | 0.42              |
| 46:DZ:150:LEU:H   | 46:DZ:150:LEU:CD1 | 2.33                     | 0.42              |
| 1:AA:453:A:N6     | 1:AA:454:C:N4     | 2.67                     | 0.41              |
| 1:AA:768:A:N3     | 1:AA:1512:U:O2'   | 2.51                     | 0.41              |
| 1:AA:925:G:H1     | 1:AA:1391:U:H3    | 1.67                     | 0.41              |
| 2:AB:231:GLU:H    | 2:AB:231:GLU:HG2  | 1.53                     | 0.41              |
| 3:AC:11:ARG:O     | 3:AC:12:LEU:C     | 2.62                     | 0.41              |
| 3:AC:134:ILE:C    | 3:AC:136:GLN:N    | 2.76                     | 0.41              |
| 4:AD:77:ASN:O     | 4:AD:80:GLU:HB2   | 2.20                     | 0.41              |
| 6:AF:54:LYS:HA    | 6:AF:54:LYS:HD3   | 1.95                     | 0.41              |
| 7:AG:99:LEU:O     | 7:AG:102:ARG:HB3  | 2.20                     | 0.41              |
| 15:AO:63:ARG:HG2  | 15:AO:67:LEU:CD1  | 2.50                     | 0.41              |
| 20:AT:36:LEU:O    | 20:AT:55:ILE:CG2  | 2.68                     | 0.41              |
| 23:AW:38:A:C6     | 23:AW:39:U:C4     | 3.08                     | 0.41              |
| 25:BA:28:A:N6     | 25:BA:512:G:H1'   | 2.34                     | 0.41              |
| 25:BA:411:G:H5''  | 25:BA:412:A:OP1   | 2.20                     | 0.41              |
| 25:BA:603:A:O2'   | 25:BA:604:G:O5'   | 2.32                     | 0.41              |
| 25:BA:627:A:N6    | 36:BP:116:GLY:HA2 | 2.35                     | 0.41              |
| 25:BA:1264:G:H2'  | 25:BA:2014:A:N6   | 2.35                     | 0.41              |
| 25:BA:1456:G:C4   | 25:BA:1457:A:N7   | 2.87                     | 0.41              |
| 25:BA:1472:A:H2'  | 25:BA:1473:G:O4'  | 2.20                     | 0.41              |
| 25:BA:2494:G:HO2' | 37:BQ:80:GLU:HA   | 1.84                     | 0.41              |
| 28:BD:69:ARG:HE   | 28:BD:69:ARG:HB2  | 1.68                     | 0.41              |
| 30:BF:7:TYR:OH    | 30:BF:10:PRO:HG3  | 2.20                     | 0.41              |
| 30:BF:64:ILE:HG22 | 30:BF:65:TRP:N    | 2.34                     | 0.41              |
| 30:BF:182:ASN:O   | 30:BF:182:ASN:OD1 | 2.37                     | 0.41              |
| 30:BF:199:TRP:CH2 | 30:BF:203:GLN:HG2 | 2.55                     | 0.41              |
| 33:BI:96:ASP:O    | 33:BI:97:ILE:C    | 2.60                     | 0.41              |
| 34:BN:1:MET:HB3   | 34:BN:1:MET:HE2   | 1.72                     | 0.41              |
| 34:BN:12:ARG:O    | 34:BN:13:TRP:O    | 2.37                     | 0.41              |
| 35:BO:19:ILE:O    | 35:BO:19:ILE:CG1  | 2.67                     | 0.41              |
| 38:BR:28:LEU:HD23 | 38:BR:28:LEU:HA   | 1.62                     | 0.41              |
| 39:BS:28:VAL:CG1  | 39:BS:89:ARG:HG3  | 2.50                     | 0.41              |
| 41:BU:21:ALA:O    | 41:BU:22:LYS:C    | 2.63                     | 0.41              |
| 42:BV:20:LEU:CB   | 42:BV:21:ARG:HD3  | 2.49                     | 0.41              |
| 44:BX:63:LYS:HA   | 44:BX:72:LYS:HA   | 2.02                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 45:BY:30:VAL:HG12  | 45:BY:31:LEU:H     | 1.85                     | 0.41              |
| 46:BZ:33:LEU:HD12  | 46:BZ:33:LEU:HA    | 1.86                     | 0.41              |
| 46:BZ:141:VAL:O    | 46:BZ:141:VAL:HG13 | 2.20                     | 0.41              |
| 48:B1:75:GLU:OE2   | 48:B1:75:GLU:HA    | 2.18                     | 0.41              |
| 51:B4:60:GLU:O     | 51:B4:61:VAL:CB    | 2.64                     | 0.41              |
| 52:B5:57:VAL:HG23  | 52:B5:58:LEU:N     | 2.32                     | 0.41              |
| 54:B7:23:ARG:O     | 54:B7:28:ARG:NH1   | 2.52                     | 0.41              |
| 1:CA:375:U:H4'     | 16:CP:17:TYR:CE2   | 2.55                     | 0.41              |
| 1:CA:486:U:H2'     | 1:CA:487:A:O4'     | 2.20                     | 0.41              |
| 1:CA:1052:U:H2'    | 1:CA:1055:A:OP1    | 2.20                     | 0.41              |
| 1:CA:1216:G:H5''   | 14:CN:5:ALA:HB2    | 2.02                     | 0.41              |
| 1:CA:1306:A:N6     | 1:CA:1331:G:H1'    | 2.34                     | 0.41              |
| 2:CB:115:LEU:HD12  | 2:CB:115:LEU:C     | 2.44                     | 0.41              |
| 3:CC:22:TRP:CH2    | 3:CC:32:LEU:HB3    | 2.55                     | 0.41              |
| 4:CD:94:LEU:H      | 4:CD:94:LEU:HG     | 1.59                     | 0.41              |
| 5:CE:153:LYS:HB3   | 5:CE:154:GLY:H     | 1.62                     | 0.41              |
| 6:CF:1:MET:CE      | 6:CF:67:MET:HA     | 2.50                     | 0.41              |
| 9:CI:47:LEU:C      | 9:CI:49:PRO:HD2    | 2.45                     | 0.41              |
| 10:CJ:55:LYS:HE2   | 10:CJ:55:LYS:HB3   | 1.83                     | 0.41              |
| 10:CJ:84:GLN:CD    | 10:CJ:84:GLN:H     | 2.28                     | 0.41              |
| 11:CK:31:THR:HG23  | 11:CK:31:THR:O     | 2.19                     | 0.41              |
| 13:CM:100:GLY:O    | 13:CM:101:GLN:O    | 2.38                     | 0.41              |
| 14:CN:50:LYS:O     | 14:CN:52:GLN:N     | 2.52                     | 0.41              |
| 19:CS:29:ARG:N     | 19:CS:29:ARG:HD2   | 2.35                     | 0.41              |
| 19:CS:50:ALA:HB1   | 19:CS:57:HIS:HB3   | 2.02                     | 0.41              |
| 23:CW:5:G:C2       | 23:CW:69:G:N2      | 2.88                     | 0.41              |
| 25:DA:61:G:C4      | 49:D2:47:ASN:OD1   | 2.73                     | 0.41              |
| 25:DA:1022:G:O6    | 34:DN:66:LYS:HE3   | 2.20                     | 0.41              |
| 25:DA:1251:C:OP1   | 41:DU:10:ARG:HG3   | 2.19                     | 0.41              |
| 25:DA:2208:A:H1'   | 25:DA:2219:G:N3    | 2.35                     | 0.41              |
| 25:DA:2286:A:H5''  | 25:DA:2287:A:O4'   | 2.19                     | 0.41              |
| 25:DA:2398:U:H5'   | 25:DA:2399:G:OP2   | 2.20                     | 0.41              |
| 25:DA:2422:A:H4'   | 25:DA:2423:U:OP1   | 2.20                     | 0.41              |
| 25:DA:2838:G:C1'   | 38:DR:45:ARG:HH11  | 2.33                     | 0.41              |
| 26:DB:13:A:O2'     | 26:DB:14:U:H5''    | 2.20                     | 0.41              |
| 26:DB:56:G:H5''    | 26:DB:57:A:OP1     | 2.20                     | 0.41              |
| 28:DD:69:ARG:HD2   | 28:DD:119:ALA:HB2  | 2.02                     | 0.41              |
| 28:DD:182:LEU:HD23 | 28:DD:182:LEU:HA   | 1.79                     | 0.41              |
| 30:DF:107:LYS:CE   | 30:DF:206:ILE:HD13 | 2.50                     | 0.41              |
| 31:DG:102:PHE:HZ   | 31:DG:157:ILE:HD13 | 1.85                     | 0.41              |
| 32:DH:107:VAL:HG23 | 32:DH:109:PHE:CE1  | 2.55                     | 0.41              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 34:DN:2:LYS:O      | 34:DN:4:TYR:CE1   | 2.73                     | 0.41              |
| 34:DN:120:LEU:HD11 | 34:DN:122:VAL:CG2 | 2.50                     | 0.41              |
| 36:DP:56:SER:O     | 36:DP:57:THR:HG22 | 2.20                     | 0.41              |
| 36:DP:106:LEU:O    | 36:DP:107:LYS:CB  | 2.68                     | 0.41              |
| 37:DQ:5:ARG:HG3    | 37:DQ:5:ARG:H     | 1.50                     | 0.41              |
| 37:DQ:85:LYS:CG    | 47:D0:7:LEU:HD13  | 2.49                     | 0.41              |
| 43:DW:5:ALA:HB1    | 43:DW:50:VAL:CG2  | 2.50                     | 0.41              |
| 43:DW:82:LEU:HD23  | 43:DW:82:LEU:HA   | 1.63                     | 0.41              |
| 44:DX:59:VAL:O     | 44:DX:59:VAL:HG12 | 2.20                     | 0.41              |
| 53:D6:14:THR:C     | 53:D6:16:CYS:H    | 2.28                     | 0.41              |
| 53:D6:41:PRO:HD3   | 53:D6:46:HIS:HA   | 2.02                     | 0.41              |
| 55:D8:6:THR:HA     | 55:D8:61:LEU:HD11 | 2.01                     | 0.41              |
| 1:AA:442:C:H42     | 1:AA:492:G:H1     | 1.68                     | 0.41              |
| 1:AA:1278:U:H6     | 1:AA:1278:U:H3'   | 1.85                     | 0.41              |
| 2:AB:18:GLY:O      | 2:AB:204:ASN:OD1  | 2.38                     | 0.41              |
| 2:AB:20:GLU:HG2    | 2:AB:20:GLU:H     | 1.53                     | 0.41              |
| 2:AB:93:VAL:O      | 2:AB:93:VAL:CG2   | 2.67                     | 0.41              |
| 2:AB:118:LEU:HB3   | 2:AB:142:LEU:HD13 | 2.02                     | 0.41              |
| 2:AB:194:PRO:O     | 2:AB:195:ASP:C    | 2.63                     | 0.41              |
| 3:AC:142:MET:O     | 3:AC:143:GLU:C    | 2.63                     | 0.41              |
| 4:AD:23:GLY:O      | 4:AD:27:TYR:CD1   | 2.73                     | 0.41              |
| 4:AD:117:ALA:O     | 4:AD:121:VAL:HG23 | 2.19                     | 0.41              |
| 15:AO:71:GLN:HG2   | 15:AO:78:TYR:CE2  | 2.55                     | 0.41              |
| 17:AQ:85:VAL:CG1   | 17:AQ:89:LEU:HD12 | 2.47                     | 0.41              |
| 20:AT:37:SER:O     | 20:AT:40:ALA:HB3  | 2.20                     | 0.41              |
| 23:AW:24:G:C6      | 23:AW:25:C:C4     | 3.08                     | 0.41              |
| 23:AW:43:C:H2'     | 23:AW:43:C:O2     | 2.19                     | 0.41              |
| 23:AW:71:G:N3      | 23:AW:71:G:H2'    | 2.35                     | 0.41              |
| 25:BA:196:A:C2     | 25:BA:805:G:C6    | 3.09                     | 0.41              |
| 25:BA:215:G:H4'    | 25:BA:216:A:H4'   | 2.01                     | 0.41              |
| 25:BA:241:A:H8     | 25:BA:241:A:O5'   | 2.03                     | 0.41              |
| 25:BA:242:G:C8     | 55:B8:5:LYS:HA    | 2.55                     | 0.41              |
| 25:BA:311:A:N7     | 25:BA:332:A:C6    | 2.88                     | 0.41              |
| 25:BA:333:G:C6     | 25:BA:334:C:N4    | 2.88                     | 0.41              |
| 25:BA:586:A:N1     | 25:BA:809:G:O2'   | 2.48                     | 0.41              |
| 25:BA:873:G:H4'    | 37:BQ:63:LYS:HE3  | 2.03                     | 0.41              |
| 25:BA:1549:C:O2'   | 25:BA:1550:C:H5'  | 2.20                     | 0.41              |
| 25:BA:2448:A:H5'   | 25:BA:2449:U:OP2  | 2.20                     | 0.41              |
| 25:BA:2503:A:O2'   | 25:BA:2504:U:P    | 2.79                     | 0.41              |
| 26:BB:66:A:C6      | 26:BB:108:U:C2    | 3.08                     | 0.41              |
| 28:BD:24:ILE:CG1   | 28:BD:25:THR:N    | 2.72                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 28:BD:45:ASN:OD1   | 28:BD:45:ASN:N     | 2.52                     | 0.41              |
| 28:BD:155:LEU:HD23 | 28:BD:177:LEU:CD2  | 2.48                     | 0.41              |
| 31:BG:81:LYS:O     | 31:BG:82:LEU:C     | 2.62                     | 0.41              |
| 32:BH:43:VAL:HG11  | 32:BH:52:VAL:HA    | 2.01                     | 0.41              |
| 33:BI:101:LEU:HD13 | 33:BI:101:LEU:HA   | 1.78                     | 0.41              |
| 34:BN:33:LEU:O     | 34:BN:35:ARG:O     | 2.38                     | 0.41              |
| 36:BP:1:MET:HB2    | 36:BP:2:LYS:H      | 1.66                     | 0.41              |
| 36:BP:111:ARG:HA   | 36:BP:128:HIS:CE1  | 2.56                     | 0.41              |
| 37:BQ:1:MET:HE1    | 37:BQ:44:ALA:HB1   | 2.02                     | 0.41              |
| 37:BQ:84:GLY:O     | 37:BQ:85:LYS:HB2   | 2.19                     | 0.41              |
| 38:BR:11:ASN:C     | 38:BR:12:ARG:CG    | 2.93                     | 0.41              |
| 40:BT:27:THR:O     | 40:BT:28:VAL:CB    | 2.65                     | 0.41              |
| 40:BT:30:VAL:HG21  | 40:BT:83:ILE:HG13  | 2.02                     | 0.41              |
| 42:BV:21:ARG:HD3   | 42:BV:21:ARG:N     | 2.34                     | 0.41              |
| 43:BW:19:LEU:HD23  | 52:B5:25:LEU:HG    | 2.01                     | 0.41              |
| 43:BW:70:TYR:HE2   | 43:BW:108:GLY:C    | 2.28                     | 0.41              |
| 45:BY:14:LEU:HG    | 45:BY:15:VAL:H     | 1.81                     | 0.41              |
| 45:BY:100:ALA:O    | 45:BY:101:LYS:O    | 2.38                     | 0.41              |
| 46:BZ:129:SER:O    | 46:BZ:133:ILE:HG13 | 2.20                     | 0.41              |
| 53:B6:15:GLU:HB3   | 53:B6:18:ARG:HG2   | 2.02                     | 0.41              |
| 1:CA:119:A:H5'     | 1:CA:120:A:C4      | 2.55                     | 0.41              |
| 1:CA:250:A:O2'     | 1:CA:251:G:OP2     | 2.39                     | 0.41              |
| 1:CA:274:A:O2'     | 1:CA:275:G:H5''    | 2.20                     | 0.41              |
| 1:CA:708:C:H2'     | 1:CA:709:G:H8      | 1.85                     | 0.41              |
| 1:CA:792:A:N3      | 1:CA:794:A:C5      | 2.88                     | 0.41              |
| 1:CA:913:A:O2'     | 1:CA:914:A:O5'     | 2.37                     | 0.41              |
| 1:CA:947:G:C6      | 1:CA:948:C:C4      | 3.08                     | 0.41              |
| 1:CA:1029:C:O2'    | 1:CA:1032:G:N2     | 2.41                     | 0.41              |
| 2:CB:22:LYS:C      | 2:CB:24:TRP:HD1    | 2.26                     | 0.41              |
| 4:CD:2:GLY:O       | 4:CD:3:ARG:C       | 2.62                     | 0.41              |
| 4:CD:156:GLU:O     | 4:CD:159:ARG:HB2   | 2.19                     | 0.41              |
| 4:CD:171:GLY:HA3   | 4:CD:173:TRP:CZ3   | 2.55                     | 0.41              |
| 9:CI:86:VAL:HB     | 9:CI:96:LEU:HD22   | 2.02                     | 0.41              |
| 10:CJ:85:LEU:C     | 10:CJ:87:THR:H     | 2.27                     | 0.41              |
| 11:CK:21:ILE:CA    | 11:CK:30:VAL:HG12  | 2.49                     | 0.41              |
| 13:CM:53:VAL:HG12  | 13:CM:57:ARG:HH12  | 1.84                     | 0.41              |
| 15:CO:11:VAL:O     | 15:CO:14:GLU:HB3   | 2.19                     | 0.41              |
| 16:CP:71:ARG:HG3   | 16:CP:72:ARG:N     | 2.35                     | 0.41              |
| 17:CQ:27:PHE:HB2   | 17:CQ:28:PRO:CD    | 2.50                     | 0.41              |
| 20:CT:82:SER:O     | 20:CT:85:MET:CG    | 2.65                     | 0.41              |
| 25:DA:77:C:P       | 49:D2:59:ARG:HH11  | 2.43                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:DA:301:G:H2'   | 25:DA:302:C:C6     | 2.55                     | 0.41              |
| 25:DA:498:G:N2    | 45:DY:47:LYS:NZ    | 2.69                     | 0.41              |
| 25:DA:553:G:H2'   | 25:DA:554:U:O4'    | 2.19                     | 0.41              |
| 25:DA:859:G:O2'   | 25:DA:860:U:H5     | 2.03                     | 0.41              |
| 25:DA:1020:A:H4'  | 25:DA:1021:A:O5'   | 2.19                     | 0.41              |
| 25:DA:1025:G:C4   | 25:DA:1135:C:H1'   | 2.55                     | 0.41              |
| 25:DA:1364:G:OP2  | 48:D1:3:LYS:HD2    | 2.21                     | 0.41              |
| 27:DC:212:VAL:O   | 27:DC:213:TYR:CB   | 2.68                     | 0.41              |
| 28:DD:25:THR:C    | 28:DD:27:THR:H     | 2.28                     | 0.41              |
| 28:DD:28:GLU:H    | 28:DD:28:GLU:CD    | 2.28                     | 0.41              |
| 29:DE:108:SER:O   | 29:DE:162:ALA:HA   | 2.20                     | 0.41              |
| 31:DG:55:LYS:NZ   | 31:DG:148:MET:HE2  | 2.34                     | 0.41              |
| 31:DG:83:ARG:HG2  | 31:DG:83:ARG:HH11  | 1.85                     | 0.41              |
| 31:DG:83:ARG:HB2  | 31:DG:86:MET:HE3   | 2.02                     | 0.41              |
| 32:DH:136:ILE:O   | 32:DH:136:ILE:CG2  | 2.68                     | 0.41              |
| 36:DP:101:VAL:CG1 | 36:DP:102:ARG:N    | 2.83                     | 0.41              |
| 43:DW:82:LEU:HB2  | 43:DW:98:LYS:HB2   | 2.01                     | 0.41              |
| 45:DY:39:VAL:C    | 45:DY:40:GLU:OE2   | 2.63                     | 0.41              |
| 46:DZ:98:MET:O    | 46:DZ:98:MET:HG3   | 2.20                     | 0.41              |
| 46:DZ:119:GLU:O   | 46:DZ:119:GLU:HG3  | 2.20                     | 0.41              |
| 46:DZ:151:HIS:HB3 | 46:DZ:170:THR:HG23 | 2.02                     | 0.41              |
| 47:D0:51:VAL:C    | 47:D0:62:LEU:HD12  | 2.45                     | 0.41              |
| 48:D1:83:GLU:HB2  | 48:D1:84:GLY:H     | 1.63                     | 0.41              |
| 51:D4:14:ILE:HA   | 51:D4:31:ILE:HB    | 2.01                     | 0.41              |
| 55:D8:29:LYS:HD3  | 55:D8:44:LYS:HG2   | 2.02                     | 0.41              |
| 55:D8:57:ARG:O    | 55:D8:59:LYS:N     | 2.53                     | 0.41              |
| 1:AA:324:G:P      | 20:AT:70:SER:HB2   | 2.60                     | 0.41              |
| 2:AB:36:ARG:NE    | 2:AB:36:ARG:CA     | 2.83                     | 0.41              |
| 2:AB:144:ARG:HA   | 2:AB:147:LYS:HB2   | 2.01                     | 0.41              |
| 3:AC:29:TYR:O     | 3:AC:33:LEU:N      | 2.51                     | 0.41              |
| 3:AC:175:LEU:H    | 3:AC:175:LEU:CD1   | 2.21                     | 0.41              |
| 4:AD:7:PRO:HB3    | 4:AD:10:ARG:HD2    | 2.03                     | 0.41              |
| 4:AD:54:TYR:O     | 4:AD:55:ALA:C      | 2.62                     | 0.41              |
| 4:AD:133:VAL:HG21 | 4:AD:138:TYR:CD1   | 2.56                     | 0.41              |
| 5:AE:147:ASP:HA   | 5:AE:150:ARG:NE    | 2.36                     | 0.41              |
| 6:AF:68:PRO:O     | 6:AF:69:GLU:C      | 2.63                     | 0.41              |
| 9:AI:33:PHE:CZ    | 9:AI:47:LEU:HD13   | 2.55                     | 0.41              |
| 11:AK:80:VAL:O    | 11:AK:80:VAL:HG23  | 2.19                     | 0.41              |
| 11:AK:87:THR:CG2  | 11:AK:88:GLY:N     | 2.83                     | 0.41              |
| 15:AO:56:LEU:O    | 15:AO:57:LEU:C     | 2.62                     | 0.41              |
| 16:AP:39:TYR:CD2  | 16:AP:73:LEU:HD11  | 2.54                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 19:AS:6:LYS:HE3   | 19:AS:6:LYS:HB3    | 1.55                     | 0.41              |
| 25:BA:49:A:N6     | 25:BA:177:G:C4     | 2.88                     | 0.41              |
| 25:BA:330:A:O2'   | 25:BA:331:A:C8     | 2.72                     | 0.41              |
| 25:BA:548:A:C5    | 25:BA:549:G:H1'    | 2.56                     | 0.41              |
| 25:BA:668:G:C5    | 25:BA:670:A:C5     | 3.08                     | 0.41              |
| 25:BA:797:C:OP1   | 30:BF:60:SER:OG    | 2.30                     | 0.41              |
| 25:BA:890:A:H2'   | 25:BA:892:G:H5'    | 2.01                     | 0.41              |
| 25:BA:1020:A:N1   | 25:BA:1141:U:H2'   | 2.35                     | 0.41              |
| 25:BA:1248:G:H2'  | 41:BU:3:ARG:HA     | 2.01                     | 0.41              |
| 25:BA:1288:U:C2   | 25:BA:1327:C:C2    | 3.08                     | 0.41              |
| 25:BA:1963:U:C4'  | 25:BA:1964:G:OP1   | 2.67                     | 0.41              |
| 25:BA:2198:A:C1'  | 33:BI:28:ASN:O     | 2.63                     | 0.41              |
| 25:BA:2262:U:H4'  | 25:BA:2328:A:C2    | 2.55                     | 0.41              |
| 25:BA:2313:C:H5'  | 31:BG:40:ASN:ND2   | 2.36                     | 0.41              |
| 25:BA:2334:G:H1'  | 39:BS:15:ARG:HG3   | 2.01                     | 0.41              |
| 29:BE:119:ARG:HG2 | 29:BE:160:TYR:CB   | 2.50                     | 0.41              |
| 30:BF:168:ARG:HA  | 30:BF:175:THR:HG21 | 2.02                     | 0.41              |
| 33:BI:72:LEU:HD11 | 33:BI:138:ILE:CA   | 2.50                     | 0.41              |
| 34:BN:135:PRO:O   | 34:BN:136:GLU:O    | 2.38                     | 0.41              |
| 38:BR:20:LEU:HD12 | 38:BR:20:LEU:HA    | 1.57                     | 0.41              |
| 39:BS:39:ILE:O    | 39:BS:47:THR:HG23  | 2.21                     | 0.41              |
| 42:BV:15:GLU:O    | 42:BV:16:PRO:C     | 2.64                     | 0.41              |
| 42:BV:52:VAL:O    | 42:BV:55:ALA:HB3   | 2.20                     | 0.41              |
| 43:BW:1:MET:HE2   | 43:BW:2:GLU:O      | 2.20                     | 0.41              |
| 43:BW:38:TYR:HE2  | 52:B5:40:LYS:HA    | 1.85                     | 0.41              |
| 48:B1:40:ARG:HD3  | 48:B1:40:ARG:O     | 2.20                     | 0.41              |
| 48:B1:75:GLU:O    | 48:B1:77:ALA:N     | 2.52                     | 0.41              |
| 50:B3:50:VAL:O    | 50:B3:51:ALA:C     | 2.63                     | 0.41              |
| 1:CA:243:A:O2'    | 1:CA:244:U:OP2     | 2.30                     | 0.41              |
| 1:CA:529:G:O6     | 12:CL:49:ASN:HA    | 2.20                     | 0.41              |
| 1:CA:1251:A:H2'   | 1:CA:1252:A:O4'    | 2.21                     | 0.41              |
| 2:CB:92:TYR:CE2   | 2:CB:151:GLY:HA2   | 2.55                     | 0.41              |
| 4:CD:19:LEU:HB3   | 4:CD:21:LEU:HD11   | 1.99                     | 0.41              |
| 4:CD:58:LEU:HD22  | 4:CD:58:LEU:O      | 2.20                     | 0.41              |
| 5:CE:115:VAL:CG1  | 5:CE:116:THR:H     | 2.28                     | 0.41              |
| 7:CG:99:LEU:HD23  | 7:CG:99:LEU:HA     | 1.91                     | 0.41              |
| 7:CG:106:GLN:O    | 7:CG:110:GLN:HG3   | 2.21                     | 0.41              |
| 9:CI:9:ARG:CD     | 9:CI:104:ARG:HH11  | 2.33                     | 0.41              |
| 9:CI:44:VAL:O     | 9:CI:44:VAL:HG23   | 2.20                     | 0.41              |
| 12:CL:75:HIS:ND1  | 12:CL:75:HIS:C     | 2.78                     | 0.41              |
| 13:CM:27:LYS:O    | 13:CM:31:LYS:HG3   | 2.20                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 15:CO:39:LEU:HD23  | 15:CO:39:LEU:HA    | 1.80                     | 0.41              |
| 15:CO:75:PRO:O     | 15:CO:76:GLU:HB2   | 2.20                     | 0.41              |
| 17:CQ:4:LYS:C      | 17:CQ:5:VAL:HG23   | 2.44                     | 0.41              |
| 17:CQ:29:HIS:CE1   | 17:CQ:31:LEU:HB3   | 2.54                     | 0.41              |
| 18:CR:69:THR:O     | 18:CR:70:ILE:C     | 2.63                     | 0.41              |
| 20:CT:29:LYS:HD3   | 20:CT:66:ALA:HB2   | 1.97                     | 0.41              |
| 22:CV:19:G:C4      | 22:CV:59:A:C6      | 3.09                     | 0.41              |
| 22:CV:30:G:O6      | 22:CV:43:G:O6      | 2.38                     | 0.41              |
| 23:CW:16:U:H6      | 23:CW:17:C:H5'     | 1.84                     | 0.41              |
| 25:DA:301:G:O2'    | 25:DA:302:C:O4'    | 2.30                     | 0.41              |
| 25:DA:593:G:C1'    | 55:D8:4:MET:HE1    | 2.50                     | 0.41              |
| 25:DA:1668:A:H4'   | 25:DA:1669:A:O5'   | 2.20                     | 0.41              |
| 25:DA:2259:G:C8    | 25:DA:2427:C:C4    | 3.08                     | 0.41              |
| 25:DA:2292:C:OP1   | 39:DS:17:ARG:NH2   | 2.53                     | 0.41              |
| 27:DC:168:THR:HA   | 27:DC:173:ALA:CB   | 2.50                     | 0.41              |
| 28:DD:24:ILE:CG1   | 28:DD:25:THR:H     | 2.12                     | 0.41              |
| 29:DE:4:ILE:O      | 29:DE:4:ILE:CG2    | 2.65                     | 0.41              |
| 29:DE:54:GLN:O     | 29:DE:55:ASN:HB2   | 2.20                     | 0.41              |
| 29:DE:94:GLU:HG2   | 29:DE:177:PRO:HB3  | 2.02                     | 0.41              |
| 30:DF:29:ASN:HB3   | 30:DF:112:MET:HE1  | 2.02                     | 0.41              |
| 31:DG:63:ILE:CG2   | 31:DG:144:ILE:HD11 | 2.51                     | 0.41              |
| 32:DH:26:VAL:CG1   | 32:DH:27:LYS:N     | 2.83                     | 0.41              |
| 33:DI:67:ARG:HD2   | 33:DI:68:LEU:HD13  | 2.01                     | 0.41              |
| 33:DI:109:ILE:HG13 | 33:DI:110:ASP:N    | 2.35                     | 0.41              |
| 36:DP:38:GLN:H     | 36:DP:41:ARG:HG2   | 1.85                     | 0.41              |
| 36:DP:61:ARG:O     | 36:DP:61:ARG:CD    | 2.68                     | 0.41              |
| 36:DP:135:LEU:HD13 | 36:DP:135:LEU:O    | 2.20                     | 0.41              |
| 37:DQ:141:GLN:NE2  | 46:DZ:72:ARG:HD3   | 2.35                     | 0.41              |
| 38:DR:10:LEU:O     | 38:DR:11:ASN:C     | 2.63                     | 0.41              |
| 39:DS:46:VAL:CG1   | 39:DS:47:THR:N     | 2.82                     | 0.41              |
| 41:DU:66:ASN:HB2   | 41:DU:76:TYR:CB    | 2.45                     | 0.41              |
| 42:DV:49:THR:O     | 42:DV:50:PRO:C     | 2.60                     | 0.41              |
| 45:DY:78:ALA:HB3   | 45:DY:81:LYS:CE    | 2.49                     | 0.41              |
| 45:DY:78:ALA:CB    | 45:DY:81:LYS:HZ1   | 2.33                     | 0.41              |
| 52:D5:58:LEU:O     | 52:D5:59:GLU:OE2   | 2.39                     | 0.41              |
| 54:D7:41:ARG:HB2   | 54:D7:41:ARG:HH11  | 1.84                     | 0.41              |
| 55:D8:4:MET:O      | 55:D8:62:LEU:CD1   | 2.67                     | 0.41              |
| 1:AA:706:A:H5''    | 11:AK:22:HIS:CE1   | 2.56                     | 0.41              |
| 1:AA:860:A:H3'     | 1:AA:861:G:H8      | 1.85                     | 0.41              |
| 1:AA:862:C:H42     | 1:AA:867:G:H1      | 1.68                     | 0.41              |
| 1:AA:1070:U:H2'    | 1:AA:1071:C:C6     | 2.55                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AA:1422:G:O3'   | 35:BO:49:ARG:NH1  | 2.54                     | 0.41              |
| 2:AB:52:GLU:HG2   | 2:AB:56:ARG:HG2   | 2.02                     | 0.41              |
| 3:AC:122:GLU:O    | 3:AC:123:GLN:C    | 2.63                     | 0.41              |
| 4:AD:206:PHE:O    | 4:AD:206:PHE:CD1  | 2.73                     | 0.41              |
| 5:AE:100:VAL:HG13 | 5:AE:118:ILE:HG21 | 2.02                     | 0.41              |
| 8:AH:127:LEU:HD22 | 8:AH:127:LEU:HA   | 1.87                     | 0.41              |
| 9:AI:65:VAL:C     | 9:AI:66:ARG:HG3   | 2.45                     | 0.41              |
| 11:AK:33:THR:OG1  | 11:AK:37:GLY:C    | 2.63                     | 0.41              |
| 12:AL:60:LEU:HD13 | 12:AL:60:LEU:HA   | 1.78                     | 0.41              |
| 13:AM:96:LEU:CD2  | 13:AM:97:PRO:HD2  | 2.47                     | 0.41              |
| 13:AM:120:LYS:HA  | 13:AM:120:LYS:HD3 | 1.77                     | 0.41              |
| 17:AQ:74:LEU:O    | 17:AQ:74:LEU:HD22 | 2.21                     | 0.41              |
| 20:AT:98:PRO:C    | 20:AT:100:ILE:N   | 2.76                     | 0.41              |
| 23:AW:16:U:C5     | 23:AW:18:G:H3'    | 2.55                     | 0.41              |
| 23:AY:31:A:C4     | 23:AY:32:U:C5     | 3.07                     | 0.41              |
| 25:BA:795:C:H2'   | 25:BA:796:C:H6    | 1.86                     | 0.41              |
| 25:BA:1114:G:H2'  | 25:BA:1115:G:H5'' | 2.02                     | 0.41              |
| 25:BA:1278:A:C5'  | 38:BR:36:THR:HG22 | 2.50                     | 0.41              |
| 25:BA:1598:C:O3'  | 44:BX:35:THR:HG22 | 2.20                     | 0.41              |
| 25:BA:1826:G:C5   | 25:BA:1827:C:C4   | 3.09                     | 0.41              |
| 25:BA:2676:C:O2   | 25:BA:2732:G:N2   | 2.50                     | 0.41              |
| 25:BA:2724:C:OP2  | 29:BE:111:ARG:NH1 | 2.53                     | 0.41              |
| 29:BE:101:ARG:HD3 | 29:BE:169:ASN:CG  | 2.45                     | 0.41              |
| 32:BH:70:THR:O    | 32:BH:72:ILE:HD12 | 2.20                     | 0.41              |
| 36:BP:34:GLY:O    | 36:BP:36:LYS:HB2  | 2.20                     | 0.41              |
| 36:BP:57:THR:HG23 | 36:BP:59:LEU:CB   | 2.46                     | 0.41              |
| 40:BT:2:ASN:HB2   | 40:BT:3:ARG:HE    | 1.85                     | 0.41              |
| 40:BT:66:VAL:HG22 | 40:BT:71:GLY:CA   | 2.50                     | 0.41              |
| 43:BW:22:ASP:HA   | 43:BW:25:ARG:NH1  | 2.35                     | 0.41              |
| 48:B1:7:ILE:HB    | 48:B1:62:VAL:HG23 | 2.01                     | 0.41              |
| 49:B2:29:LYS:CD   | 49:B2:57:ILE:HD13 | 2.45                     | 0.41              |
| 54:B7:1:MET:O     | 54:B7:2:LYS:C     | 2.63                     | 0.41              |
| 1:CA:31:G:C6      | 1:CA:48:C:N1      | 2.89                     | 0.41              |
| 1:CA:120:A:O2'    | 1:CA:122:G:OP1    | 2.38                     | 0.41              |
| 1:CA:189(K):U:H2' | 1:CA:189(L):G:H8  | 1.84                     | 0.41              |
| 1:CA:383:A:C5     | 1:CA:384:G:H1'    | 2.55                     | 0.41              |
| 1:CA:460:G:C6     | 1:CA:470:C:H5'    | 2.56                     | 0.41              |
| 1:CA:511:C:OP1    | 1:CA:511:C:C4'    | 2.67                     | 0.41              |
| 1:CA:1059:C:O2'   | 10:CJ:53:PRO:HD3  | 2.19                     | 0.41              |
| 1:CA:1270:C:OP2   | 21:CU:24:ARG:NH2  | 2.53                     | 0.41              |
| 1:CA:1297:C:H1'   | 1:CA:1298:C:H5    | 1.86                     | 0.41              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:CA:1346:A:H5''   | 9:CI:120:ARG:NH1  | 2.35                     | 0.41              |
| 1:CA:1516:G:H2'    | 1:CA:1518:A:OP2   | 2.21                     | 0.41              |
| 2:CB:90:MET:HA     | 2:CB:91:PRO:HD3   | 1.88                     | 0.41              |
| 4:CD:24:GLU:O      | 4:CD:25:ARG:C     | 2.64                     | 0.41              |
| 4:CD:73:ARG:HA     | 4:CD:73:ARG:HD3   | 1.70                     | 0.41              |
| 4:CD:101:LEU:HD23  | 4:CD:121:VAL:HG13 | 2.02                     | 0.41              |
| 4:CD:107:ARG:NH2   | 4:CD:194:LEU:HD12 | 2.35                     | 0.41              |
| 4:CD:154:ASN:O     | 4:CD:155:LEU:HD23 | 2.20                     | 0.41              |
| 4:CD:199:ASN:OD1   | 4:CD:199:ASN:C    | 2.62                     | 0.41              |
| 7:CG:69:VAL:HG12   | 7:CG:100:ALA:HA   | 2.03                     | 0.41              |
| 9:CI:60:ASP:O      | 9:CI:61:ALA:C     | 2.62                     | 0.41              |
| 9:CI:77:ILE:HG22   | 9:CI:81:ILE:HG12  | 2.02                     | 0.41              |
| 10:CJ:27:ALA:HA    | 10:CJ:30:SER:OG   | 2.20                     | 0.41              |
| 11:CK:88:GLY:O     | 11:CK:90:GLY:N    | 2.53                     | 0.41              |
| 12:CL:47:LYS:CB    | 12:CL:48:PRO:CD   | 2.70                     | 0.41              |
| 13:CM:82:MET:O     | 13:CM:83:ASP:HB2  | 2.19                     | 0.41              |
| 15:CO:15:PHE:O     | 15:CO:16:ALA:C    | 2.63                     | 0.41              |
| 22:CV:9:G:O2'      | 22:CV:10:G:N7     | 2.48                     | 0.41              |
| 22:CV:35:C:H2'     | 22:CV:36:A:O5'    | 2.20                     | 0.41              |
| 22:CV:41:C:H4'     | 23:CW:36:A:OP1    | 2.20                     | 0.41              |
| 23:CW:14:A:C6      | 23:CW:15:G:H1'    | 2.56                     | 0.41              |
| 25:DA:856:C:H1'    | 47:D0:27:GLU:HB3  | 2.02                     | 0.41              |
| 25:DA:1169:G:H1    | 25:DA:1180:C:H42  | 1.69                     | 0.41              |
| 25:DA:1191:G:OP1   | 36:DP:32:THR:HB   | 2.21                     | 0.41              |
| 25:DA:1385:G:HO2'  | 25:DA:1386:C:C5'  | 2.33                     | 0.41              |
| 25:DA:1430:C:H2'   | 25:DA:1431:U:C6   | 2.55                     | 0.41              |
| 25:DA:1865:G:H5'   | 25:DA:1866:C:OP2  | 2.20                     | 0.41              |
| 25:DA:2371:G:O4'   | 53:D6:45:LYS:HD3  | 2.21                     | 0.41              |
| 25:DA:2637:U:H5''  | 29:DE:82:ARG:NH2  | 2.34                     | 0.41              |
| 25:DA:2668:G:H2'   | 25:DA:2669:G:C8   | 2.54                     | 0.41              |
| 28:DD:24:ILE:CD1   | 28:DD:84:TYR:HB2  | 2.51                     | 0.41              |
| 29:DE:17:ASP:O     | 29:DE:18:ASP:CB   | 2.69                     | 0.41              |
| 29:DE:75:VAL:O     | 29:DE:76:ARG:C    | 2.64                     | 0.41              |
| 30:DF:31:HIS:O     | 30:DF:32:LEU:C    | 2.63                     | 0.41              |
| 30:DF:197:ASP:C    | 30:DF:199:TRP:N   | 2.78                     | 0.41              |
| 31:DG:106:LEU:HD12 | 31:DG:110:ALA:CB  | 2.50                     | 0.41              |
| 31:DG:123:ASN:C    | 31:DG:125:PHE:H   | 2.28                     | 0.41              |
| 31:DG:180:PHE:O    | 31:DG:182:LYS:N   | 2.53                     | 0.41              |
| 32:DH:32:GLU:O     | 32:DH:33:LEU:HD23 | 2.20                     | 0.41              |
| 34:DN:39:ARG:HG2   | 34:DN:39:ARG:NH1  | 2.35                     | 0.41              |
| 34:DN:51:PHE:CZ    | 34:DN:119:ARG:CD  | 3.03                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 34:DN:78:TYR:N    | 34:DN:78:TYR:CD1   | 2.88                     | 0.41              |
| 35:DO:87:ILE:HG21 | 35:DO:91:LEU:HA    | 2.02                     | 0.41              |
| 36:DP:91:PHE:HD1  | 36:DP:91:PHE:N     | 2.18                     | 0.41              |
| 36:DP:97:PRO:O    | 36:DP:98:GLU:CB    | 2.62                     | 0.41              |
| 38:DR:92:GLY:HA2  | 38:DR:94:TYR:HE1   | 1.85                     | 0.41              |
| 39:DS:110:LEU:HA  | 39:DS:112:PHE:CZ   | 2.54                     | 0.41              |
| 40:DT:77:PRO:O    | 40:DT:78:LEU:CB    | 2.69                     | 0.41              |
| 42:DV:58:VAL:HG21 | 42:DV:100:ARG:HH12 | 1.84                     | 0.41              |
| 44:DX:47:PHE:HE1  | 49:D2:33:MET:HE1   | 1.85                     | 0.41              |
| 45:DY:12:THR:HG23 | 45:DY:26:LYS:CE    | 2.50                     | 0.41              |
| 45:DY:94:LYS:NZ   | 45:DY:101:LYS:HZ3  | 2.17                     | 0.41              |
| 46:DZ:73:GLN:HB3  | 46:DZ:87:ASP:CG    | 2.45                     | 0.41              |
| 46:DZ:73:GLN:HB3  | 46:DZ:87:ASP:OD1   | 2.20                     | 0.41              |
| 46:DZ:80:ARG:HD2  | 46:DZ:80:ARG:HA    | 1.78                     | 0.41              |
| 46:DZ:168:GLU:HA  | 46:DZ:168:GLU:OE2  | 2.20                     | 0.41              |
| 55:D8:22:VAL:O    | 55:D8:49:VAL:HG22  | 2.19                     | 0.41              |
| 1:AA:21:G:H21     | 1:AA:914:A:H62     | 1.68                     | 0.41              |
| 1:AA:381:C:H2'    | 1:AA:382:A:O4'     | 2.20                     | 0.41              |
| 1:AA:687:A:H4'    | 1:AA:688:G:O5'     | 2.20                     | 0.41              |
| 1:AA:1046:A:H3'   | 1:AA:1047:G:H8     | 1.85                     | 0.41              |
| 1:AA:1225:A:N3    | 1:AA:1225:A:H2'    | 2.35                     | 0.41              |
| 2:AB:51:LEU:O     | 2:AB:55:PHE:CD2    | 2.73                     | 0.41              |
| 3:AC:21:ARG:O     | 3:AC:22:TRP:CD1    | 2.74                     | 0.41              |
| 3:AC:34:LEU:O     | 3:AC:34:LEU:HG     | 2.19                     | 0.41              |
| 4:AD:18:LYS:HG3   | 4:AD:31:CYS:SG     | 2.59                     | 0.41              |
| 4:AD:149:ALA:O    | 4:AD:152:SER:N     | 2.45                     | 0.41              |
| 4:AD:172:PRO:O    | 4:AD:187:ARG:NH1   | 2.51                     | 0.41              |
| 4:AD:192:GLU:OE2  | 4:AD:192:GLU:HA    | 2.21                     | 0.41              |
| 5:AE:30:ALA:O     | 5:AE:45:PHE:HA     | 2.21                     | 0.41              |
| 5:AE:145:LYS:O    | 5:AE:149:GLU:HG2   | 2.20                     | 0.41              |
| 9:AI:8:GLY:HA2    | 9:AI:79:LEU:CD1    | 2.46                     | 0.41              |
| 9:AI:79:LEU:C     | 9:AI:79:LEU:HD13   | 2.46                     | 0.41              |
| 10:AJ:33:GLN:HB2  | 10:AJ:75:ILE:HD13  | 2.02                     | 0.41              |
| 11:AK:73:MET:HG2  | 11:AK:103:LEU:HD21 | 2.02                     | 0.41              |
| 12:AL:82:VAL:H    | 12:AL:106:ASP:CG   | 2.27                     | 0.41              |
| 13:AM:50:GLU:H    | 13:AM:50:GLU:HG2   | 1.62                     | 0.41              |
| 17:AQ:16:GLN:O    | 17:AQ:17:LYS:HB2   | 2.20                     | 0.41              |
| 20:AT:32:ALA:O    | 20:AT:33:ILE:C     | 2.64                     | 0.41              |
| 25:BA:464:U:H4'   | 54:B7:5:TRP:CZ3    | 2.55                     | 0.41              |
| 25:BA:565:C:H4'   | 25:BA:1253:A:N6    | 2.34                     | 0.41              |
| 25:BA:729:G:P     | 28:BD:208:LYS:HZ1  | 2.44                     | 0.41              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 25:BA:740:U:H5''   | 25:BA:1784:A:H3'  | 2.02                     | 0.41              |
| 25:BA:974:G:C2     | 25:BA:989:G:C4    | 3.08                     | 0.41              |
| 25:BA:1022:G:O2'   | 25:BA:1024:G:N7   | 2.52                     | 0.41              |
| 25:BA:1291:C:H2'   | 25:BA:1292:U:C6   | 2.56                     | 0.41              |
| 25:BA:1487:G:O6    | 25:BA:1502:C:N4   | 2.49                     | 0.41              |
| 25:BA:2038:G:H2'   | 25:BA:2039:C:O4'  | 2.21                     | 0.41              |
| 26:BB:108:U:O5'    | 26:BB:108:U:H6    | 2.03                     | 0.41              |
| 27:BC:39:GLU:CD    | 27:BC:70:LYS:NZ   | 2.79                     | 0.41              |
| 28:BD:180:GLY:C    | 28:BD:181:GLU:O   | 2.62                     | 0.41              |
| 28:BD:270:ILE:HD12 | 28:BD:270:ILE:N   | 2.25                     | 0.41              |
| 29:BE:17:ASP:HB3   | 29:BE:18:ASP:H    | 1.52                     | 0.41              |
| 29:BE:92:THR:O     | 29:BE:93:VAL:C    | 2.62                     | 0.41              |
| 29:BE:110:GLY:HA2  | 29:BE:162:ALA:N   | 2.35                     | 0.41              |
| 32:BH:167:GLU:HA   | 32:BH:168:PRO:HD2 | 1.66                     | 0.41              |
| 34:BN:56:ASN:C     | 34:BN:57:ALA:O    | 2.63                     | 0.41              |
| 34:BN:57:ALA:H     | 34:BN:124:ALA:HA  | 1.86                     | 0.41              |
| 35:BO:31:LYS:HB3   | 35:BO:32:TYR:CE2  | 2.56                     | 0.41              |
| 36:BP:13:ASN:C     | 36:BP:15:ARG:N    | 2.72                     | 0.41              |
| 36:BP:50:ARG:HD3   | 55:B8:59:LYS:HD3  | 2.01                     | 0.41              |
| 36:BP:59:LEU:HD21  | 55:B8:13:ARG:NH2  | 2.30                     | 0.41              |
| 36:BP:135:LEU:HD13 | 36:BP:135:LEU:O   | 2.20                     | 0.41              |
| 37:BQ:14:ARG:CG    | 37:BQ:14:ARG:HH11 | 2.33                     | 0.41              |
| 38:BR:116:LEU:O    | 38:BR:117:VAL:O   | 2.38                     | 0.41              |
| 54:B7:39:ARG:HD3   | 54:B7:39:ARG:HA   | 1.87                     | 0.41              |
| 55:B8:15:LYS:HG2   | 55:B8:16:ILE:N    | 2.35                     | 0.41              |
| 1:CA:129(A):G:H5'' | 1:CA:130:A:O5'    | 2.21                     | 0.41              |
| 1:CA:687:A:H2      | 1:CA:704:A:C4     | 2.38                     | 0.41              |
| 1:CA:965:A:H5''    | 1:CA:966:G:OP1    | 2.20                     | 0.41              |
| 1:CA:1327:C:H2'    | 1:CA:1328:C:C6    | 2.56                     | 0.41              |
| 2:CB:211:ILE:H     | 2:CB:211:ILE:HG13 | 1.54                     | 0.41              |
| 8:CH:100:ILE:HA    | 8:CH:101:PRO:HD3  | 1.79                     | 0.41              |
| 9:CI:4:TYR:CE2     | 9:CI:88:TYR:CD2   | 3.09                     | 0.41              |
| 16:CP:3:LYS:HG2    | 16:CP:65:GLN:O    | 2.21                     | 0.41              |
| 17:CQ:33:GLY:O     | 17:CQ:34:LYS:C    | 2.62                     | 0.41              |
| 22:CV:70:C:H2'     | 22:CV:71:G:O4'    | 2.20                     | 0.41              |
| 23:CW:38:A:C2'     | 23:CW:39:U:OP1    | 2.68                     | 0.41              |
| 25:DA:271(U):G:O2' | 25:DA:9271:G:H5'  | 2.20                     | 0.41              |
| 25:DA:555:U:O2'    | 25:DA:556:G:N7    | 2.50                     | 0.41              |
| 25:DA:572:A:H5''   | 25:DA:573:G:OP2   | 2.20                     | 0.41              |
| 25:DA:573:G:O6     | 25:DA:2030:A:H3'  | 2.21                     | 0.41              |
| 25:DA:889:C:HO2'   | 25:DA:890:A:P     | 2.41                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:DA:1022:G:HO2' | 25:DA:1023:U:P    | 2.42                     | 0.41              |
| 25:DA:1027:A:N6   | 25:DA:1126:A:H1'  | 2.35                     | 0.41              |
| 25:DA:1101:U:H2'  | 25:DA:1102:C:H6   | 1.86                     | 0.41              |
| 25:DA:1149:G:H2'  | 25:DA:1150:C:C6   | 2.56                     | 0.41              |
| 25:DA:1239:G:H2'  | 25:DA:1240:U:O4'  | 2.21                     | 0.41              |
| 25:DA:1523:U:H2'  | 25:DA:1524:G:C8   | 2.55                     | 0.41              |
| 25:DA:1615:C:H2'  | 25:DA:1617:C:H5   | 1.86                     | 0.41              |
| 25:DA:1930:G:N2   | 25:DA:1968:G:H2'  | 2.35                     | 0.41              |
| 25:DA:2013:A:H4'  | 43:DW:96:ILE:HD12 | 2.02                     | 0.41              |
| 25:DA:2131:G:N7   | 25:DA:2158:A:N6   | 2.68                     | 0.41              |
| 25:DA:2415:G:H4'  | 36:DP:67:MET:N    | 2.35                     | 0.41              |
| 25:DA:2556:C:H2'  | 25:DA:2557:G:O4'  | 2.20                     | 0.41              |
| 28:DD:37:LEU:C    | 28:DD:38:LYS:O    | 2.63                     | 0.41              |
| 31:DG:31:VAL:O    | 31:DG:31:VAL:HG13 | 2.20                     | 0.41              |
| 36:DP:83:VAL:HG12 | 36:DP:112:LEU:CD2 | 2.41                     | 0.41              |
| 36:DP:124:LYS:HE3 | 36:DP:145:PRO:HD3 | 2.01                     | 0.41              |
| 37:DQ:81:VAL:HG23 | 37:DQ:82:ARG:N    | 2.36                     | 0.41              |
| 39:DS:8:GLU:HG3   | 39:DS:8:GLU:H     | 1.67                     | 0.41              |
| 39:DS:81:GLY:O    | 39:DS:82:ILE:C    | 2.63                     | 0.41              |
| 40:DT:102:ILE:HB  | 40:DT:110:ILE:CD1 | 2.49                     | 0.41              |
| 40:DT:133:GLU:OE2 | 40:DT:137:LYS:HB2 | 2.20                     | 0.41              |
| 42:DV:22:VAL:HG12 | 42:DV:23:GLU:N    | 2.35                     | 0.41              |
| 42:DV:44:LYS:HE2  | 42:DV:44:LYS:HB3  | 1.81                     | 0.41              |
| 43:DW:78:GLU:OE2  | 43:DW:99:ARG:NH1  | 2.50                     | 0.41              |
| 43:DW:87:PRO:O    | 43:DW:88:ARG:HD2  | 2.20                     | 0.41              |
| 44:DX:65:ARG:HH11 | 44:DX:65:ARG:HG2  | 1.85                     | 0.41              |
| 46:DZ:52:SER:O    | 46:DZ:53:ILE:C    | 2.64                     | 0.41              |
| 46:DZ:128:VAL:CG2 | 46:DZ:129:SER:N   | 2.84                     | 0.41              |
| 46:DZ:158:PRO:O   | 46:DZ:160:GLY:N   | 2.53                     | 0.41              |
| 48:D1:3:LYS:HG2   | 48:D1:4:VAL:H     | 1.84                     | 0.41              |
| 53:D6:28:ARG:O    | 53:D6:29:ASN:C    | 2.62                     | 0.41              |
| 54:D7:1:MET:HE2   | 54:D7:1:MET:HB2   | 1.86                     | 0.41              |
| 54:D7:25:PRO:HB3  | 54:D7:28:ARG:NH2  | 2.35                     | 0.41              |
| 1:AA:189(D):C:H1' | 1:AA:189(H):G:N2  | 2.36                     | 0.41              |
| 1:AA:242:C:O2'    | 1:AA:243:A:H5'    | 2.20                     | 0.41              |
| 1:AA:528:C:H4'    | 1:AA:535:A:C6     | 2.56                     | 0.41              |
| 1:AA:675:A:H1'    | 11:AK:116:HIS:CD2 | 2.56                     | 0.41              |
| 1:AA:1349:A:P     | 9:AI:118:LYS:NZ   | 2.94                     | 0.41              |
| 1:AA:1442(B):A:C6 | 40:BT:118:ARG:CZ  | 3.04                     | 0.41              |
| 2:AB:211:ILE:O    | 2:AB:212:GLN:C    | 2.63                     | 0.41              |
| 3:AC:180:ALA:O    | 3:AC:205:GLY:O    | 2.37                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:AD:92:VAL:HG12  | 4:AD:96:LEU:HD13  | 2.01                     | 0.41              |
| 4:AD:169:LYS:HB3  | 4:AD:169:LYS:HE2  | 1.76                     | 0.41              |
| 6:AF:23:LYS:NZ    | 6:AF:42:GLU:OE2   | 2.44                     | 0.41              |
| 7:AG:85:TYR:O     | 7:AG:87:VAL:HG23  | 2.21                     | 0.41              |
| 9:AI:3:GLN:O      | 9:AI:88:TYR:HE1   | 2.02                     | 0.41              |
| 9:AI:20:ARG:O     | 9:AI:60:ASP:HB2   | 2.20                     | 0.41              |
| 14:AN:57:ARG:O    | 14:AN:58:LYS:C    | 2.62                     | 0.41              |
| 17:AQ:7:THR:HA    | 17:AQ:58:GLU:HA   | 2.03                     | 0.41              |
| 17:AQ:51:TYR:CD1  | 17:AQ:73:VAL:HG11 | 2.56                     | 0.41              |
| 20:AT:24:LEU:O    | 20:AT:25:ARG:C    | 2.62                     | 0.41              |
| 20:AT:29:LYS:HD3  | 20:AT:66:ALA:HB2  | 2.03                     | 0.41              |
| 21:AU:6:ARG:HD3   | 21:AU:15:ARG:CZ   | 2.50                     | 0.41              |
| 25:BA:139:G:H2'   | 25:BA:140:G:N7    | 2.36                     | 0.41              |
| 25:BA:570:G:H2'   | 25:BA:2030:A:C5   | 2.55                     | 0.41              |
| 25:BA:602:G:N2    | 25:BA:656:G:C5    | 2.88                     | 0.41              |
| 25:BA:660:G:H21   | 36:BP:12:ALA:CA   | 2.34                     | 0.41              |
| 25:BA:747:U:O2    | 25:BA:2014:A:H1'  | 2.20                     | 0.41              |
| 25:BA:801:G:H5''  | 25:BA:802:A:OP2   | 2.21                     | 0.41              |
| 25:BA:813:U:H2'   | 25:BA:814:C:C6    | 2.56                     | 0.41              |
| 25:BA:1028:A:N6   | 25:BA:1125:G:H2'  | 2.36                     | 0.41              |
| 25:BA:1286:A:C6   | 25:BA:1289:C:C2   | 3.07                     | 0.41              |
| 25:BA:1332:G:N2   | 25:BA:1609:A:H2'  | 2.35                     | 0.41              |
| 25:BA:1720:U:O5'  | 25:BA:1720:U:H6   | 2.03                     | 0.41              |
| 25:BA:2056:G:C8   | 25:BA:2577:A:C6   | 3.08                     | 0.41              |
| 25:BA:2198:A:H8   | 25:BA:2198:A:O5'  | 2.03                     | 0.41              |
| 25:BA:2458:G:N7   | 25:BA:2490:G:C6   | 2.87                     | 0.41              |
| 25:BA:2758:A:H2'  | 25:BA:2759:G:O4'  | 2.21                     | 0.41              |
| 26:BB:7:G:H3'     | 26:BB:8:U:H5''    | 2.02                     | 0.41              |
| 27:BC:18:LYS:HD3  | 27:BC:19:VAL:H    | 1.85                     | 0.41              |
| 28:BD:48:ARG:CG   | 28:BD:48:ARG:HH11 | 2.34                     | 0.41              |
| 28:BD:131:LEU:HB2 | 28:BD:136:ILE:CD1 | 2.49                     | 0.41              |
| 28:BD:168:ARG:HA  | 28:BD:173:VAL:HA  | 2.03                     | 0.41              |
| 28:BD:231:HIS:ND1 | 28:BD:249:PRO:HA  | 2.35                     | 0.41              |
| 36:BP:38:GLN:HG2  | 36:BP:45:LEU:CD1  | 2.49                     | 0.41              |
| 37:BQ:16:ARG:C    | 37:BQ:17:LEU:HD23 | 2.45                     | 0.41              |
| 38:BR:60:LEU:O    | 38:BR:61:HIS:C    | 2.63                     | 0.41              |
| 39:BS:21:THR:C    | 39:BS:23:ARG:N    | 2.78                     | 0.41              |
| 39:BS:66:ALA:O    | 39:BS:69:VAL:N    | 2.54                     | 0.41              |
| 41:BU:24:TYR:O    | 41:BU:29:SER:HB3  | 2.21                     | 0.41              |
| 41:BU:92:ARG:HH12 | 42:BV:11:GLN:H    | 1.69                     | 0.41              |
| 44:BX:49:VAL:HA   | 44:BX:87:GLN:HE22 | 1.86                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 45:BY:14:LEU:HA    | 45:BY:24:VAL:HG22  | 2.02                     | 0.41              |
| 45:BY:90:LEU:CD1   | 45:BY:91:GLU:HB2   | 2.43                     | 0.41              |
| 47:B0:43:THR:O     | 47:B0:44:ARG:C     | 2.63                     | 0.41              |
| 47:B0:70:GLN:HE21  | 47:B0:80:HIS:HE2   | 1.67                     | 0.41              |
| 48:B1:80:LEU:HD23  | 48:B1:80:LEU:HA    | 1.77                     | 0.41              |
| 1:CA:280:C:H1'     | 17:CQ:38:ARG:HD3   | 2.03                     | 0.41              |
| 1:CA:627:G:H2'     | 1:CA:628:G:H8      | 1.85                     | 0.41              |
| 1:CA:1065:U:O4'    | 1:CA:1066:C:C5'    | 2.56                     | 0.41              |
| 1:CA:1096:C:H2'    | 1:CA:1097:C:C6     | 2.55                     | 0.41              |
| 1:CA:1120:G:H2'    | 1:CA:1121:U:C6     | 2.54                     | 0.41              |
| 1:CA:1407:C:O2'    | 25:DA:1912:A:N1    | 2.47                     | 0.41              |
| 4:CD:43:HIS:O      | 4:CD:44:GLY:C      | 2.61                     | 0.41              |
| 4:CD:45:GLN:HE21   | 4:CD:45:GLN:HB3    | 1.64                     | 0.41              |
| 4:CD:59:ARG:HA     | 4:CD:59:ARG:NE     | 2.35                     | 0.41              |
| 4:CD:98:GLU:O      | 4:CD:103:ASN:ND2   | 2.54                     | 0.41              |
| 4:CD:138:TYR:HE2   | 4:CD:139:ARG:O     | 2.03                     | 0.41              |
| 5:CE:112:LEU:C     | 5:CE:114:GLY:N     | 2.70                     | 0.41              |
| 11:CK:73:MET:HE1   | 11:CK:101:SER:O    | 2.20                     | 0.41              |
| 12:CL:10:LEU:HD23  | 12:CL:10:LEU:HA    | 1.93                     | 0.41              |
| 12:CL:24:VAL:HA    | 12:CL:25:PRO:HD2   | 2.01                     | 0.41              |
| 12:CL:34:ARG:HE    | 12:CL:34:ARG:HB3   | 1.56                     | 0.41              |
| 12:CL:69:TYR:HB2   | 12:CL:90:VAL:HG23  | 2.01                     | 0.41              |
| 13:CM:15:VAL:HG12  | 13:CM:19:LEU:CD2   | 2.50                     | 0.41              |
| 13:CM:44:ARG:O     | 13:CM:45:VAL:C     | 2.64                     | 0.41              |
| 13:CM:122:LYS:HG3  | 13:CM:123:ALA:N    | 2.35                     | 0.41              |
| 15:CO:33:THR:O     | 15:CO:36:ILE:N     | 2.54                     | 0.41              |
| 17:CQ:70:ARG:C     | 17:CQ:71:PHE:CD2   | 2.94                     | 0.41              |
| 22:CV:19:G:N2      | 22:CV:59:A:C8      | 2.89                     | 0.41              |
| 22:CV:41:C:H5'     | 23:CW:35:A:O3'     | 2.20                     | 0.41              |
| 25:DA:841:A:H2'    | 25:DA:842:G:C8     | 2.56                     | 0.41              |
| 25:DA:848:G:O6     | 25:DA:928:G:H2'    | 2.21                     | 0.41              |
| 25:DA:870:A:OP1    | 37:DQ:6:ARG:NH2    | 2.40                     | 0.41              |
| 25:DA:1835:G:H2'   | 25:DA:1835:G:N3    | 2.36                     | 0.41              |
| 25:DA:2396:G:OP1   | 48:D1:25:LYS:NZ    | 2.49                     | 0.41              |
| 25:DA:2563:U:H4'   | 35:DO:28:SER:HA    | 2.03                     | 0.41              |
| 25:DA:2740:A:H2'   | 25:DA:2741:A:C8    | 2.55                     | 0.41              |
| 28:DD:125:ILE:HG22 | 28:DD:125:ILE:O    | 2.21                     | 0.41              |
| 28:DD:253:GLN:H    | 28:DD:253:GLN:HG2  | 1.60                     | 0.41              |
| 31:DG:7:LEU:HD22   | 31:DG:100:TRP:CE3  | 2.56                     | 0.41              |
| 31:DG:111:LEU:HD13 | 31:DG:120:LEU:HD21 | 2.03                     | 0.41              |
| 32:DH:103:LEU:O    | 32:DH:103:LEU:HD23 | 2.21                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 33:DI:47:LEU:O    | 33:DI:51:ILE:HG13  | 2.20                     | 0.41              |
| 34:DN:76:SER:O    | 34:DN:78:TYR:N     | 2.54                     | 0.41              |
| 35:DO:27:GLY:C    | 35:DO:29:ASN:N     | 2.78                     | 0.41              |
| 37:DQ:77:LYS:O    | 37:DQ:78:PRO:O     | 2.37                     | 0.41              |
| 38:DR:16:HIS:C    | 38:DR:16:HIS:HD1   | 2.29                     | 0.41              |
| 38:DR:27:SER:HB3  | 38:DR:34:ILE:HD12  | 2.02                     | 0.41              |
| 38:DR:80:PHE:HD1  | 38:DR:80:PHE:HA    | 1.69                     | 0.41              |
| 39:DS:86:ALA:O    | 39:DS:87:PHE:CB    | 2.64                     | 0.41              |
| 40:DT:33:LYS:HG3  | 40:DT:43:GLN:HB2   | 1.98                     | 0.41              |
| 40:DT:38:ASN:O    | 40:DT:39:ARG:CB    | 2.68                     | 0.41              |
| 41:DU:79:PHE:CE1  | 41:DU:106:PHE:CZ   | 3.09                     | 0.41              |
| 44:DX:18:TYR:O    | 44:DX:20:GLY:N     | 2.53                     | 0.41              |
| 46:DZ:39:VAL:CG1  | 46:DZ:88:PHE:HE1   | 2.33                     | 0.41              |
| 46:DZ:41:LEU:O    | 46:DZ:43:GLU:N     | 2.53                     | 0.41              |
| 46:DZ:136:PHE:C   | 46:DZ:137:ILE:HD13 | 2.45                     | 0.41              |
| 53:D6:20:ASN:C    | 53:D6:21:TYR:CG    | 2.98                     | 0.41              |
| 54:D7:19:ARG:HG2  | 54:D7:19:ARG:NH1   | 2.36                     | 0.41              |
| 1:AA:736:C:H2'    | 1:AA:737:A:C8      | 2.55                     | 0.41              |
| 1:AA:1049:U:C2    | 1:AA:1201:A:C1'    | 3.04                     | 0.41              |
| 1:AA:1067:A:H1'   | 1:AA:1068:G:C8     | 2.55                     | 0.41              |
| 1:AA:1231:G:C5'   | 9:AI:128:ARG:HG3   | 2.50                     | 0.41              |
| 1:AA:1427:U:H2'   | 1:AA:1428:A:C8     | 2.55                     | 0.41              |
| 3:AC:147:LYS:HG3  | 3:AC:204:LEU:O     | 2.21                     | 0.41              |
| 5:AE:147:ASP:HA   | 5:AE:150:ARG:HE    | 1.85                     | 0.41              |
| 8:AH:36:LEU:CA    | 8:AH:39:LEU:HD23   | 2.48                     | 0.41              |
| 10:AJ:87:THR:OG1  | 10:AJ:88:LEU:N     | 2.54                     | 0.41              |
| 12:AL:46:LYS:HD3  | 12:AL:47:LYS:HG3   | 2.02                     | 0.41              |
| 13:AM:83:ASP:OD2  | 13:AM:83:ASP:N     | 2.51                     | 0.41              |
| 15:AO:32:LEU:HD13 | 15:AO:63:ARG:HB2   | 2.02                     | 0.41              |
| 15:AO:64:ARG:HG2  | 15:AO:65:ARG:N     | 2.35                     | 0.41              |
| 22:AV:4:G:HO2'    | 22:AV:5:G:P        | 2.44                     | 0.41              |
| 23:AY:36:A:C4     | 23:AY:37:A:C8      | 3.08                     | 0.41              |
| 25:BA:196:A:C2    | 25:BA:805:G:N1     | 2.89                     | 0.41              |
| 25:BA:319:C:H2'   | 25:BA:320:A:C8     | 2.56                     | 0.41              |
| 25:BA:340:A:C8    | 25:BA:341:G:N7     | 2.89                     | 0.41              |
| 25:BA:547:A:H2'   | 25:BA:548:A:C8     | 2.56                     | 0.41              |
| 25:BA:586:A:H5'   | 30:BF:89:VAL:HG21  | 2.03                     | 0.41              |
| 25:BA:636:G:C8    | 36:BP:115:LEU:HD21 | 2.56                     | 0.41              |
| 25:BA:1754:C:H2'  | 25:BA:1755:A:O4'   | 2.20                     | 0.41              |
| 25:BA:1803:A:H4'  | 28:BD:259:THR:CG2  | 2.50                     | 0.41              |
| 25:BA:2166:G:H2'  | 25:BA:2167:U:O4'   | 2.21                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:BA:2250:G:C6    | 37:BQ:83:MET:HB3   | 2.56                     | 0.41              |
| 25:BA:2331:G:O3'   | 47:B0:43:THR:HG22  | 2.20                     | 0.41              |
| 26:BB:64:C:H2'     | 26:BB:65:C:C6      | 2.55                     | 0.41              |
| 27:BC:58:VAL:CG2   | 27:BC:166:ASP:H    | 2.04                     | 0.41              |
| 27:BC:73:ARG:O     | 27:BC:75:LEU:N     | 2.53                     | 0.41              |
| 29:BE:3:GLY:CA     | 29:BE:81:ILE:HG21  | 2.41                     | 0.41              |
| 29:BE:13:ARG:HH21  | 40:BT:77:PRO:HB3   | 1.85                     | 0.41              |
| 30:BF:9:ILE:O      | 30:BF:128:ALA:HB2  | 2.20                     | 0.41              |
| 30:BF:142:TRP:CE3  | 30:BF:143:ALA:HA   | 2.55                     | 0.41              |
| 31:BG:107:LEU:HD23 | 31:BG:111:LEU:CD1  | 2.48                     | 0.41              |
| 32:BH:64:LEU:HD23  | 32:BH:67:LEU:HD23  | 2.03                     | 0.41              |
| 32:BH:156:ALA:HB3  | 32:BH:159:GLU:CB   | 2.50                     | 0.41              |
| 33:BI:77:LEU:HD22  | 33:BI:101:LEU:HD11 | 1.95                     | 0.41              |
| 36:BP:91:PHE:HD1   | 36:BP:91:PHE:N     | 2.18                     | 0.41              |
| 37:BQ:51:ARG:CG    | 37:BQ:51:ARG:HH11  | 2.33                     | 0.41              |
| 37:BQ:141:GLN:C    | 46:BZ:53:ILE:O     | 2.64                     | 0.41              |
| 38:BR:101:ALA:HB2  | 52:B5:44:THR:HB    | 2.02                     | 0.41              |
| 40:BT:72:VAL:CG1   | 40:BT:73:GLU:N     | 2.84                     | 0.41              |
| 43:BW:29:LEU:HD21  | 43:BW:33:ARG:NH1   | 2.36                     | 0.41              |
| 45:BY:2:ARG:C      | 45:BY:4:LYS:N      | 2.78                     | 0.41              |
| 46:BZ:4:ARG:HG3    | 46:BZ:58:VAL:O     | 2.21                     | 0.41              |
| 46:BZ:5:LEU:CD1    | 46:BZ:6:LYS:H      | 2.28                     | 0.41              |
| 46:BZ:70:LEU:HD23  | 46:BZ:70:LEU:HA    | 1.65                     | 0.41              |
| 49:B2:25:VAL:O     | 49:B2:26:ARG:C     | 2.64                     | 0.41              |
| 55:B8:16:ILE:O     | 55:B8:16:ILE:HG23  | 2.20                     | 0.41              |
| 55:B8:59:LYS:HB2   | 55:B8:59:LYS:HE3   | 1.26                     | 0.41              |
| 1:CA:17:U:O4'      | 1:CA:1080:A:H1'    | 2.21                     | 0.41              |
| 1:CA:966:G:O2'     | 9:CI:127:LYS:O     | 2.39                     | 0.41              |
| 1:CA:1065:U:H5'    | 1:CA:1066:C:C6     | 2.55                     | 0.41              |
| 1:CA:1081:G:OP1    | 5:CE:18:ARG:HG2    | 2.21                     | 0.41              |
| 1:CA:1128:C:H42    | 1:CA:1143:G:H1     | 1.68                     | 0.41              |
| 1:CA:1213:A:N1     | 1:CA:1215:G:H1'    | 2.36                     | 0.41              |
| 2:CB:51:LEU:HB3    | 2:CB:55:PHE:CE2    | 2.56                     | 0.41              |
| 2:CB:101:MET:C     | 2:CB:102:LEU:HD12  | 2.46                     | 0.41              |
| 8:CH:112:LEU:HD11  | 8:CH:114:THR:HG23  | 2.03                     | 0.41              |
| 9:CI:18:PHE:HD1    | 9:CI:62:TYR:CD2    | 2.39                     | 0.41              |
| 10:CJ:23:ILE:H     | 10:CJ:23:ILE:HG13  | 1.71                     | 0.41              |
| 13:CM:15:VAL:HG11  | 13:CM:34:LEU:HD21  | 2.03                     | 0.41              |
| 13:CM:27:LYS:HB3   | 13:CM:31:LYS:HE3   | 2.03                     | 0.41              |
| 25:DA:49:A:H5'     | 25:DA:51:G:O4'     | 2.21                     | 0.41              |
| 25:DA:563:G:C6     | 25:DA:2018:G:C5    | 3.09                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:DA:774:A:H2    | 25:DA:787:U:O2'    | 2.03                     | 0.41              |
| 25:DA:2286:A:OP2  | 53:D6:30:THR:OG1   | 2.39                     | 0.41              |
| 25:DA:2306:C:O5'  | 25:DA:2306:C:H6    | 2.03                     | 0.41              |
| 25:DA:2370:G:H21  | 53:D6:45:LYS:HE2   | 1.85                     | 0.41              |
| 25:DA:2481:G:O2'  | 25:DA:2482:G:P     | 2.79                     | 0.41              |
| 25:DA:2581:G:H5'' | 25:DA:2582:G:OP1   | 2.21                     | 0.41              |
| 25:DA:2835:A:H62  | 25:DA:2878:U:H3'   | 1.86                     | 0.41              |
| 25:DA:2835:A:N6   | 25:DA:2878:U:H3'   | 2.36                     | 0.41              |
| 25:DA:2854:G:H2'  | 25:DA:2855:C:C6    | 2.56                     | 0.41              |
| 26:DB:91:C:OP1    | 37:DQ:16:ARG:HG3   | 2.20                     | 0.41              |
| 28:DD:94:LEU:CD2  | 28:DD:95:LEU:N     | 2.79                     | 0.41              |
| 29:DE:78:LEU:H    | 29:DE:78:LEU:HG    | 1.62                     | 0.41              |
| 30:DF:68:LYS:HG2  | 30:DF:69:HIS:CD2   | 2.55                     | 0.41              |
| 31:DG:115:ARG:CG  | 31:DG:115:ARG:NH1  | 2.81                     | 0.41              |
| 32:DH:135:GLY:HA3 | 32:DH:141:VAL:CG2  | 2.46                     | 0.41              |
| 33:DI:1:MET:HE3   | 33:DI:26:ALA:CB    | 2.48                     | 0.41              |
| 33:DI:38:LEU:C    | 33:DI:40:THR:H     | 2.27                     | 0.41              |
| 34:DN:91:LEU:O    | 34:DN:92:ALA:C     | 2.62                     | 0.41              |
| 34:DN:123:TYR:CZ  | 34:DN:129:PRO:HD2  | 2.56                     | 0.41              |
| 36:DP:79:ARG:O    | 36:DP:111:ARG:CB   | 2.59                     | 0.41              |
| 36:DP:95:VAL:HG23 | 36:DP:125:VAL:HG23 | 2.03                     | 0.41              |
| 38:DR:63:ARG:NH1  | 38:DR:80:PHE:CD2   | 2.87                     | 0.41              |
| 39:DS:102:ALA:O   | 39:DS:105:ALA:HB3  | 2.20                     | 0.41              |
| 40:DT:131:ALA:O   | 40:DT:133:GLU:N    | 2.54                     | 0.41              |
| 41:DU:80:ILE:HD13 | 41:DU:80:ILE:HA    | 1.93                     | 0.41              |
| 42:DV:15:GLU:O    | 42:DV:18:LEU:HB2   | 2.21                     | 0.41              |
| 45:DY:86:ARG:HD2  | 45:DY:86:ARG:HA    | 1.68                     | 0.41              |
| 47:D0:46:LYS:HD2  | 47:D0:78:TYR:CE1   | 2.55                     | 0.41              |
| 49:D2:32:LEU:CB   | 49:D2:53:LEU:HD13  | 2.51                     | 0.41              |
| 53:D6:15:GLU:O    | 53:D6:16:CYS:SG    | 2.76                     | 0.41              |
| 1:AA:243:A:C6     | 1:AA:281:G:C2      | 3.09                     | 0.41              |
| 1:AA:266:G:O2'    | 1:AA:267:C:OP2     | 2.30                     | 0.41              |
| 1:AA:328:C:O2     | 1:AA:328:C:C2'     | 2.51                     | 0.41              |
| 1:AA:362:G:N2     | 1:AA:365:U:OP2     | 2.52                     | 0.41              |
| 1:AA:878:G:P      | 8:AH:88:LYS:HD3    | 2.60                     | 0.41              |
| 1:AA:1048:G:N1    | 1:AA:1210:C:C4     | 2.89                     | 0.41              |
| 1:AA:1048:G:OP1   | 14:AN:4:LYS:HB2    | 2.20                     | 0.41              |
| 1:AA:1139:G:H1'   | 1:AA:1141:C:N4     | 2.35                     | 0.41              |
| 1:AA:1310:G:H5'   | 13:AM:77:ASN:OD1   | 2.21                     | 0.41              |
| 1:AA:1372:U:H2'   | 1:AA:1373:G:O4'    | 2.20                     | 0.41              |
| 2:AB:178:ARG:NH1  | 2:AB:196:LEU:O     | 2.45                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:AC:18:TRP:CE3    | 3:AC:18:TRP:N      | 2.86                     | 0.41              |
| 6:AF:25:ILE:HD13   | 6:AF:25:ILE:HA     | 1.86                     | 0.41              |
| 8:AH:2:LEU:HD13    | 8:AH:3:THR:N       | 2.35                     | 0.41              |
| 8:AH:127:LEU:HD12  | 8:AH:129:VAL:HG11  | 2.02                     | 0.41              |
| 11:AK:33:THR:OG1   | 11:AK:37:GLY:CA    | 2.68                     | 0.41              |
| 13:AM:105:THR:O    | 13:AM:106:ASN:C    | 2.64                     | 0.41              |
| 16:AP:72:ARG:O     | 16:AP:73:LEU:C     | 2.64                     | 0.41              |
| 19:AS:47:HIS:O     | 19:AS:62:ILE:CG2   | 2.69                     | 0.41              |
| 22:AV:21:U:H5''    | 22:AV:22:A:OP2     | 2.21                     | 0.41              |
| 23:AW:16:U:O4      | 23:AW:18:G:H2'     | 2.21                     | 0.41              |
| 25:BA:372:G:HO2'   | 25:BA:373:U:P      | 2.43                     | 0.41              |
| 25:BA:482:A:H1'    | 25:BA:498:G:N2     | 2.35                     | 0.41              |
| 25:BA:494:G:O2'    | 43:BW:5:ALA:O      | 2.39                     | 0.41              |
| 25:BA:571:A:H5''   | 25:BA:975:C:C4     | 2.55                     | 0.41              |
| 25:BA:804:A:H2'    | 25:BA:806:C:N4     | 2.36                     | 0.41              |
| 25:BA:811:U:H4'    | 25:BA:1251:C:O4'   | 2.21                     | 0.41              |
| 25:BA:1264:G:C6    | 25:BA:1265:A:N6    | 2.88                     | 0.41              |
| 25:BA:1339:G:H5''  | 44:BX:16:LYS:HD2   | 2.01                     | 0.41              |
| 25:BA:1608:A:HO2'  | 25:BA:1610:A:P     | 2.44                     | 0.41              |
| 25:BA:2050:C:N4    | 25:BA:2051:A:C6    | 2.89                     | 0.41              |
| 25:BA:2230:G:H1'   | 48:B1:45:ASN:CB    | 2.50                     | 0.41              |
| 25:BA:2287:A:H2    | 25:BA:2346:A:H2    | 1.60                     | 0.41              |
| 25:BA:2366:A:H3'   | 25:BA:2367:G:H8    | 1.86                     | 0.41              |
| 25:BA:2453:A:C2    | 25:BA:2504:U:C4    | 3.08                     | 0.41              |
| 25:BA:2619:C:H2'   | 25:BA:2620:C:H6    | 1.86                     | 0.41              |
| 25:BA:2805:G:H2'   | 25:BA:2807:G:O4'   | 2.21                     | 0.41              |
| 28:BD:2:ALA:O      | 28:BD:3:VAL:HB     | 2.21                     | 0.41              |
| 28:BD:31:LYS:O     | 28:BD:32:SER:C     | 2.63                     | 0.41              |
| 28:BD:73:VAL:C     | 28:BD:75:ILE:N     | 2.79                     | 0.41              |
| 28:BD:182:LEU:HD23 | 28:BD:182:LEU:HA   | 1.65                     | 0.41              |
| 31:BG:25:TYR:CD1   | 31:BG:30:GLU:HG2   | 2.56                     | 0.41              |
| 31:BG:96:ARG:O     | 31:BG:99:MET:HB3   | 2.21                     | 0.41              |
| 32:BH:121:ILE:HG22 | 32:BH:133:VAL:HG12 | 2.02                     | 0.41              |
| 32:BH:159:GLU:HG3  | 32:BH:160:LYS:HG3  | 2.03                     | 0.41              |
| 33:BI:64:GLU:C     | 33:BI:66:GLU:H     | 2.29                     | 0.41              |
| 33:BI:127:VAL:O    | 33:BI:127:VAL:HG12 | 2.21                     | 0.41              |
| 33:BI:136:VAL:HG23 | 33:BI:137:PRO:N    | 2.35                     | 0.41              |
| 34:BN:28:THR:CG2   | 34:BN:29:LYS:N     | 2.83                     | 0.41              |
| 34:BN:87:LEU:O     | 34:BN:90:MET:HB2   | 2.21                     | 0.41              |
| 34:BN:90:MET:HB3   | 34:BN:98:VAL:CG2   | 2.50                     | 0.41              |
| 35:BO:88:ASN:HB3   | 35:BO:94:ARG:HG2   | 2.03                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 37:BQ:21:THR:C     | 37:BQ:23:GLY:N     | 2.78                     | 0.41              |
| 38:BR:95:THR:O     | 38:BR:95:THR:CG2   | 2.68                     | 0.41              |
| 40:BT:76:PHE:HA    | 40:BT:77:PRO:HD3   | 1.93                     | 0.41              |
| 41:BU:103:PRO:O    | 41:BU:106:PHE:HB3  | 2.21                     | 0.41              |
| 43:BW:88:ARG:HB2   | 43:BW:92:ARG:HB2   | 2.03                     | 0.41              |
| 45:BY:86:ARG:CZ    | 45:BY:95:LYS:HZ2   | 2.33                     | 0.41              |
| 48:B1:29:GLY:C     | 48:B1:30:VAL:CG2   | 2.94                     | 0.41              |
| 49:B2:47:ASN:O     | 49:B2:48:HIS:C     | 2.63                     | 0.41              |
| 56:B9:7:VAL:HG13   | 56:B9:34:GLN:CD    | 2.45                     | 0.41              |
| 1:CA:177:C:OP1     | 20:CT:65:LYS:NZ    | 2.34                     | 0.41              |
| 1:CA:529:G:H4'     | 1:CA:533:A:C4      | 2.56                     | 0.41              |
| 1:CA:1308:U:H2'    | 1:CA:1309:G:C8     | 2.56                     | 0.41              |
| 1:CA:1321:C:H3'    | 1:CA:1322:C:H5''   | 2.02                     | 0.41              |
| 3:CC:90:GLU:HA     | 3:CC:90:GLU:OE1    | 2.20                     | 0.41              |
| 5:CE:147:ASP:OD2   | 5:CE:147:ASP:N     | 2.47                     | 0.41              |
| 12:CL:104:VAL:O    | 12:CL:105:TYR:C    | 2.64                     | 0.41              |
| 13:CM:108:ARG:HH11 | 13:CM:108:ARG:CG   | 2.33                     | 0.41              |
| 14:CN:7:ILE:HG12   | 14:CN:7:ILE:H      | 1.69                     | 0.41              |
| 15:CO:57:LEU:HD23  | 15:CO:57:LEU:HA    | 1.81                     | 0.41              |
| 16:CP:36:ILE:CG1   | 16:CP:37:GLY:N     | 2.83                     | 0.41              |
| 17:CQ:74:LEU:HD22  | 17:CQ:74:LEU:HA    | 1.87                     | 0.41              |
| 19:CS:60:VAL:HG22  | 19:CS:61:TYR:O     | 2.20                     | 0.41              |
| 23:CW:36:A:C6      | 23:CW:37:A:C6      | 3.08                     | 0.41              |
| 25:DA:42:G:H2'     | 25:DA:43:A:O4'     | 2.21                     | 0.41              |
| 25:DA:144:C:H2'    | 25:DA:145:G:C8     | 2.55                     | 0.41              |
| 25:DA:9271:G:C4    | 25:DA:9272:G:C8    | 3.08                     | 0.41              |
| 25:DA:458:G:O3'    | 25:DA:459:U:C6     | 2.70                     | 0.41              |
| 25:DA:1047:G:C5    | 25:DA:1110:G:O6    | 2.73                     | 0.41              |
| 25:DA:1500:G:O2'   | 28:DD:100:GLY:O    | 2.32                     | 0.41              |
| 25:DA:1665:A:H4'   | 35:DO:67:LYS:HB2   | 2.01                     | 0.41              |
| 25:DA:1999:C:H5''  | 25:DA:2723:C:O2'   | 2.21                     | 0.41              |
| 25:DA:2282:G:H5''  | 25:DA:2283:C:O4'   | 2.21                     | 0.41              |
| 29:DE:108:SER:OG   | 29:DE:163:GLU:HG2  | 2.20                     | 0.41              |
| 29:DE:116:VAL:HG23 | 29:DE:120:TRP:HB2  | 2.03                     | 0.41              |
| 30:DF:150:GLY:HA2  | 30:DF:172:TRP:CE3  | 2.56                     | 0.41              |
| 31:DG:39:ILE:HB    | 31:DG:92:VAL:HG13  | 2.03                     | 0.41              |
| 31:DG:85:GLY:O     | 31:DG:86:MET:CB    | 2.68                     | 0.41              |
| 31:DG:110:ALA:C    | 31:DG:112:PRO:CD   | 2.93                     | 0.41              |
| 33:DI:144:VAL:C    | 33:DI:145:VAL:HG22 | 2.46                     | 0.41              |
| 33:DI:144:VAL:O    | 33:DI:145:VAL:HG22 | 2.21                     | 0.41              |
| 36:DP:20:GLY:HA2   | 36:DP:27:HIS:O     | 2.21                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 36:DP:42:SER:O    | 36:DP:44:GLY:N    | 2.54                     | 0.41              |
| 37:DQ:33:GLY:HA2  | 37:DQ:105:GLU:HA  | 2.02                     | 0.41              |
| 38:DR:16:HIS:O    | 38:DR:17:ARG:C    | 2.63                     | 0.41              |
| 39:DS:106:ARG:HG3 | 39:DS:106:ARG:H   | 1.67                     | 0.41              |
| 40:DT:28:VAL:HG22 | 40:DT:46:GLU:HG3  | 2.01                     | 0.41              |
| 40:DT:28:VAL:HG11 | 40:DT:46:GLU:OE1  | 2.21                     | 0.41              |
| 44:DX:35:THR:HG22 | 44:DX:36:LYS:N    | 2.36                     | 0.41              |
| 44:DX:42:ALA:O    | 44:DX:46:ALA:HB2  | 2.21                     | 0.41              |
| 48:D1:51:VAL:HG21 | 48:D1:74:VAL:HG21 | 2.03                     | 0.41              |
| 49:D2:3:LEU:CD2   | 49:D2:7:ARG:HH11  | 2.33                     | 0.41              |
| 49:D2:45:SER:O    | 49:D2:46:GLN:NE2  | 2.53                     | 0.41              |
| 53:D6:30:THR:HB   | 53:D6:31:PRO:CD   | 2.42                     | 0.41              |
| 54:D7:23:ARG:O    | 54:D7:28:ARG:NH1  | 2.53                     | 0.41              |
| 55:D8:14:VAL:CG2  | 55:D8:22:VAL:CG1  | 2.99                     | 0.41              |
| 1:AA:246:A:O2'    | 1:AA:247:G:O4'    | 2.35                     | 0.41              |
| 1:AA:371:G:O2'    | 1:AA:373:A:N7     | 2.54                     | 0.41              |
| 1:AA:617:G:H1     | 1:AA:623:C:H42    | 1.68                     | 0.41              |
| 1:AA:644:G:H5'    | 8:AH:92:ARG:NH2   | 2.36                     | 0.41              |
| 1:AA:913:A:HO2'   | 1:AA:914:A:P      | 2.42                     | 0.41              |
| 1:AA:972:C:O3'    | 10:AJ:57:LYS:HG3  | 2.21                     | 0.41              |
| 1:AA:1125:U:C2'   | 1:AA:1126:U:OP2   | 2.68                     | 0.41              |
| 1:AA:1151:A:H2'   | 1:AA:1152:A:H8    | 1.83                     | 0.41              |
| 1:AA:1329:A:OP1   | 13:AM:26:GLY:HA3  | 2.21                     | 0.41              |
| 1:AA:1399:C:C2    | 1:AA:1502:A:N6    | 2.89                     | 0.41              |
| 2:AB:69:LEU:HD13  | 2:AB:70:PHE:N     | 2.36                     | 0.41              |
| 2:AB:185:ILE:HG12 | 2:AB:199:TYR:HB2  | 2.02                     | 0.41              |
| 3:AC:70:VAL:O     | 3:AC:106:VAL:HG23 | 2.20                     | 0.41              |
| 3:AC:101:LEU:C    | 3:AC:101:LEU:CD2  | 2.93                     | 0.41              |
| 3:AC:150:LYS:HG3  | 3:AC:169:ALA:HB2  | 2.02                     | 0.41              |
| 3:AC:178:LEU:HD13 | 3:AC:178:LEU:HA   | 1.94                     | 0.41              |
| 4:AD:179:GLU:C    | 4:AD:181:MET:H    | 2.29                     | 0.41              |
| 5:AE:76:ILE:HG22  | 5:AE:93:PRO:HB3   | 2.01                     | 0.41              |
| 7:AG:20:ASP:HB3   | 7:AG:23:VAL:HB    | 2.03                     | 0.41              |
| 7:AG:113:GLU:HB2  | 7:AG:118:VAL:HG21 | 2.02                     | 0.41              |
| 8:AH:35:ILE:HG23  | 8:AH:111:ILE:CD1  | 2.50                     | 0.41              |
| 8:AH:85:ARG:HD3   | 8:AH:85:ARG:C     | 2.46                     | 0.41              |
| 9:AI:53:VAL:O     | 9:AI:54:ASP:CB    | 2.68                     | 0.41              |
| 9:AI:126:SER:O    | 9:AI:127:LYS:CB   | 2.69                     | 0.41              |
| 13:AM:23:TYR:HE1  | 13:AM:71:ARG:HA   | 1.86                     | 0.41              |
| 13:AM:57:ARG:HH12 | 51:B4:60:GLU:CA   | 2.33                     | 0.41              |
| 13:AM:57:ARG:NH1  | 51:B4:60:GLU:CB   | 2.84                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 14:AN:36:PHE:CD1   | 14:AN:36:PHE:C     | 2.98                     | 0.41              |
| 14:AN:42:ILE:O     | 14:AN:43:CYS:C     | 2.64                     | 0.41              |
| 19:AS:13:ASP:O     | 19:AS:14:HIS:C     | 2.64                     | 0.41              |
| 24:AX:15:A:H8      | 24:AX:15:A:O5'     | 2.04                     | 0.41              |
| 25:BA:118:A:N3     | 25:BA:178:G:H1'    | 2.35                     | 0.41              |
| 25:BA:214:G:H1'    | 25:BA:216:A:O2'    | 2.21                     | 0.41              |
| 25:BA:448:U:O4     | 25:BA:583:G:H1'    | 2.19                     | 0.41              |
| 25:BA:662:G:P      | 36:BP:15:ARG:HE    | 2.44                     | 0.41              |
| 25:BA:700:G:H2'    | 25:BA:701:G:O4'    | 2.21                     | 0.41              |
| 25:BA:747:U:C4     | 25:BA:2613:U:C4    | 3.08                     | 0.41              |
| 25:BA:747:U:C6     | 52:B5:2:ALA:HB3    | 2.56                     | 0.41              |
| 25:BA:959:A:C6     | 25:BA:960:A:C6     | 3.09                     | 0.41              |
| 25:BA:1051:G:O2'   | 25:BA:1052:C:OP1   | 2.31                     | 0.41              |
| 25:BA:1445:A:N3    | 25:BA:1445:A:H2'   | 2.35                     | 0.41              |
| 25:BA:1554:A:H5''  | 25:BA:1555:G:OP2   | 2.20                     | 0.41              |
| 25:BA:1826:G:H4'   | 28:BD:242:ARG:NH2  | 2.22                     | 0.41              |
| 25:BA:2061:G:O2'   | 25:BA:2062:A:OP2   | 2.30                     | 0.41              |
| 25:BA:2178:C:H1'   | 27:BC:172:HIS:CB   | 2.50                     | 0.41              |
| 25:BA:2228:G:C5    | 25:BA:2229:C:C4    | 3.09                     | 0.41              |
| 25:BA:2277:G:H5''  | 37:BQ:87:LYS:HB3   | 2.03                     | 0.41              |
| 25:BA:2287:A:N6    | 25:BA:2289:G:C2    | 2.88                     | 0.41              |
| 25:BA:2345:G:O2'   | 25:BA:2382:G:H5'   | 2.20                     | 0.41              |
| 25:BA:2350:C:H2'   | 25:BA:2351:G:O4'   | 2.21                     | 0.41              |
| 25:BA:2461:C:H2'   | 25:BA:2462:U:C6    | 2.56                     | 0.41              |
| 25:BA:2702:U:H6    | 25:BA:2702:U:OP1   | 2.03                     | 0.41              |
| 25:BA:2892:A:C5    | 25:BA:2893:G:H1'   | 2.55                     | 0.41              |
| 26:BB:50:G:OP2     | 39:BS:62:LYS:HG3   | 2.21                     | 0.41              |
| 28:BD:198:ASN:O    | 28:BD:198:ASN:CG   | 2.63                     | 0.41              |
| 29:BE:201:THR:HG21 | 29:BE:203:LYS:HG2  | 2.03                     | 0.41              |
| 30:BF:36:VAL:HB    | 30:BF:183:VAL:HG21 | 2.01                     | 0.41              |
| 30:BF:42:ALA:O     | 30:BF:45:ARG:CB    | 2.69                     | 0.41              |
| 31:BG:4:ASP:C      | 31:BG:5:VAL:CG1    | 2.94                     | 0.41              |
| 31:BG:19:LEU:HD21  | 31:BG:171:ALA:HB1  | 2.01                     | 0.41              |
| 31:BG:60:LEU:CD1   | 31:BG:92:VAL:HG11  | 2.50                     | 0.41              |
| 32:BH:55:PRO:HB2   | 32:BH:56:SER:H     | 1.61                     | 0.41              |
| 32:BH:159:GLU:HG3  | 32:BH:160:LYS:HG2  | 2.02                     | 0.41              |
| 33:BI:77:LEU:CD2   | 33:BI:101:LEU:HA   | 2.50                     | 0.41              |
| 33:BI:77:LEU:HD13  | 33:BI:105:HIS:NE2  | 2.36                     | 0.41              |
| 34:BN:133:GLN:HG2  | 34:BN:134:ARG:N    | 2.36                     | 0.41              |
| 35:BO:35:VAL:HG21  | 35:BO:69:ILE:HD13  | 2.01                     | 0.41              |
| 35:BO:64:ARG:HD3   | 35:BO:79:PHE:CD2   | 2.55                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 36:BP:42:SER:O     | 36:BP:44:GLY:N     | 2.54                     | 0.41              |
| 36:BP:71:VAL:CG2   | 36:BP:72:PRO:CD    | 2.99                     | 0.41              |
| 36:BP:79:ARG:O     | 36:BP:111:ARG:CB   | 2.59                     | 0.41              |
| 36:BP:95:VAL:HG23  | 36:BP:125:VAL:HG23 | 2.03                     | 0.41              |
| 36:BP:127:ALA:HB3  | 36:BP:130:PHE:CE2  | 2.56                     | 0.41              |
| 37:BQ:42:ILE:HD13  | 37:BQ:97:VAL:CB    | 2.48                     | 0.41              |
| 37:BQ:109:VAL:HG13 | 37:BQ:113:GLN:HB3  | 2.02                     | 0.41              |
| 38:BR:103:ARG:HB2  | 38:BR:109:ALA:N    | 2.36                     | 0.41              |
| 39:BS:26:LEU:HG    | 39:BS:39:ILE:HD11  | 2.03                     | 0.41              |
| 39:BS:86:ALA:N     | 39:BS:106:ARG:HG3  | 2.36                     | 0.41              |
| 40:BT:65:LYS:O     | 40:BT:72:VAL:N     | 2.49                     | 0.41              |
| 40:BT:66:VAL:HG22  | 40:BT:71:GLY:HA2   | 2.03                     | 0.41              |
| 40:BT:94:ALA:C     | 40:BT:96:ARG:H     | 2.29                     | 0.41              |
| 43:BW:48:ALA:C     | 43:BW:50:VAL:N     | 2.78                     | 0.41              |
| 46:BZ:5:LEU:HD12   | 46:BZ:6:LYS:N      | 2.28                     | 0.41              |
| 46:BZ:97:GLU:HA    | 46:BZ:126:VAL:O    | 2.21                     | 0.41              |
| 48:B1:23:LYS:HD3   | 48:B1:28:GLY:CA    | 2.50                     | 0.41              |
| 49:B2:16:LEU:O     | 49:B2:17:SER:CB    | 2.68                     | 0.41              |
| 50:B3:5:LYS:HG3    | 50:B3:36:VAL:HG12  | 2.02                     | 0.41              |
| 50:B3:44:ARG:O     | 50:B3:48:GLU:HG2   | 2.21                     | 0.41              |
| 50:B3:58:VAL:C     | 50:B3:59:VAL:HG22  | 2.45                     | 0.41              |
| 52:B5:46:CYS:HB3   | 52:B5:49:CYS:HB2   | 2.03                     | 0.41              |
| 1:CA:45:U:H2'      | 1:CA:46:G:C8       | 2.56                     | 0.41              |
| 1:CA:59:A:H3'      | 1:CA:331:G:H22     | 1.86                     | 0.41              |
| 1:CA:267:C:OP2     | 17:CQ:67:LYS:HD2   | 2.21                     | 0.41              |
| 1:CA:985:C:H2'     | 1:CA:986:A:C8      | 2.56                     | 0.41              |
| 1:CA:1315:U:H2'    | 1:CA:1316:G:O4'    | 2.21                     | 0.41              |
| 1:CA:1456:G:C2     | 1:CA:1457:G:C4     | 3.09                     | 0.41              |
| 2:CB:157:ARG:O     | 2:CB:158:LEU:C     | 2.63                     | 0.41              |
| 2:CB:216:SER:C     | 2:CB:218:ALA:N     | 2.78                     | 0.41              |
| 3:CC:114:PRO:O     | 3:CC:118:GLN:HG3   | 2.21                     | 0.41              |
| 4:CD:15:GLU:HG2    | 4:CD:63:LYS:HA     | 2.02                     | 0.41              |
| 4:CD:66:ARG:C      | 4:CD:69:GLY:H      | 2.28                     | 0.41              |
| 4:CD:172:PRO:C     | 4:CD:174:LEU:H     | 2.29                     | 0.41              |
| 4:CD:176:LEU:HD12  | 4:CD:177:ASP:N     | 2.14                     | 0.41              |
| 6:CF:23:LYS:HE2    | 6:CF:23:LYS:HB3    | 1.71                     | 0.41              |
| 7:CG:22:LEU:HD12   | 7:CG:101:LEU:HD11  | 2.02                     | 0.41              |
| 7:CG:25:ALA:HA     | 7:CG:28:ASN:HD22   | 1.86                     | 0.41              |
| 8:CH:22:GLU:O      | 8:CH:63:LEU:HD22   | 2.20                     | 0.41              |
| 8:CH:29:SER:HB3    | 8:CH:32:LYS:CG     | 2.50                     | 0.41              |
| 8:CH:44:PHE:HE2    | 8:CH:109:ILE:HG21  | 1.85                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 8:CH:89:PRO:HA    | 8:CH:92:ARG:NH1    | 2.35                     | 0.41              |
| 10:CJ:13:HIS:O    | 10:CJ:13:HIS:CG    | 2.74                     | 0.41              |
| 10:CJ:54:PHE:CG   | 10:CJ:55:LYS:HG2   | 2.56                     | 0.41              |
| 11:CK:81:ASP:OD2  | 11:CK:107:SER:HB3  | 2.20                     | 0.41              |
| 11:CK:85:ARG:HG2  | 11:CK:111:ASP:O    | 2.21                     | 0.41              |
| 11:CK:110:ASP:OD2 | 11:CK:110:ASP:C    | 2.64                     | 0.41              |
| 12:CL:77:LEU:HA   | 12:CL:77:LEU:HD23  | 1.70                     | 0.41              |
| 13:CM:83:ASP:N    | 13:CM:93:ARG:NH2   | 2.65                     | 0.41              |
| 13:CM:108:ARG:H   | 13:CM:108:ARG:CD   | 2.25                     | 0.41              |
| 15:CO:56:LEU:HD21 | 25:DA:715:G:C4     | 2.55                     | 0.41              |
| 16:CP:79:VAL:HB   | 16:CP:80:PHE:HD1   | 1.86                     | 0.41              |
| 18:CR:45:SER:C    | 18:CR:47:THR:N     | 2.79                     | 0.41              |
| 22:CV:41:C:C2'    | 22:CV:42:C:C5'     | 2.96                     | 0.41              |
| 23:CW:59:U:C4     | 23:CW:60:U:C4      | 3.09                     | 0.41              |
| 25:DA:49:A:H5''   | 25:DA:50:U:O5'     | 2.20                     | 0.41              |
| 25:DA:77:C:O4'    | 49:D2:62:THR:HG21  | 2.21                     | 0.41              |
| 25:DA:241:A:O3'   | 25:DA:242:G:C4'    | 2.69                     | 0.41              |
| 25:DA:247:G:N7    | 25:DA:249:C:C2     | 2.88                     | 0.41              |
| 25:DA:9271:G:C2   | 25:DA:9272:G:C4    | 3.09                     | 0.41              |
| 25:DA:272(E):G:C2 | 25:DA:364:C:N3     | 2.89                     | 0.41              |
| 25:DA:329:G:H4'   | 25:DA:330:A:OP1    | 2.19                     | 0.41              |
| 25:DA:818:G:H4'   | 25:DA:838:C:O3'    | 2.21                     | 0.41              |
| 25:DA:978:G:C2    | 25:DA:986:C:C2     | 3.09                     | 0.41              |
| 25:DA:1153:C:H2'  | 25:DA:1154:G:O4'   | 2.21                     | 0.41              |
| 25:DA:1340:U:H1'  | 25:DA:1603:A:C5'   | 2.51                     | 0.41              |
| 25:DA:1427:A:C4'  | 25:DA:1428:C:OP1   | 2.69                     | 0.41              |
| 25:DA:1567:A:H1'  | 25:DA:1568:G:N1    | 2.36                     | 0.41              |
| 25:DA:1667:G:N2   | 25:DA:1992:G:OP2   | 2.33                     | 0.41              |
| 25:DA:2173:A:H3'  | 25:DA:2174:C:C6    | 2.56                     | 0.41              |
| 25:DA:2177:C:H1'  | 27:DC:44:HIS:CD2   | 2.55                     | 0.41              |
| 25:DA:2197:U:O2'  | 25:DA:2198:A:C8    | 2.69                     | 0.41              |
| 26:DB:60:C:H2'    | 26:DB:61:G:H8      | 1.86                     | 0.41              |
| 27:DC:58:VAL:HB   | 27:DC:59:ARG:H     | 1.76                     | 0.41              |
| 27:DC:147:PHE:O   | 27:DC:148:ASN:CB   | 2.69                     | 0.41              |
| 28:DD:10:THR:CG2  | 28:DD:13:ARG:HB3   | 2.29                     | 0.41              |
| 28:DD:35:LYS:HB2  | 28:DD:36:PRO:HD3   | 2.03                     | 0.41              |
| 28:DD:153:ALA:C   | 28:DD:154:LYS:HG2  | 2.45                     | 0.41              |
| 29:DE:37:ARG:HA   | 29:DE:42:ASP:OD2   | 2.21                     | 0.41              |
| 29:DE:84:PHE:O    | 29:DE:84:PHE:CG    | 2.73                     | 0.41              |
| 29:DE:144:ARG:HB3 | 29:DE:145:LYS:H    | 1.32                     | 0.41              |
| 29:DE:176:ILE:N   | 29:DE:176:ILE:HD12 | 2.36                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 30:DF:188:ARG:CG  | 36:DP:3:LEU:HD11  | 2.35                     | 0.41              |
| 31:DG:16:ARG:NH1  | 31:DG:16:ARG:CG   | 2.75                     | 0.41              |
| 31:DG:49:ASP:HB3  | 31:DG:52:ILE:CG1  | 2.51                     | 0.41              |
| 31:DG:60:LEU:C    | 31:DG:62:LEU:N    | 2.79                     | 0.41              |
| 32:DH:55:PRO:HG2  | 32:DH:61:HIS:CE1  | 2.55                     | 0.41              |
| 32:DH:59:ARG:NH1  | 32:DH:59:ARG:CG   | 2.83                     | 0.41              |
| 32:DH:86:GLU:HB2  | 32:DH:87:LEU:H    | 1.56                     | 0.41              |
| 32:DH:89:ILE:CD1  | 32:DH:89:ILE:N    | 2.84                     | 0.41              |
| 33:DI:29:TYR:O    | 33:DI:33:ARG:HB2  | 2.20                     | 0.41              |
| 33:DI:37:VAL:CG1  | 33:DI:38:LEU:N    | 2.84                     | 0.41              |
| 33:DI:94:ALA:O    | 33:DI:95:LYS:C    | 2.64                     | 0.41              |
| 34:DN:18:ALA:O    | 34:DN:21:LYS:N    | 2.53                     | 0.41              |
| 36:DP:52:GLU:O    | 36:DP:53:GLY:C    | 2.64                     | 0.41              |
| 36:DP:111:ARG:HA  | 36:DP:128:HIS:CE1 | 2.55                     | 0.41              |
| 37:DQ:35:VAL:HA   | 37:DQ:102:VAL:HA  | 2.02                     | 0.41              |
| 37:DQ:38:GLU:HB2  | 37:DQ:39:PRO:HD2  | 2.03                     | 0.41              |
| 37:DQ:137:TYR:O   | 37:DQ:138:ASP:C   | 2.63                     | 0.41              |
| 38:DR:18:LEU:HD11 | 38:DR:22:ARG:NH2  | 2.36                     | 0.41              |
| 39:DS:52:SER:O    | 39:DS:56:LEU:HD21 | 2.21                     | 0.41              |
| 40:DT:19:LEU:HA   | 40:DT:20:PRO:HD3  | 1.84                     | 0.41              |
| 40:DT:24:PRO:HD2  | 40:DT:52:ILE:HD12 | 1.95                     | 0.41              |
| 40:DT:50:ILE:HA   | 40:DT:99:LEU:CD1  | 2.51                     | 0.41              |
| 40:DT:65:LYS:HD2  | 40:DT:65:LYS:HA   | 1.65                     | 0.41              |
| 40:DT:93:ARG:O    | 40:DT:94:ALA:C    | 2.63                     | 0.41              |
| 41:DU:61:TRP:O    | 41:DU:64:ARG:N    | 2.54                     | 0.41              |
| 42:DV:98:GLU:HB3  | 42:DV:100:ARG:HG3 | 2.02                     | 0.41              |
| 43:DW:20:VAL:HG11 | 43:DW:44:ALA:HA   | 2.03                     | 0.41              |
| 45:DY:65:ALA:HA   | 45:DY:66:PRO:HD3  | 1.93                     | 0.41              |
| 46:DZ:29:TYR:OH   | 46:DZ:87:ASP:OD1  | 2.36                     | 0.41              |
| 48:D1:66:HIS:O    | 48:D1:67:ILE:C    | 2.64                     | 0.41              |
| 48:D1:90:ILE:O    | 48:D1:93:GLU:N    | 2.54                     | 0.41              |
| 48:D1:93:GLU:C    | 48:D1:95:LEU:H    | 2.29                     | 0.41              |
| 49:D2:16:LEU:HD23 | 49:D2:16:LEU:HA   | 1.82                     | 0.41              |
| 55:D8:23:VAL:CG1  | 55:D8:46:ARG:NH1  | 2.82                     | 0.41              |
| 1:AA:38:G:H4'     | 1:AA:547:A:N6     | 2.35                     | 0.41              |
| 1:AA:551:U:H2'    | 1:AA:552:U:C6     | 2.56                     | 0.41              |
| 1:AA:811:C:O2'    | 1:AA:901:A:N1     | 2.49                     | 0.41              |
| 1:AA:1189:C:H5''  | 3:AC:5:ILE:HG21   | 2.03                     | 0.41              |
| 2:AB:134:GLU:OE1  | 2:AB:137:ARG:HD2  | 2.21                     | 0.41              |
| 2:AB:236:TYR:CD1  | 2:AB:236:TYR:N    | 2.88                     | 0.41              |
| 3:AC:8:ILE:O      | 3:AC:10:PHE:N     | 2.54                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:AD:63:LYS:O     | 4:AD:64:LEU:C     | 2.64                     | 0.41              |
| 4:AD:140:VAL:HG12 | 4:AD:141:ARG:N    | 2.36                     | 0.41              |
| 4:AD:168:ARG:HH21 | 6:CF:18:GLN:HE21  | 1.66                     | 0.41              |
| 7:AG:15:ASP:CA    | 7:AG:24:THR:CG2   | 2.99                     | 0.41              |
| 7:AG:145:ALA:C    | 7:AG:147:ALA:N    | 2.75                     | 0.41              |
| 8:AH:11:THR:O     | 8:AH:11:THR:HG22  | 2.21                     | 0.41              |
| 11:AK:111:ASP:HA  | 18:AR:84:LYS:HD2  | 2.02                     | 0.41              |
| 11:AK:124:LYS:HD2 | 11:AK:125:PHE:CE1 | 2.43                     | 0.41              |
| 12:AL:53:ARG:NH1  | 12:AL:92:ASP:HB3  | 2.35                     | 0.41              |
| 13:AM:18:ALA:CB   | 13:AM:45:VAL:HG21 | 2.51                     | 0.41              |
| 15:AO:47:LYS:H    | 15:AO:47:LYS:HG2  | 1.58                     | 0.41              |
| 15:AO:70:LEU:O    | 15:AO:71:GLN:C    | 2.64                     | 0.41              |
| 19:AS:19:VAL:HG11 | 19:AS:44:MET:HG3  | 2.02                     | 0.41              |
| 19:AS:45:VAL:HG23 | 19:AS:46:GLY:N    | 2.35                     | 0.41              |
| 23:AW:15:G:H21    | 23:AW:59:U:H1'    | 1.86                     | 0.41              |
| 25:BA:601:C:C4'   | 30:BF:104:LYS:HZ3 | 2.34                     | 0.41              |
| 25:BA:729:G:P     | 28:BD:208:LYS:NZ  | 2.94                     | 0.41              |
| 25:BA:810:U:H6    | 25:BA:810:U:O5'   | 2.04                     | 0.41              |
| 25:BA:1012:U:C4   | 34:BN:28:THR:HG21 | 2.55                     | 0.41              |
| 25:BA:1819:A:C1'  | 25:BA:1821:A:C6   | 2.91                     | 0.41              |
| 25:BA:1902:C:C2'  | 28:BD:244:ARG:HG3 | 2.51                     | 0.41              |
| 25:BA:1964:G:O2'  | 25:BA:1967:C:OP2  | 2.39                     | 0.41              |
| 25:BA:2077:A:H2'  | 25:BA:2078:C:H6   | 1.86                     | 0.41              |
| 25:BA:2490:G:H4'  | 25:BA:2491:U:O5'  | 2.21                     | 0.41              |
| 25:BA:2579:C:H2'  | 25:BA:2580:U:O4'  | 2.21                     | 0.41              |
| 25:BA:2691:C:C5   | 25:BA:2872:G:N1   | 2.89                     | 0.41              |
| 26:BB:51:G:H2'    | 26:BB:52:A:H1'    | 2.03                     | 0.41              |
| 26:BB:105:A:OP1   | 46:BZ:72:ARG:NH1  | 2.54                     | 0.41              |
| 29:BE:91:VAL:CG1  | 29:BE:95:ILE:HG12 | 2.48                     | 0.41              |
| 31:BG:11:TYR:O    | 31:BG:16:ARG:HB2  | 2.21                     | 0.41              |
| 31:BG:117:PHE:HE1 | 31:BG:119:GLY:C   | 2.28                     | 0.41              |
| 31:BG:117:PHE:CD1 | 31:BG:119:GLY:N   | 2.83                     | 0.41              |
| 32:BH:88:LEU:HD23 | 32:BH:165:ALA:HA  | 2.03                     | 0.41              |
| 33:BI:5:LEU:N     | 33:BI:5:LEU:HD12  | 2.36                     | 0.41              |
| 34:BN:58:ASP:O    | 34:BN:59:LYS:HB2  | 2.21                     | 0.41              |
| 36:BP:88:LEU:HD11 | 36:BP:95:VAL:CB   | 2.51                     | 0.41              |
| 37:BQ:37:LEU:HD23 | 37:BQ:37:LEU:HA   | 1.90                     | 0.41              |
| 41:BU:94:ASN:C    | 41:BU:94:ASN:ND2  | 2.79                     | 0.41              |
| 44:BX:13:LEU:HA   | 44:BX:18:TYR:HE1  | 1.86                     | 0.41              |
| 46:BZ:103:ARG:O   | 46:BZ:138:GLU:HA  | 2.21                     | 0.41              |
| 48:B1:49:VAL:HG21 | 48:B1:67:ILE:HG23 | 2.01                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 48:B1:84:GLY:O    | 48:B1:86:SER:N    | 2.54                     | 0.41              |
| 1:CA:119:A:H5''   | 1:CA:120:A:O5'    | 2.21                     | 0.41              |
| 1:CA:160:A:N6     | 1:CA:347:G:H1'    | 2.36                     | 0.41              |
| 1:CA:252:U:H2'    | 1:CA:275:G:N2     | 2.36                     | 0.41              |
| 1:CA:751:U:H4'    | 15:CO:24:SER:HA   | 2.03                     | 0.41              |
| 1:CA:1191:A:H5''  | 3:CC:4:LYS:HZ1    | 1.86                     | 0.41              |
| 1:CA:1336:C:H1'   | 1:CA:1337:G:N1    | 2.36                     | 0.41              |
| 1:CA:1414:U:H2'   | 1:CA:1415:G:H8    | 1.86                     | 0.41              |
| 2:CB:224:GLN:HA   | 2:CB:229:VAL:CG2  | 2.48                     | 0.41              |
| 3:CC:130:VAL:O    | 3:CC:130:VAL:HG12 | 2.21                     | 0.41              |
| 3:CC:144:SER:O    | 3:CC:144:SER:OG   | 2.39                     | 0.41              |
| 4:CD:4:TYR:O      | 4:CD:5:ILE:CB     | 2.65                     | 0.41              |
| 4:CD:108:LEU:HD12 | 4:CD:108:LEU:HA   | 1.84                     | 0.41              |
| 5:CE:90:VAL:C     | 5:CE:91:LEU:HD13  | 2.46                     | 0.41              |
| 6:CF:9:VAL:HB     | 6:CF:87:ARG:HB2   | 2.03                     | 0.41              |
| 6:CF:100:ASN:ND2  | 18:CR:26:LEU:O    | 2.53                     | 0.41              |
| 7:CG:126:ASP:O    | 7:CG:129:GLU:HB3  | 2.21                     | 0.41              |
| 8:CH:81:HIS:HB2   | 8:CH:138:TRP:OXT  | 2.21                     | 0.41              |
| 8:CH:97:VAL:HG13  | 8:CH:98:LYS:N     | 2.36                     | 0.41              |
| 9:CI:33:PHE:HD2   | 9:CI:34:ASN:OD1   | 2.03                     | 0.41              |
| 9:CI:104:ARG:O    | 9:CI:104:ARG:HD2  | 2.21                     | 0.41              |
| 10:CJ:78:ASN:ND2  | 10:CJ:80:LYS:CB   | 2.65                     | 0.41              |
| 11:CK:21:ILE:CG1  | 11:CK:30:VAL:HG12 | 2.50                     | 0.41              |
| 12:CL:58:VAL:HG21 | 12:CL:85:ILE:HD11 | 2.04                     | 0.41              |
| 14:CN:23:ARG:NH1  | 14:CN:30:ALA:HB2  | 2.35                     | 0.41              |
| 17:CQ:95:TYR:HD1  | 17:CQ:95:TYR:HA   | 1.73                     | 0.41              |
| 25:DA:242:G:O2'   | 25:DA:243:U:P     | 2.78                     | 0.41              |
| 25:DA:307:G:H21   | 25:DA:330:A:N6    | 2.14                     | 0.41              |
| 25:DA:675:A:N3    | 25:DA:2443:C:O2'  | 2.51                     | 0.41              |
| 25:DA:685:A:O2'   | 25:DA:689:A:N6    | 2.54                     | 0.41              |
| 25:DA:807:U:O2'   | 25:DA:2060:A:N1   | 2.40                     | 0.41              |
| 25:DA:846:C:O2'   | 25:DA:847:U:O5'   | 2.31                     | 0.41              |
| 25:DA:863:A:H2'   | 25:DA:864:G:C8    | 2.56                     | 0.41              |
| 25:DA:1268:A:H2'  | 25:DA:1269:A:O4'  | 2.21                     | 0.41              |
| 25:DA:1472:A:H2'  | 25:DA:1473:G:O4'  | 2.21                     | 0.41              |
| 25:DA:1694:C:O4'  | 25:DA:1695:G:C2   | 2.74                     | 0.41              |
| 25:DA:1971:A:N9   | 28:DD:241:PRO:HB3 | 2.36                     | 0.41              |
| 25:DA:2123:G:H2'  | 25:DA:2124:G:C8   | 2.56                     | 0.41              |
| 25:DA:2735:G:H2'  | 25:DA:2736:G:C8   | 2.56                     | 0.41              |
| 29:DE:54:GLN:O    | 29:DE:75:VAL:HG23 | 2.21                     | 0.41              |
| 32:DH:83:TYR:HA   | 32:DH:135:GLY:H   | 1.86                     | 0.41              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 32:DH:152:ARG:CG   | 32:DH:153:LYS:HE3 | 2.50                     | 0.41              |
| 33:DI:40:THR:C     | 33:DI:42:SER:H    | 2.29                     | 0.41              |
| 33:DI:56:LYS:HG3   | 33:DI:57:ARG:N    | 2.34                     | 0.41              |
| 34:DN:104:LYS:C    | 34:DN:106:MET:H   | 2.29                     | 0.41              |
| 36:DP:55:ARG:O     | 36:DP:57:THR:N    | 2.54                     | 0.41              |
| 37:DQ:57:HIS:CE1   | 37:DQ:116:GLU:HB3 | 2.56                     | 0.41              |
| 38:DR:41:ALA:O     | 38:DR:44:LEU:N    | 2.54                     | 0.41              |
| 42:DV:30:GLY:O     | 42:DV:60:GLU:OE2  | 2.39                     | 0.41              |
| 45:DY:38:ILE:HG22  | 45:DY:66:PRO:CA   | 2.50                     | 0.41              |
| 46:DZ:112:ARG:HD2  | 46:DZ:112:ARG:N   | 2.36                     | 0.41              |
| 47:D0:23:VAL:HG22  | 47:D0:38:VAL:HG22 | 2.02                     | 0.41              |
| 51:D4:8:LYS:HE2    | 51:D4:8:LYS:HB2   | 1.81                     | 0.41              |
| 55:D8:6:THR:CB     | 55:D8:63:PRO:HG3  | 2.50                     | 0.41              |
| 55:D8:39:LYS:O     | 55:D8:43:GLN:HG3  | 2.21                     | 0.41              |
| 1:AA:920:U:H2'     | 1:AA:921:U:C6     | 2.55                     | 0.40              |
| 2:AB:24:TRP:CG     | 2:AB:40:HIS:NE2   | 2.89                     | 0.40              |
| 2:AB:30:ARG:C      | 2:AB:32:ILE:H     | 2.29                     | 0.40              |
| 2:AB:215:LEU:HA    | 2:AB:215:LEU:HD23 | 1.84                     | 0.40              |
| 4:AD:50:ARG:HA     | 4:AD:51:PRO:HD3   | 1.86                     | 0.40              |
| 4:AD:182:LYS:HB3   | 4:AD:182:LYS:HE2  | 1.79                     | 0.40              |
| 12:AL:7:ILE:O      | 12:AL:10:LEU:N    | 2.53                     | 0.40              |
| 12:AL:41:ARG:HG2   | 12:AL:42:THR:H    | 1.86                     | 0.40              |
| 12:AL:83:VAL:O     | 12:AL:83:VAL:HG12 | 2.21                     | 0.40              |
| 15:AO:64:ARG:HH11  | 15:AO:64:ARG:HG3  | 1.85                     | 0.40              |
| 23:AW:34:G:C8      | 24:AX:14:A:C2     | 3.08                     | 0.40              |
| 23:AW:64:A:C6      | 23:AW:65:G:C6     | 3.08                     | 0.40              |
| 25:BA:61:G:C5      | 49:B2:47:ASN:ND2  | 2.89                     | 0.40              |
| 25:BA:253:C:OP2    | 55:B8:5:LYS:NZ    | 2.52                     | 0.40              |
| 25:BA:297:C:H2'    | 25:BA:298:G:O4'   | 2.21                     | 0.40              |
| 25:BA:671:C:O2'    | 25:BA:672:C:H5'   | 2.20                     | 0.40              |
| 25:BA:900:A:H3'    | 25:BA:901:A:H8    | 1.85                     | 0.40              |
| 25:BA:1011:G:O2'   | 25:BA:1013:C:O4'  | 2.32                     | 0.40              |
| 25:BA:1142(A):A:C5 | 25:BA:1144:G:C5   | 3.09                     | 0.40              |
| 25:BA:1340:U:O2'   | 25:BA:1602:U:H5'' | 2.21                     | 0.40              |
| 25:BA:1568:G:O5'   | 28:BD:61:LEU:HB2  | 2.21                     | 0.40              |
| 25:BA:2126:A:OP2   | 25:BA:2126:A:C8   | 2.73                     | 0.40              |
| 25:BA:2865:U:H3'   | 25:BA:2866:U:O2   | 2.20                     | 0.40              |
| 26:BB:6:C:C2       | 26:BB:116:G:N2    | 2.89                     | 0.40              |
| 26:BB:60:C:H2'     | 26:BB:61:G:H8     | 1.86                     | 0.40              |
| 27:BC:64:LEU:O     | 27:BC:66:HIS:N    | 2.53                     | 0.40              |
| 33:BI:72:LEU:HD21  | 33:BI:138:ILE:HB  | 2.04                     | 0.40              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 36:BP:69:GLY:C     | 36:BP:70:GLN:CD     | 2.89                     | 0.40              |
| 38:BR:103:ARG:HA   | 38:BR:111:LEU:HD22  | 2.02                     | 0.40              |
| 41:BU:95:LEU:C     | 41:BU:97:ASP:H      | 2.28                     | 0.40              |
| 42:BV:59:ALA:HB1   | 42:BV:94:LEU:HD13   | 2.02                     | 0.40              |
| 45:BY:19:LYS:HG2   | 45:BY:20:TYR:CD2    | 2.56                     | 0.40              |
| 46:BZ:48:PHE:CZ    | 46:BZ:52:SER:HA     | 2.57                     | 0.40              |
| 47:B0:25:ARG:HA    | 47:B0:29:GLN:HE22   | 1.85                     | 0.40              |
| 53:B6:9:LEU:HD13   | 53:B6:28:ARG:HD2    | 2.03                     | 0.40              |
| 1:CA:119:A:H4'     | 1:CA:120:A:C8       | 2.56                     | 0.40              |
| 1:CA:484:G:H1'     | 1:CA:486:U:C4       | 2.56                     | 0.40              |
| 4:CD:22:LYS:HE3    | 4:CD:22:LYS:HB3     | 1.86                     | 0.40              |
| 8:CH:6:ILE:H       | 8:CH:6:ILE:HD12     | 1.86                     | 0.40              |
| 10:CJ:7:LYS:HB2    | 10:CJ:97:GLU:HB2    | 2.02                     | 0.40              |
| 12:CL:6:THR:HG23   | 12:CL:9:GLN:OE1     | 2.21                     | 0.40              |
| 12:CL:77:LEU:HD23  | 12:CL:77:LEU:N      | 2.34                     | 0.40              |
| 12:CL:126:LYS:CE   | 12:CL:127:GLU:H     | 2.34                     | 0.40              |
| 12:CL:126:LYS:HE2  | 12:CL:127:GLU:H     | 1.85                     | 0.40              |
| 15:CO:62:GLN:O     | 15:CO:65:ARG:N      | 2.52                     | 0.40              |
| 19:CS:28:LYS:HB3   | 19:CS:29:ARG:HD2    | 2.03                     | 0.40              |
| 20:CT:14:LYS:O     | 20:CT:15:ARG:C      | 2.62                     | 0.40              |
| 22:CV:54:G:C4      | 22:CV:55:U:H5       | 2.34                     | 0.40              |
| 25:DA:271(M):G:H2' | 25:DA:271(N):U:H5'' | 2.03                     | 0.40              |
| 25:DA:272(B):G:H2' | 25:DA:272(C):G:H8   | 1.87                     | 0.40              |
| 25:DA:1270:C:N4    | 25:DA:1648:C:H41    | 2.19                     | 0.40              |
| 25:DA:1412:A:H2'   | 25:DA:1413:G:C8     | 2.56                     | 0.40              |
| 25:DA:1550:C:H2'   | 25:DA:1551:C:H6     | 1.86                     | 0.40              |
| 25:DA:1688:U:H1'   | 25:DA:1701:A:C6     | 2.56                     | 0.40              |
| 25:DA:1838:C:N4    | 25:DA:1898:U:H2'    | 2.36                     | 0.40              |
| 25:DA:1995:U:H2'   | 25:DA:1996:C:C5     | 2.57                     | 0.40              |
| 25:DA:2359:C:H2'   | 25:DA:2360:A:O4'    | 2.20                     | 0.40              |
| 26:DB:13:A:H2'     | 26:DB:70:C:O2'      | 2.21                     | 0.40              |
| 27:DC:20:TYR:CG    | 27:DC:21:THR:N      | 2.88                     | 0.40              |
| 28:DD:250:TRP:HE3  | 28:DD:252:TRP:NE1   | 2.19                     | 0.40              |
| 29:DE:116:VAL:HG22 | 29:DE:122:PHE:HB2   | 2.03                     | 0.40              |
| 30:DF:36:VAL:HG11  | 30:DF:183:VAL:HG11  | 2.02                     | 0.40              |
| 32:DH:26:VAL:HG11  | 32:DH:33:LEU:HB2    | 2.03                     | 0.40              |
| 32:DH:85:LYS:HD2   | 32:DH:85:LYS:HA     | 1.70                     | 0.40              |
| 33:DI:144:VAL:CG2  | 33:DI:145:VAL:N     | 2.82                     | 0.40              |
| 36:DP:138:LEU:C    | 36:DP:140:ALA:N     | 2.77                     | 0.40              |
| 39:DS:14:VAL:HG13  | 39:DS:15:ARG:N      | 2.35                     | 0.40              |
| 40:DT:35:LYS:O     | 40:DT:36:GLU:CB     | 2.67                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 41:DU:92:ARG:HH12 | 42:DV:11:GLN:H    | 1.67                     | 0.40              |
| 45:DY:39:VAL:C    | 45:DY:40:GLU:CD   | 2.88                     | 0.40              |
| 46:DZ:22:GLY:O    | 46:DZ:23:LYS:CG   | 2.69                     | 0.40              |
| 46:DZ:104:PHE:O   | 46:DZ:105:VAL:C   | 2.64                     | 0.40              |
| 50:D3:36:VAL:O    | 50:D3:36:VAL:CG2  | 2.67                     | 0.40              |
| 1:AA:160:A:H1'    | 1:AA:344:A:C5     | 2.56                     | 0.40              |
| 1:AA:530:G:O2'    | 23:AY:35:A:O4'    | 2.37                     | 0.40              |
| 1:AA:925:G:H1'    | 1:AA:1502:A:N9    | 2.35                     | 0.40              |
| 1:AA:1029:C:H4'   | 1:AA:1033:G:H22   | 1.86                     | 0.40              |
| 1:AA:1287:A:H2    | 1:AA:1353:G:H1'   | 1.85                     | 0.40              |
| 1:AA:1291:G:C6    | 1:AA:1292:U:C4    | 3.10                     | 0.40              |
| 1:AA:1380:U:H1'   | 1:AA:1381:U:H5    | 1.86                     | 0.40              |
| 1:AA:1442(B):A:N1 | 40:BT:118:ARG:CZ  | 2.85                     | 0.40              |
| 2:AB:142:LEU:O    | 2:AB:146:GLN:HB2  | 2.22                     | 0.40              |
| 2:AB:144:ARG:O    | 2:AB:147:LYS:N    | 2.55                     | 0.40              |
| 3:AC:92:ALA:HB2   | 3:AC:99:VAL:HG11  | 2.03                     | 0.40              |
| 4:AD:42:GLN:C     | 4:AD:43:HIS:ND1   | 2.80                     | 0.40              |
| 7:AG:3:ARG:HH11   | 7:AG:3:ARG:CG     | 2.35                     | 0.40              |
| 7:AG:6:ARG:O      | 7:AG:7:ALA:O      | 2.39                     | 0.40              |
| 7:AG:24:THR:O     | 7:AG:27:ILE:N     | 2.54                     | 0.40              |
| 7:AG:69:VAL:HG11  | 7:AG:104:LEU:HD22 | 2.03                     | 0.40              |
| 8:AH:4:ASP:HA     | 8:AH:5:PRO:HD3    | 1.88                     | 0.40              |
| 10:AJ:38:ILE:HG13 | 10:AJ:71:LEU:O    | 2.21                     | 0.40              |
| 11:AK:70:LYS:HE3  | 11:AK:70:LYS:HB2  | 1.67                     | 0.40              |
| 12:AL:85:ILE:HA   | 12:AL:85:ILE:HD12 | 1.83                     | 0.40              |
| 13:AM:35:GLU:C    | 13:AM:37:THR:H    | 2.29                     | 0.40              |
| 13:AM:118:ALA:CB  | 22:AV:29:C:O3'    | 2.68                     | 0.40              |
| 16:AP:11:SER:HB2  | 16:AP:14:ASN:CB   | 2.51                     | 0.40              |
| 22:AV:55:U:C2'    | 22:AV:56:U:C5'    | 2.93                     | 0.40              |
| 23:AW:72:C:N4     | 23:AW:73:A:C6     | 2.89                     | 0.40              |
| 25:BA:210:C:OP1   | 54:B7:29:LYS:HE2  | 2.22                     | 0.40              |
| 25:BA:533:G:N3    | 41:BU:45:TYR:CE1  | 2.89                     | 0.40              |
| 25:BA:846:C:O2'   | 25:BA:847:U:O5'   | 2.36                     | 0.40              |
| 25:BA:1003:G:O2'  | 25:BA:1010:A:N1   | 2.51                     | 0.40              |
| 25:BA:1043:C:H6   | 25:BA:1043:C:O5'  | 2.04                     | 0.40              |
| 25:BA:1211:U:H4'  | 25:BA:1212:G:OP2  | 2.21                     | 0.40              |
| 25:BA:2119:A:C6   | 25:BA:2171:A:C6   | 3.09                     | 0.40              |
| 25:BA:2245:U:H5'' | 25:BA:2246:G:H5'  | 2.02                     | 0.40              |
| 25:BA:2283:C:H5'' | 25:BA:2283:C:H6   | 1.86                     | 0.40              |
| 25:BA:2561:A:H4'  | 35:BO:40:VAL:HG11 | 2.03                     | 0.40              |
| 25:BA:2572:A:N7   | 29:BE:145:LYS:HB2 | 2.36                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:BA:2576:G:O2'  | 25:BA:2579:C:OP2  | 2.30                     | 0.40              |
| 26:BB:75:G:H22    | 46:BZ:73:GLN:HE21 | 1.69                     | 0.40              |
| 27:BC:56:GLN:NE2  | 27:BC:173:ALA:HB1 | 2.37                     | 0.40              |
| 28:BD:19:ALA:CB   | 28:BD:21:PHE:CE2  | 2.99                     | 0.40              |
| 28:BD:22:SER:O    | 28:BD:24:ILE:N    | 2.54                     | 0.40              |
| 29:BE:12:THR:O    | 29:BE:23:VAL:CG2  | 2.67                     | 0.40              |
| 30:BF:96:ASP:OD1  | 30:BF:96:ASP:C    | 2.64                     | 0.40              |
| 30:BF:157:VAL:HA  | 30:BF:176:LEU:O   | 2.22                     | 0.40              |
| 31:BG:150:ASP:O   | 31:BG:151:ALA:CB  | 2.69                     | 0.40              |
| 33:BI:2:LYS:HA    | 33:BI:20:ASP:HB3  | 2.03                     | 0.40              |
| 33:BI:72:LEU:HD13 | 33:BI:73:GLU:N    | 2.37                     | 0.40              |
| 35:BO:26:LYS:HB3  | 35:BO:27:GLY:H    | 1.59                     | 0.40              |
| 37:BQ:26:TYR:HB2  | 37:BQ:137:TYR:HD1 | 1.85                     | 0.40              |
| 41:BU:10:ARG:O    | 41:BU:11:ARG:C    | 2.60                     | 0.40              |
| 41:BU:83:LEU:HA   | 41:BU:83:LEU:HD12 | 1.75                     | 0.40              |
| 42:BV:1:MET:SD    | 42:BV:42:GLY:HA3  | 2.62                     | 0.40              |
| 42:BV:51:VAL:HG12 | 42:BV:52:VAL:N    | 2.35                     | 0.40              |
| 45:BY:12:THR:O    | 45:BY:13:VAL:HG13 | 2.20                     | 0.40              |
| 45:BY:12:THR:O    | 45:BY:13:VAL:CG1  | 2.70                     | 0.40              |
| 46:BZ:29:TYR:CD1  | 46:BZ:29:TYR:O    | 2.74                     | 0.40              |
| 49:B2:32:LEU:HG   | 49:B2:53:LEU:HD13 | 2.03                     | 0.40              |
| 53:B6:19:ARG:CG   | 53:B6:20:ASN:H    | 2.29                     | 0.40              |
| 54:B7:12:ARG:CD   | 54:B7:46:VAL:HG21 | 2.51                     | 0.40              |
| 55:B8:51:ALA:CA   | 55:B8:53:PRO:HD2  | 2.51                     | 0.40              |
| 55:B8:61:LEU:H    | 55:B8:61:LEU:HG   | 1.23                     | 0.40              |
| 1:CA:136:C:O2'    | 16:CP:65:GLN:OE1  | 2.38                     | 0.40              |
| 1:CA:452:A:H4'    | 16:CP:72:ARG:CZ   | 2.51                     | 0.40              |
| 1:CA:495:A:H1'    | 1:CA:496:A:C8     | 2.57                     | 0.40              |
| 1:CA:1002:G:H2'   | 1:CA:1002:G:N3    | 2.36                     | 0.40              |
| 2:CB:178:ARG:NH2  | 8:CH:74:PRO:HG3   | 2.36                     | 0.40              |
| 4:CD:105:VAL:HG21 | 4:CD:126:ILE:HG13 | 2.04                     | 0.40              |
| 4:CD:190:ASP:CG   | 4:CD:191:ARG:N    | 2.78                     | 0.40              |
| 7:CG:80:VAL:HG21  | 7:CG:85:TYR:HD1   | 1.86                     | 0.40              |
| 7:CG:111:ARG:HA   | 7:CG:112:PRO:HD3  | 1.91                     | 0.40              |
| 10:CJ:40:LEU:H    | 10:CJ:40:LEU:HD23 | 1.86                     | 0.40              |
| 12:CL:27:LEU:O    | 12:CL:28:LYS:C    | 2.63                     | 0.40              |
| 12:CL:59:ARG:HA   | 12:CL:65:GLU:HA   | 2.03                     | 0.40              |
| 13:CM:54:VAL:HG12 | 13:CM:58:GLU:OE2  | 2.21                     | 0.40              |
| 15:CO:15:PHE:CE1  | 15:CO:30:ALA:HB1  | 2.57                     | 0.40              |
| 21:CU:6:ARG:CG    | 21:CU:15:ARG:NH1  | 2.84                     | 0.40              |
| 22:CV:28:U:C2'    | 22:CV:29:C:H5'    | 2.50                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:CW:3:C:H2'      | 23:CW:3:C:O2       | 2.21                     | 0.40              |
| 25:DA:271(R):G:H2' | 25:DA:271(S):G:C8  | 2.55                     | 0.40              |
| 25:DA:287:C:H2'    | 25:DA:288:C:O4'    | 2.22                     | 0.40              |
| 25:DA:975:C:O2     | 25:DA:975:C:H2'    | 2.21                     | 0.40              |
| 25:DA:1354:A:H2'   | 25:DA:1355:G:O4'   | 2.22                     | 0.40              |
| 25:DA:1708:C:H42   | 25:DA:1750:G:H1    | 1.70                     | 0.40              |
| 27:DC:47:LEU:H     | 27:DC:47:LEU:HD23  | 1.87                     | 0.40              |
| 28:DD:57:GLY:O     | 28:DD:58:HIS:C     | 2.64                     | 0.40              |
| 28:DD:147:LEU:HD13 | 28:DD:155:LEU:HD21 | 2.04                     | 0.40              |
| 29:DE:2:LYS:O      | 29:DE:199:ARG:HA   | 2.21                     | 0.40              |
| 29:DE:181:LEU:HA   | 29:DE:181:LEU:HD12 | 1.84                     | 0.40              |
| 31:DG:115:ARG:HH11 | 31:DG:115:ARG:CB   | 2.33                     | 0.40              |
| 32:DH:121:ILE:HG22 | 32:DH:122:THR:N    | 2.36                     | 0.40              |
| 32:DH:126:PRO:HB2  | 32:DH:130:ARG:HH12 | 1.86                     | 0.40              |
| 33:DI:77:LEU:HD13  | 33:DI:78:THR:O     | 2.21                     | 0.40              |
| 33:DI:127:VAL:HG13 | 33:DI:139:GLN:CB   | 2.52                     | 0.40              |
| 34:DN:117:PHE:CD2  | 34:DN:117:PHE:O    | 2.74                     | 0.40              |
| 35:DO:104:ARG:NH2  | 40:DT:33:LYS:HE3   | 2.37                     | 0.40              |
| 36:DP:127:ALA:HB3  | 36:DP:130:PHE:CE2  | 2.56                     | 0.40              |
| 39:DS:24:LEU:CD1   | 39:DS:41:ASP:HB2   | 2.51                     | 0.40              |
| 40:DT:27:THR:O     | 40:DT:28:VAL:HB    | 2.21                     | 0.40              |
| 43:DW:87:PRO:HA    | 43:DW:93:ALA:HA    | 2.02                     | 0.40              |
| 44:DX:60:ARG:CZ    | 54:D7:47:ARG:NH2   | 2.84                     | 0.40              |
| 47:D0:34:GLY:O     | 47:D0:35:ASN:C     | 2.65                     | 0.40              |
| 49:D2:16:LEU:HD12  | 49:D2:21:LEU:CD2   | 2.51                     | 0.40              |
| 52:D5:56:LYS:HD2   | 52:D5:56:LYS:N     | 2.27                     | 0.40              |
| 54:D7:20:ALA:O     | 54:D7:21:ARG:C     | 2.62                     | 0.40              |
| 54:D7:34:ARG:NH1   | 54:D7:41:ARG:O     | 2.55                     | 0.40              |
| 1:AA:945:G:C2      | 1:AA:1337:G:C2     | 3.09                     | 0.40              |
| 2:AB:17:PHE:N      | 2:AB:17:PHE:CD2    | 2.90                     | 0.40              |
| 2:AB:56:ARG:O      | 2:AB:60:ASP:HB3    | 2.21                     | 0.40              |
| 2:AB:223:ILE:H     | 2:AB:223:ILE:HG12  | 1.47                     | 0.40              |
| 3:AC:108:ASN:HA    | 3:AC:109:PRO:HD3   | 1.77                     | 0.40              |
| 4:AD:101:LEU:HB3   | 4:AD:102:ASP:H     | 1.67                     | 0.40              |
| 5:AE:55:VAL:HG12   | 5:AE:56:GLN:N      | 2.36                     | 0.40              |
| 8:AH:106:GLY:C     | 8:AH:108:GLY:N     | 2.79                     | 0.40              |
| 10:AJ:40:LEU:O     | 10:AJ:41:PRO:C     | 2.65                     | 0.40              |
| 11:AK:97:ALA:O     | 11:AK:101:SER:HB3  | 2.22                     | 0.40              |
| 12:AL:81:SER:CA    | 12:AL:106:ASP:OD2  | 2.65                     | 0.40              |
| 14:AN:4:LYS:C      | 14:AN:6:LEU:N      | 2.78                     | 0.40              |
| 16:AP:20:VAL:HG21  | 16:AP:32:TYR:CD1   | 2.56                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 17:AQ:79:SER:O    | 17:AQ:80:GLY:C    | 2.65                     | 0.40              |
| 22:AV:67:C:H6     | 22:AV:67:C:O5'    | 2.04                     | 0.40              |
| 23:AW:34:G:C8     | 24:AX:14:A:C6     | 3.10                     | 0.40              |
| 23:AW:34:G:O2'    | 23:AW:35:A:H5'    | 2.21                     | 0.40              |
| 23:AW:43:C:H2'    | 23:AW:44:G:H5'    | 2.04                     | 0.40              |
| 24:AX:16:A:C2     | 24:AX:17:U:C2     | 3.10                     | 0.40              |
| 25:BA:34:C:H3'    | 25:BA:34:C:C6     | 2.56                     | 0.40              |
| 25:BA:74:A:C4'    | 25:BA:75:G:O5'    | 2.70                     | 0.40              |
| 25:BA:287:C:H2'   | 25:BA:288:C:O4'   | 2.21                     | 0.40              |
| 25:BA:354:G:H2'   | 25:BA:355:G:O4'   | 2.21                     | 0.40              |
| 25:BA:435:C:C2'   | 25:BA:436:C:H5'   | 2.51                     | 0.40              |
| 25:BA:670:A:OP2   | 25:BA:670:A:H8    | 2.01                     | 0.40              |
| 25:BA:709:U:H2'   | 25:BA:710:G:C8    | 2.56                     | 0.40              |
| 25:BA:747:U:N3    | 52:B5:2:ALA:N     | 2.69                     | 0.40              |
| 25:BA:1299:G:C5   | 25:BA:1639:U:C5   | 3.09                     | 0.40              |
| 25:BA:1314:C:H42  | 25:BA:1338:G:H1   | 1.70                     | 0.40              |
| 25:BA:1464:C:H2'  | 25:BA:1465:G:H8   | 1.86                     | 0.40              |
| 28:BD:31:LYS:HZ1  | 28:BD:102:LYS:HZ1 | 1.65                     | 0.40              |
| 29:BE:57:LYS:HA   | 29:BE:57:LYS:HD2  | 1.46                     | 0.40              |
| 32:BH:25:LYS:H    | 32:BH:25:LYS:CD   | 2.05                     | 0.40              |
| 32:BH:88:LEU:H    | 32:BH:88:LEU:HD22 | 1.86                     | 0.40              |
| 33:BI:1:MET:C     | 33:BI:20:ASP:HB2  | 2.46                     | 0.40              |
| 33:BI:23:PRO:O    | 33:BI:27:ARG:HB2  | 2.22                     | 0.40              |
| 33:BI:58:LEU:HD23 | 33:BI:58:LEU:O    | 2.22                     | 0.40              |
| 35:BO:114:ILE:O   | 35:BO:115:VAL:O   | 2.38                     | 0.40              |
| 36:BP:85:LEU:HD23 | 36:BP:85:LEU:N    | 2.32                     | 0.40              |
| 37:BQ:42:ILE:HA   | 37:BQ:46:GLN:OE1  | 2.21                     | 0.40              |
| 37:BQ:59:ARG:O    | 37:BQ:60:ARG:CB   | 2.69                     | 0.40              |
| 40:BT:33:LYS:HD2  | 40:BT:43:GLN:OE1  | 2.21                     | 0.40              |
| 41:BU:94:ASN:C    | 41:BU:96:ALA:H    | 2.28                     | 0.40              |
| 42:BV:18:LEU:HD13 | 42:BV:96:ILE:HG12 | 2.04                     | 0.40              |
| 42:BV:71:LEU:HD23 | 42:BV:71:LEU:HA   | 1.92                     | 0.40              |
| 43:BW:15:ARG:O    | 43:BW:19:LEU:HD13 | 2.21                     | 0.40              |
| 43:BW:35:ILE:O    | 43:BW:36:LEU:C    | 2.64                     | 0.40              |
| 44:BX:65:ARG:HG3  | 44:BX:70:LEU:HA   | 2.02                     | 0.40              |
| 45:BY:46:LYS:HD2  | 45:BY:47:LYS:HZ2  | 1.86                     | 0.40              |
| 46:BZ:76:LEU:HA   | 46:BZ:83:PRO:HA   | 2.03                     | 0.40              |
| 46:BZ:166:SER:CB  | 46:BZ:167:PRO:C   | 2.95                     | 0.40              |
| 47:B0:45:PHE:CE1  | 47:B0:77:ARG:NH1  | 2.89                     | 0.40              |
| 48:B1:29:GLY:C    | 48:B1:30:VAL:HG22 | 2.46                     | 0.40              |
| 49:B2:69:ARG:O    | 49:B2:70:GLN:HB3  | 2.22                     | 0.40              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 55:B8:13:ARG:O    | 55:B8:13:ARG:HG3   | 2.20                     | 0.40              |
| 55:B8:16:ILE:CG2  | 55:B8:64:TYR:CD2   | 3.01                     | 0.40              |
| 1:CA:90:U:H5''    | 1:CA:91:C:H5'      | 2.04                     | 0.40              |
| 1:CA:240:C:H2'    | 1:CA:241:C:C6      | 2.55                     | 0.40              |
| 1:CA:436:C:H2'    | 1:CA:437:U:C6      | 2.56                     | 0.40              |
| 1:CA:470:C:H6     | 1:CA:470:C:O5'     | 2.04                     | 0.40              |
| 1:CA:870:U:C5'    | 1:CA:871:U:H5'     | 2.47                     | 0.40              |
| 1:CA:913:A:H1'    | 1:CA:914:A:C1'     | 2.50                     | 0.40              |
| 1:CA:1346:A:N1    | 1:CA:1374:A:H5''   | 2.36                     | 0.40              |
| 2:CB:31:TYR:HE2   | 2:CB:46:LYS:NZ     | 2.19                     | 0.40              |
| 2:CB:71:VAL:HA    | 2:CB:93:VAL:CG2    | 2.41                     | 0.40              |
| 3:CC:31:HIS:HA    | 3:CC:34:LEU:HB3    | 2.04                     | 0.40              |
| 4:CD:3:ARG:HB3    | 4:CD:118:ARG:NE    | 2.35                     | 0.40              |
| 4:CD:50:ARG:HA    | 4:CD:51:PRO:HD3    | 1.82                     | 0.40              |
| 4:CD:68:TYR:O     | 4:CD:69:GLY:C      | 2.64                     | 0.40              |
| 5:CE:63:ARG:C     | 5:CE:65:ASN:N      | 2.80                     | 0.40              |
| 12:CL:64:TYR:HB3  | 12:CL:65:GLU:H     | 1.43                     | 0.40              |
| 12:CL:68:ALA:HA   | 12:CL:98:TYR:O     | 2.22                     | 0.40              |
| 16:CP:9:PHE:HD2   | 16:CP:9:PHE:N      | 2.14                     | 0.40              |
| 16:CP:81:ARG:C    | 16:CP:82:GLN:HE21  | 2.28                     | 0.40              |
| 19:CS:10:PHE:HZ   | 19:CS:70:LYS:CE    | 2.35                     | 0.40              |
| 22:CV:1:C:O2'     | 22:CV:2:G:H5'      | 2.21                     | 0.40              |
| 22:CV:41:C:H2'    | 22:CV:42:C:H6      | 1.86                     | 0.40              |
| 25:DA:464:U:H2'   | 25:DA:465:G:O4'    | 2.20                     | 0.40              |
| 25:DA:669:G:N3    | 25:DA:669:G:H2'    | 2.37                     | 0.40              |
| 25:DA:738:G:C6    | 25:DA:739:G:C2     | 3.08                     | 0.40              |
| 25:DA:1151:G:O2'  | 41:DU:77:SER:O     | 2.38                     | 0.40              |
| 25:DA:1286:A:C4   | 25:DA:1329:U:C4    | 3.10                     | 0.40              |
| 25:DA:1373:A:H2'  | 25:DA:1374:G:O4'   | 2.20                     | 0.40              |
| 25:DA:1568:G:H5'  | 28:DD:60:ARG:HA    | 2.04                     | 0.40              |
| 25:DA:2476:A:H3'  | 25:DA:2476:A:N3    | 2.36                     | 0.40              |
| 27:DC:127:LEU:O   | 27:DC:129:ARG:N    | 2.55                     | 0.40              |
| 28:DD:16:MET:HE2  | 28:DD:208:LYS:HD2  | 2.03                     | 0.40              |
| 31:DG:102:PHE:CZ  | 31:DG:157:ILE:HD13 | 2.56                     | 0.40              |
| 33:DI:69:LYS:C    | 33:DI:71:ILE:H     | 2.28                     | 0.40              |
| 33:DI:132:PRO:C   | 33:DI:133:HIS:O    | 2.64                     | 0.40              |
| 33:DI:144:VAL:O   | 33:DI:145:VAL:CG2  | 2.69                     | 0.40              |
| 36:DP:121:LYS:O   | 36:DP:123:LEU:HD23 | 2.21                     | 0.40              |
| 43:DW:69:LEU:HD23 | 43:DW:69:LEU:HA    | 1.82                     | 0.40              |
| 45:DY:42:VAL:CG1  | 45:DY:43:ASN:N     | 2.83                     | 0.40              |
| 51:D4:4:GLY:C     | 51:D4:6:HIS:H      | 2.30                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 55:D8:53:PRO:C    | 55:D8:55:ALA:N    | 2.77                     | 0.40              |
| 1:AA:764:C:H2'    | 1:AA:765:G:O4'    | 2.21                     | 0.40              |
| 2:AB:52:GLU:O     | 2:AB:56:ARG:N     | 2.55                     | 0.40              |
| 2:AB:194:PRO:O    | 2:AB:196:LEU:N    | 2.54                     | 0.40              |
| 3:AC:59:ARG:O     | 10:AJ:93:GLY:HA2  | 2.21                     | 0.40              |
| 3:AC:97:LYS:HB3   | 3:AC:97:LYS:HZ2   | 1.87                     | 0.40              |
| 4:AD:138:TYR:HD2  | 4:AD:139:ARG:N    | 2.19                     | 0.40              |
| 6:AF:89:MET:HG2   | 6:AF:91:VAL:HG23  | 2.03                     | 0.40              |
| 9:AI:85:LEU:HD11  | 9:AI:95:LYS:NZ    | 2.37                     | 0.40              |
| 11:AK:27:ASN:OD1  | 11:AK:28:THR:N    | 2.55                     | 0.40              |
| 13:AM:19:LEU:O    | 13:AM:20:THR:C    | 2.64                     | 0.40              |
| 13:AM:123:ALA:HA  | 13:AM:124:PRO:HD3 | 1.83                     | 0.40              |
| 19:AS:13:ASP:C    | 19:AS:15:LEU:N    | 2.79                     | 0.40              |
| 20:AT:45:GLN:HA   | 20:AT:91:LEU:HD13 | 2.00                     | 0.40              |
| 23:AW:19:G:H4'    | 23:AW:20:U:OP2    | 2.21                     | 0.40              |
| 23:AY:30:G:O6     | 23:AY:40:C:N4     | 2.50                     | 0.40              |
| 25:BA:50:U:H5''   | 25:BA:51:G:OP2    | 2.20                     | 0.40              |
| 25:BA:271(D):G:H1 | 25:BA:271(T):C:N4 | 2.09                     | 0.40              |
| 25:BA:464:U:C2    | 25:BA:788:A:C6    | 3.10                     | 0.40              |
| 25:BA:1813:G:H4'  | 28:BD:44:ASN:O    | 2.21                     | 0.40              |
| 25:BA:2127:G:C6   | 25:BA:2162:G:C4   | 3.09                     | 0.40              |
| 26:BB:24:G:H5'    | 26:BB:25:A:H8     | 1.86                     | 0.40              |
| 27:BC:212:VAL:O   | 27:BC:213:TYR:CB  | 2.68                     | 0.40              |
| 28:BD:139:GLY:HA2 | 28:BD:165:ILE:O   | 2.21                     | 0.40              |
| 29:BE:85:ASN:HA   | 29:BE:86:PRO:HD3  | 1.76                     | 0.40              |
| 29:BE:97:LYS:HE2  | 29:BE:97:LYS:HB3  | 1.70                     | 0.40              |
| 30:BF:8:GLN:O     | 30:BF:9:ILE:C     | 2.65                     | 0.40              |
| 30:BF:153:SER:N   | 30:BF:190:GLU:OE2 | 2.51                     | 0.40              |
| 32:BH:88:LEU:HD22 | 32:BH:164:TYR:O   | 2.21                     | 0.40              |
| 33:BI:69:LYS:HE3  | 33:BI:73:GLU:OE1  | 2.22                     | 0.40              |
| 34:BN:15:LEU:HD22 | 34:BN:53:VAL:HB   | 2.03                     | 0.40              |
| 35:BO:85:VAL:HG11 | 35:BO:114:ILE:CD1 | 2.31                     | 0.40              |
| 36:BP:84:ASN:CB   | 36:BP:116:GLY:HA3 | 2.51                     | 0.40              |
| 37:BQ:32:TYR:OH   | 37:BQ:111:GLU:HA  | 2.22                     | 0.40              |
| 37:BQ:85:LYS:HG3  | 47:B0:7:LEU:HD22  | 2.04                     | 0.40              |
| 38:BR:8:ARG:HB3   | 38:BR:9:LYS:H     | 1.64                     | 0.40              |
| 40:BT:34:VAL:HG13 | 40:BT:39:ARG:CG   | 2.35                     | 0.40              |
| 41:BU:10:ARG:HH11 | 41:BU:10:ARG:HD2  | 1.75                     | 0.40              |
| 43:BW:70:TYR:N    | 43:BW:70:TYR:CD2  | 2.89                     | 0.40              |
| 44:BX:64:LYS:NZ   | 44:BX:73:ARG:NE   | 2.53                     | 0.40              |
| 45:BY:11:ASP:OD1  | 45:BY:12:THR:N    | 2.54                     | 0.40              |

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| Atom-1            | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 46:BZ:108:PRO:C   | 46:BZ:110:GLY:N     | 2.80                     | 0.40              |
| 52:B5:20:ARG:O    | 52:B5:21:SER:C      | 2.63                     | 0.40              |
| 54:B7:15:THR:HG22 | 54:B7:16:HIS:CD2    | 2.56                     | 0.40              |
| 1:CA:230:G:O2'    | 16:CP:25:ARG:NH2    | 2.54                     | 0.40              |
| 1:CA:1502:A:H3'   | 1:CA:1504:G:N7      | 2.37                     | 0.40              |
| 1:CA:1521:G:H2'   | 1:CA:1522:U:C6      | 2.56                     | 0.40              |
| 2:CB:28:PHE:CE2   | 2:CB:31:TYR:HB2     | 2.57                     | 0.40              |
| 2:CB:82:ARG:O     | 2:CB:83:MET:C       | 2.63                     | 0.40              |
| 3:CC:15:THR:HB    | 3:CC:16:ARG:H       | 1.41                     | 0.40              |
| 3:CC:52:LEU:C     | 3:CC:54:ARG:H       | 2.28                     | 0.40              |
| 4:CD:25:ARG:NH1   | 4:CD:30:LYS:HB2     | 2.35                     | 0.40              |
| 7:CG:107:ALA:O    | 7:CG:108:ALA:C      | 2.65                     | 0.40              |
| 10:CJ:63:PHE:CD2  | 10:CJ:63:PHE:N      | 2.90                     | 0.40              |
| 11:CK:32:ILE:HD11 | 11:CK:68:ALA:HB1    | 2.02                     | 0.40              |
| 14:CN:53:LEU:HD23 | 14:CN:53:LEU:HA     | 1.66                     | 0.40              |
| 16:CP:19:ILE:HD13 | 16:CP:19:ILE:HA     | 1.81                     | 0.40              |
| 16:CP:52:ASP:C    | 16:CP:52:ASP:OD2    | 2.65                     | 0.40              |
| 16:CP:73:LEU:HD23 | 16:CP:73:LEU:N      | 2.36                     | 0.40              |
| 18:CR:75:ILE:HG22 | 18:CR:76:LEU:HD22   | 2.03                     | 0.40              |
| 22:CV:56:U:O2     | 22:CV:58:A:C8       | 2.75                     | 0.40              |
| 23:CW:16:U:H6     | 23:CW:17:C:C5'      | 2.35                     | 0.40              |
| 24:CX:16:A:O2'    | 24:CX:17:U:H5'      | 2.22                     | 0.40              |
| 23:CY:37:A:H2'    | 23:CY:38:A:O4'      | 2.22                     | 0.40              |
| 25:DA:13:A:C5     | 25:DA:525:U:N3      | 2.90                     | 0.40              |
| 25:DA:185:U:H2'   | 25:DA:186:G:C8      | 2.57                     | 0.40              |
| 25:DA:372:G:O2'   | 25:DA:373:U:OP2     | 2.40                     | 0.40              |
| 25:DA:673:C:OP1   | 30:DF:54:ARG:HD2    | 2.21                     | 0.40              |
| 25:DA:1022:G:O2'  | 25:DA:1023:U:P      | 2.79                     | 0.40              |
| 25:DA:1024:G:H3'  | 25:DA:1025:G:H5''   | 2.03                     | 0.40              |
| 25:DA:1110:G:H2'  | 25:DA:1111:A:C8     | 2.53                     | 0.40              |
| 25:DA:1113:U:H2'  | 25:DA:1114:G:H8     | 1.85                     | 0.40              |
| 25:DA:1565:C:O2'  | 25:DA:1566:A:C8     | 2.75                     | 0.40              |
| 25:DA:2520:C:C4   | 25:DA:2567:G:C8     | 3.10                     | 0.40              |
| 25:DA:2547:U:H2'  | 25:DA:2548:G:C8     | 2.56                     | 0.40              |
| 25:DA:2668:G:HO2' | 25:DA:2669:G:P      | 2.45                     | 0.40              |
| 25:DA:2693:A:H2'  | 25:DA:2694:G:C8     | 2.57                     | 0.40              |
| 25:DA:2712:U:O2'  | 25:DA:2712(A):A:O5' | 2.40                     | 0.40              |
| 28:DD:142:VAL:CG2 | 28:DD:191:ALA:HB1   | 2.51                     | 0.40              |
| 29:DE:10:GLY:HA3  | 40:DT:8:LYS:HD2     | 2.03                     | 0.40              |
| 30:DF:12:LEU:O    | 30:DF:127:GLU:HB2   | 2.22                     | 0.40              |
| 31:DG:53:LEU:HD23 | 31:DG:54:GLU:CA     | 2.52                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:DG:58:GLN:HE22  | 31:DG:148:MET:CE   | 2.30                     | 0.40              |
| 31:DG:82:LEU:HA    | 31:DG:86:MET:SD    | 2.61                     | 0.40              |
| 31:DG:83:ARG:N     | 31:DG:86:MET:HE3   | 2.36                     | 0.40              |
| 32:DH:92:ILE:H     | 32:DH:92:ILE:CD1   | 2.14                     | 0.40              |
| 32:DH:101:ARG:HG2  | 32:DH:117:PRO:CG   | 2.46                     | 0.40              |
| 33:DI:57:ARG:C     | 33:DI:57:ARG:HD3   | 2.46                     | 0.40              |
| 33:DI:140:LEU:HD23 | 33:DI:140:LEU:N    | 2.36                     | 0.40              |
| 34:DN:43:THR:HB    | 34:DN:46:VAL:HG11  | 2.04                     | 0.40              |
| 35:DO:60:ALA:HB1   | 35:DO:85:VAL:O     | 2.21                     | 0.40              |
| 35:DO:77:ILE:HD12  | 40:DT:73:GLU:O     | 2.21                     | 0.40              |
| 38:DR:95:THR:C     | 38:DR:117:VAL:HG23 | 2.46                     | 0.40              |
| 38:DR:104:ARG:HD3  | 38:DR:111:LEU:HD21 | 2.04                     | 0.40              |
| 38:DR:117:VAL:O    | 38:DR:118:GLU:HB2  | 2.21                     | 0.40              |
| 45:DY:95:LYS:C     | 45:DY:96:ILE:O     | 2.64                     | 0.40              |
| 45:DY:101:LYS:HG2  | 45:DY:101:LYS:O    | 2.21                     | 0.40              |
| 50:D3:26:LEU:HD21  | 50:D3:46:ASN:HB2   | 2.03                     | 0.40              |
| 1:AA:7:G:O2'       | 1:AA:8:A:OP1       | 2.31                     | 0.40              |
| 1:AA:1029:C:C4'    | 1:AA:1033:G:H22    | 2.34                     | 0.40              |
| 1:AA:1112:C:C2     | 3:AC:178:LEU:HB2   | 2.57                     | 0.40              |
| 1:AA:1190:G:H5'    | 3:AC:176:HIS:NE2   | 2.37                     | 0.40              |
| 1:AA:1265:G:H2'    | 1:AA:1266:G:H8     | 1.85                     | 0.40              |
| 5:AE:143:ARG:NH1   | 8:AH:77:GLU:OE1    | 2.54                     | 0.40              |
| 6:AF:60:PHE:CZ     | 18:AR:78:LEU:CD2   | 3.03                     | 0.40              |
| 10:AJ:8:LEU:CD2    | 10:AJ:96:ILE:HG22  | 2.50                     | 0.40              |
| 10:AJ:12:ASP:C     | 10:AJ:14:LYS:H     | 2.29                     | 0.40              |
| 10:AJ:29:ARG:NH1   | 1:CA:1163:C:H5''   | 2.31                     | 0.40              |
| 10:AJ:30:SER:CB    | 10:AJ:80:LYS:HD3   | 2.52                     | 0.40              |
| 10:AJ:79:ARG:HD3   | 10:AJ:79:ARG:HA    | 1.79                     | 0.40              |
| 11:AK:120:ARG:HA   | 11:AK:121:PRO:HD3  | 1.90                     | 0.40              |
| 12:AL:20:LYS:HB3   | 12:AL:20:LYS:HE2   | 1.88                     | 0.40              |
| 13:AM:3:ARG:NE     | 31:BG:113:ARG:NH2  | 2.69                     | 0.40              |
| 13:AM:76:ALA:O     | 13:AM:79:LYS:HB2   | 2.21                     | 0.40              |
| 13:AM:91:ARG:HB2   | 13:AM:92:HIS:H     | 1.74                     | 0.40              |
| 13:AM:91:ARG:O     | 13:AM:95:GLY:N     | 2.54                     | 0.40              |
| 14:AN:28:GLY:O     | 14:AN:29:ARG:C     | 2.65                     | 0.40              |
| 19:AS:7:LYS:HD3    | 19:AS:7:LYS:N      | 2.36                     | 0.40              |
| 20:AT:56:MET:HE2   | 20:AT:56:MET:HB3   | 1.83                     | 0.40              |
| 25:BA:205:G:HO2'   | 25:BA:206:U:P      | 2.44                     | 0.40              |
| 25:BA:480:A:H1'    | 45:BY:44:ILE:HG21  | 2.04                     | 0.40              |
| 25:BA:487:C:H1'    | 43:BW:53:SER:HB2   | 2.02                     | 0.40              |
| 25:BA:708:C:N4     | 25:BA:723:G:H1     | 2.19                     | 0.40              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 25:BA:932:G:H4'    | 25:BA:933:A:O5'   | 2.21                     | 0.40              |
| 25:BA:1021:A:C2    | 25:BA:1023:U:C2   | 3.09                     | 0.40              |
| 25:BA:1275:A:N9    | 38:BR:16:HIS:HD2  | 2.19                     | 0.40              |
| 25:BA:1278:A:OP1   | 38:BR:36:THR:HG22 | 2.21                     | 0.40              |
| 25:BA:1337:G:H2'   | 25:BA:1338:G:C8   | 2.56                     | 0.40              |
| 25:BA:1673:U:H2'   | 25:BA:1674:G:H5'  | 2.04                     | 0.40              |
| 25:BA:1721:G:C6    | 25:BA:1739:U:OP2  | 2.75                     | 0.40              |
| 25:BA:2016:U:H2'   | 25:BA:2017:U:O4'  | 2.21                     | 0.40              |
| 26:BB:66:A:N6      | 26:BB:108:U:C2    | 2.90                     | 0.40              |
| 27:BC:20:TYR:N     | 27:BC:20:TYR:CD1  | 2.90                     | 0.40              |
| 28:BD:7:LYS:O      | 28:BD:9:TYR:CD1   | 2.75                     | 0.40              |
| 28:BD:24:ILE:HD12  | 28:BD:84:TYR:HB2  | 2.04                     | 0.40              |
| 29:BE:82:ARG:HB3   | 29:BE:83:ASP:H    | 1.42                     | 0.40              |
| 30:BF:7:TYR:HB3    | 30:BF:16:GLY:C    | 2.46                     | 0.40              |
| 30:BF:45:ARG:HG3   | 30:BF:46:ARG:N    | 2.33                     | 0.40              |
| 30:BF:192:LEU:HD23 | 30:BF:193:VAL:H   | 1.86                     | 0.40              |
| 32:BH:137:ASP:OD1  | 32:BH:138:LYS:N   | 2.50                     | 0.40              |
| 32:BH:151:ILE:O    | 32:BH:152:ARG:CG  | 2.69                     | 0.40              |
| 34:BN:35:ARG:C     | 34:BN:37:LYS:N    | 2.80                     | 0.40              |
| 40:BT:50:ILE:HD12  | 40:BT:99:LEU:CD1  | 2.47                     | 0.40              |
| 42:BV:52:VAL:HG13  | 42:BV:55:ALA:CB   | 2.50                     | 0.40              |
| 45:BY:40:GLU:OE2   | 45:BY:40:GLU:CA   | 2.43                     | 0.40              |
| 48:B1:27:GLU:HB2   | 48:B1:28:GLY:H    | 1.73                     | 0.40              |
| 48:B1:66:HIS:C     | 48:B1:68:PRO:HD2  | 2.45                     | 0.40              |
| 52:B5:34:PRO:HB2   | 52:B5:35:GLU:H    | 1.75                     | 0.40              |
| 54:B7:29:LYS:HG2   | 54:B7:29:LYS:O    | 2.20                     | 0.40              |
| 1:CA:458:C:H2'     | 1:CA:460:G:C8     | 2.55                     | 0.40              |
| 1:CA:729:A:H2'     | 1:CA:730:G:C8     | 2.55                     | 0.40              |
| 1:CA:979:C:OP1     | 1:CA:1223:C:N4    | 2.54                     | 0.40              |
| 1:CA:1427:U:H2'    | 1:CA:1428:A:C8    | 2.56                     | 0.40              |
| 3:CC:85:ARG:C      | 3:CC:87:LEU:N     | 2.80                     | 0.40              |
| 3:CC:131:ARG:NH2   | 3:CC:167:TRP:O    | 2.51                     | 0.40              |
| 4:CD:101:LEU:CD1   | 4:CD:105:VAL:HG23 | 2.50                     | 0.40              |
| 6:CF:1:MET:HE3     | 6:CF:67:MET:C     | 2.46                     | 0.40              |
| 7:CG:95:ARG:O      | 7:CG:96:GLN:C     | 2.64                     | 0.40              |
| 8:CH:10:LEU:N      | 8:CH:10:LEU:HD23  | 2.35                     | 0.40              |
| 10:CJ:6:ILE:HD11   | 10:CJ:72:VAL:CG1  | 2.51                     | 0.40              |
| 14:CN:37:PHE:C     | 14:CN:39:LEU:N    | 2.79                     | 0.40              |
| 14:CN:53:LEU:HA    | 14:CN:54:PRO:HD3  | 1.80                     | 0.40              |
| 20:CT:84:LEU:C     | 20:CT:85:MET:HG2  | 2.46                     | 0.40              |
| 23:CY:36:A:H2'     | 23:CY:37:A:O5'    | 2.22                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:DA:76:C:O3'     | 49:D2:59:ARG:HG2   | 2.21                     | 0.40              |
| 25:DA:207:A:H2'    | 25:DA:208:C:O4'    | 2.21                     | 0.40              |
| 25:DA:613:G:N2     | 25:DA:615:G:C5     | 2.89                     | 0.40              |
| 25:DA:814:C:N4     | 36:DP:24:GLY:O     | 2.50                     | 0.40              |
| 25:DA:995:C:OP2    | 41:DU:54:LYS:NZ    | 2.50                     | 0.40              |
| 25:DA:1001:A:H2'   | 25:DA:1002:G:O4'   | 2.21                     | 0.40              |
| 25:DA:1116:C:H2'   | 25:DA:1117:G:C8    | 2.57                     | 0.40              |
| 25:DA:1313:U:H2'   | 25:DA:1610:A:C2    | 2.56                     | 0.40              |
| 25:DA:1353:A:H4'   | 28:DD:38:LYS:NZ    | 2.37                     | 0.40              |
| 25:DA:1540:U:O4    | 25:DA:1541:G:N1    | 2.54                     | 0.40              |
| 25:DA:2296:U:H4'   | 25:DA:2297:C:OP1   | 2.21                     | 0.40              |
| 28:DD:48:ARG:HG3   | 28:DD:48:ARG:HH11  | 1.87                     | 0.40              |
| 29:DE:72:VAL:O     | 29:DE:73:GLU:C     | 2.63                     | 0.40              |
| 29:DE:77:ILE:H     | 29:DE:77:ILE:HG13  | 1.63                     | 0.40              |
| 29:DE:97:LYS:H     | 29:DE:100:GLU:CD   | 2.29                     | 0.40              |
| 30:DF:33:LEU:HD12  | 30:DF:33:LEU:HA    | 1.94                     | 0.40              |
| 30:DF:119:ARG:HG2  | 30:DF:119:ARG:NH1  | 2.36                     | 0.40              |
| 30:DF:122:LYS:HA   | 30:DF:122:LYS:HD3  | 1.91                     | 0.40              |
| 30:DF:157:VAL:HG11 | 30:DF:181:LEU:HD23 | 2.02                     | 0.40              |
| 31:DG:54:GLU:HA    | 31:DG:57:ALA:HB3   | 2.02                     | 0.40              |
| 31:DG:77:ILE:O     | 31:DG:78:SER:C     | 2.65                     | 0.40              |
| 31:DG:161:THR:HG22 | 31:DG:163:ALA:H    | 1.87                     | 0.40              |
| 32:DH:117:PRO:HB3  | 32:DH:123:PHE:CD1  | 2.57                     | 0.40              |
| 32:DH:121:ILE:CG2  | 32:DH:122:THR:N    | 2.84                     | 0.40              |
| 33:DI:78:THR:O     | 33:DI:79:ILE:HB    | 2.21                     | 0.40              |
| 34:DN:60:ILE:H     | 34:DN:60:ILE:HG13  | 1.63                     | 0.40              |
| 34:DN:82:LEU:HD12  | 34:DN:82:LEU:HA    | 1.82                     | 0.40              |
| 35:DO:29:ASN:O     | 35:DO:29:ASN:ND2   | 2.42                     | 0.40              |
| 35:DO:47:ILE:CG2   | 35:DO:48:PRO:N     | 2.85                     | 0.40              |
| 37:DQ:10:ARG:HG3   | 37:DQ:10:ARG:HH11  | 1.87                     | 0.40              |
| 39:DS:103:GLU:OE1  | 39:DS:103:GLU:CA   | 2.70                     | 0.40              |
| 42:DV:35:LEU:HD21  | 42:DV:57:VAL:CG2   | 2.29                     | 0.40              |
| 46:DZ:101:PRO:HA   | 46:DZ:123:ASP:HB3  | 2.04                     | 0.40              |
| 46:DZ:117:LEU:HD13 | 46:DZ:144:LEU:HB3  | 2.02                     | 0.40              |
| 46:DZ:137:ILE:O    | 46:DZ:138:GLU:C    | 2.64                     | 0.40              |
| 47:D0:27:GLU:HB2   | 47:D0:69:PHE:HD1   | 1.87                     | 0.40              |
| 47:D0:45:PHE:N     | 47:D0:45:PHE:HD1   | 2.19                     | 0.40              |
| 48:D1:4:VAL:HG22   | 48:D1:5:CYS:N      | 2.36                     | 0.40              |
| 49:D2:67:LYS:O     | 49:D2:69:ARG:N     | 2.52                     | 0.40              |
| 53:D6:41:PRO:CG    | 53:D6:46:HIS:N     | 2.84                     | 0.40              |

All (8) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

| Atom-1            | Atom-2                  | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------------|--------------------------|-------------------|
| 50:B3:1:MET:N     | 36:DP:122:PRO:CG[3_455] | 1.46                     | 0.74              |
| 50:B3:1:MET:N     | 36:DP:122:PRO:CD[3_455] | 1.64                     | 0.56              |
| 42:DV:50:PRO:CG   | 52:D5:58:LEU:O[4_445]   | 1.80                     | 0.40              |
| 42:DV:48:GLY:O    | 52:D5:58:LEU:CD1[4_445] | 1.84                     | 0.36              |
| 25:BA:1593:G:O2'  | 26:BB:54:G:OP1[1_655]   | 2.09                     | 0.11              |
| 42:DV:6:LYS:CE    | 52:D5:60:VAL:CG1[4_445] | 2.12                     | 0.08              |
| 32:BH:130:ARG:NH1 | 1:CA:82:U:O2[2_455]     | 2.18                     | 0.02              |
| 50:B3:1:MET:CG    | 36:DP:122:PRO:CG[3_455] | 2.19                     | 0.01              |

## 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 X-ray entries followed by that with respect to entries of similar resolution.

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 |    |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 2   | AB    | 233/256 (91%) | 159 (68%) | 53 (23%) | 21 (9%)  | 0           | 7  |
| 2   | CB    | 233/256 (91%) | 158 (68%) | 45 (19%) | 30 (13%) | 0           | 3  |
| 3   | AC    | 205/239 (86%) | 129 (63%) | 54 (26%) | 22 (11%) | 0           | 5  |
| 3   | CC    | 205/239 (86%) | 135 (66%) | 52 (25%) | 18 (9%)  | 0           | 7  |
| 4   | AD    | 206/209 (99%) | 142 (69%) | 43 (21%) | 21 (10%) | 0           | 6  |
| 4   | CD    | 206/209 (99%) | 141 (68%) | 47 (23%) | 18 (9%)  | 0           | 7  |
| 5   | AE    | 149/162 (92%) | 117 (78%) | 20 (13%) | 12 (8%)  | 1           | 8  |
| 5   | CE    | 149/162 (92%) | 113 (76%) | 22 (15%) | 14 (9%)  | 0           | 6  |
| 6   | AF    | 99/101 (98%)  | 63 (64%)  | 29 (29%) | 7 (7%)   | 1           | 10 |
| 6   | CF    | 99/101 (98%)  | 80 (81%)  | 14 (14%) | 5 (5%)   | 1           | 15 |
| 7   | AG    | 153/156 (98%) | 116 (76%) | 26 (17%) | 11 (7%)  | 1           | 9  |
| 7   | CG    | 153/156 (98%) | 117 (76%) | 29 (19%) | 7 (5%)   | 2           | 17 |
| 8   | AH    | 136/138 (99%) | 96 (71%)  | 35 (26%) | 5 (4%)   | 2           | 21 |
| 8   | CH    | 136/138 (99%) | 102 (75%) | 28 (21%) | 6 (4%)   | 2           | 17 |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 9   | AI    | 125/128 (98%) | 84 (67%)  | 32 (26%) | 9 (7%)   | 1           | 9  |
| 9   | CI    | 125/128 (98%) | 87 (70%)  | 23 (18%) | 15 (12%) | 0           | 4  |
| 10  | AJ    | 97/105 (92%)  | 59 (61%)  | 31 (32%) | 7 (7%)   | 1           | 9  |
| 10  | CJ    | 97/105 (92%)  | 60 (62%)  | 25 (26%) | 12 (12%) | 0           | 4  |
| 11  | AK    | 117/129 (91%) | 92 (79%)  | 19 (16%) | 6 (5%)   | 1           | 15 |
| 11  | CK    | 117/129 (91%) | 92 (79%)  | 23 (20%) | 2 (2%)   | 7           | 35 |
| 12  | AL    | 123/132 (93%) | 78 (63%)  | 25 (20%) | 20 (16%) | 0           | 2  |
| 12  | CL    | 123/132 (93%) | 91 (74%)  | 20 (16%) | 12 (10%) | 0           | 6  |
| 13  | AM    | 123/126 (98%) | 82 (67%)  | 23 (19%) | 18 (15%) | 0           | 3  |
| 13  | CM    | 123/126 (98%) | 78 (63%)  | 22 (18%) | 23 (19%) | 0           | 1  |
| 14  | AN    | 58/61 (95%)   | 40 (69%)  | 11 (19%) | 7 (12%)  | 0           | 4  |
| 14  | CN    | 58/61 (95%)   | 37 (64%)  | 14 (24%) | 7 (12%)  | 0           | 4  |
| 15  | AO    | 86/89 (97%)   | 65 (76%)  | 20 (23%) | 1 (1%)   | 10          | 42 |
| 15  | CO    | 86/89 (97%)   | 55 (64%)  | 25 (29%) | 6 (7%)   | 1           | 10 |
| 16  | AP    | 82/88 (93%)   | 53 (65%)  | 25 (30%) | 4 (5%)   | 1           | 16 |
| 16  | CP    | 82/88 (93%)   | 66 (80%)  | 13 (16%) | 3 (4%)   | 2           | 21 |
| 17  | AQ    | 98/105 (93%)  | 79 (81%)  | 13 (13%) | 6 (6%)   | 1           | 12 |
| 17  | CQ    | 98/105 (93%)  | 77 (79%)  | 15 (15%) | 6 (6%)   | 1           | 12 |
| 18  | AR    | 68/88 (77%)   | 49 (72%)  | 12 (18%) | 7 (10%)  | 0           | 5  |
| 18  | CR    | 68/88 (77%)   | 49 (72%)  | 11 (16%) | 8 (12%)  | 0           | 4  |
| 19  | AS    | 77/93 (83%)   | 56 (73%)  | 15 (20%) | 6 (8%)   | 1           | 8  |
| 19  | CS    | 77/93 (83%)   | 47 (61%)  | 17 (22%) | 13 (17%) | 0           | 2  |
| 20  | AT    | 97/106 (92%)  | 68 (70%)  | 22 (23%) | 7 (7%)   | 1           | 9  |
| 20  | CT    | 97/106 (92%)  | 67 (69%)  | 18 (19%) | 12 (12%) | 0           | 4  |
| 21  | AU    | 23/27 (85%)   | 15 (65%)  | 4 (17%)  | 4 (17%)  | 0           | 2  |
| 21  | CU    | 23/27 (85%)   | 18 (78%)  | 3 (13%)  | 2 (9%)   | 0           | 7  |
| 27  | BC    | 183/229 (80%) | 85 (46%)  | 52 (28%) | 46 (25%) | 0           | 0  |
| 27  | DC    | 183/229 (80%) | 87 (48%)  | 45 (25%) | 51 (28%) | 0           | 0  |
| 28  | BD    | 270/276 (98%) | 200 (74%) | 38 (14%) | 32 (12%) | 0           | 4  |
| 28  | DD    | 270/276 (98%) | 202 (75%) | 44 (16%) | 24 (9%)  | 0           | 7  |
| 29  | BE    | 203/206 (98%) | 145 (71%) | 36 (18%) | 22 (11%) | 0           | 5  |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 29  | DE    | 203/206 (98%) | 134 (66%) | 36 (18%) | 33 (16%) | 0           | 2  |
| 30  | BF    | 206/210 (98%) | 142 (69%) | 44 (21%) | 20 (10%) | 0           | 6  |
| 30  | DF    | 200/210 (95%) | 160 (80%) | 29 (14%) | 11 (6%)  | 1           | 13 |
| 31  | BG    | 179/182 (98%) | 121 (68%) | 36 (20%) | 22 (12%) | 0           | 4  |
| 31  | DG    | 179/182 (98%) | 124 (69%) | 30 (17%) | 25 (14%) | 0           | 3  |
| 32  | BH    | 158/180 (88%) | 96 (61%)  | 37 (23%) | 25 (16%) | 0           | 2  |
| 32  | DH    | 166/180 (92%) | 96 (58%)  | 42 (25%) | 28 (17%) | 0           | 2  |
| 33  | BI    | 143/148 (97%) | 101 (71%) | 26 (18%) | 16 (11%) | 0           | 4  |
| 33  | DI    | 144/148 (97%) | 78 (54%)  | 39 (27%) | 27 (19%) | 0           | 1  |
| 34  | BN    | 137/140 (98%) | 91 (66%)  | 24 (18%) | 22 (16%) | 0           | 2  |
| 34  | DN    | 137/140 (98%) | 86 (63%)  | 39 (28%) | 12 (9%)  | 0           | 7  |
| 35  | BO    | 120/122 (98%) | 95 (79%)  | 17 (14%) | 8 (7%)   | 1           | 11 |
| 35  | DO    | 120/122 (98%) | 97 (81%)  | 18 (15%) | 5 (4%)   | 2           | 18 |
| 36  | BP    | 148/150 (99%) | 86 (58%)  | 26 (18%) | 36 (24%) | 0           | 0  |
| 36  | DP    | 148/150 (99%) | 86 (58%)  | 23 (16%) | 39 (26%) | 0           | 0  |
| 37  | BQ    | 139/141 (99%) | 104 (75%) | 24 (17%) | 11 (8%)  | 1           | 8  |
| 37  | DQ    | 139/141 (99%) | 109 (78%) | 18 (13%) | 12 (9%)  | 0           | 7  |
| 38  | BR    | 115/118 (98%) | 78 (68%)  | 25 (22%) | 12 (10%) | 0           | 5  |
| 38  | DR    | 116/118 (98%) | 86 (74%)  | 20 (17%) | 10 (9%)  | 0           | 7  |
| 39  | BS    | 97/112 (87%)  | 53 (55%)  | 16 (16%) | 28 (29%) | 0           | 0  |
| 39  | DS    | 109/112 (97%) | 71 (65%)  | 21 (19%) | 17 (16%) | 0           | 2  |
| 40  | BT    | 136/146 (93%) | 90 (66%)  | 28 (21%) | 18 (13%) | 0           | 3  |
| 40  | DT    | 136/146 (93%) | 95 (70%)  | 19 (14%) | 22 (16%) | 0           | 2  |
| 41  | BU    | 115/118 (98%) | 73 (64%)  | 30 (26%) | 12 (10%) | 0           | 5  |
| 41  | DU    | 115/118 (98%) | 75 (65%)  | 30 (26%) | 10 (9%)  | 0           | 7  |
| 42  | BV    | 99/101 (98%)  | 75 (76%)  | 9 (9%)   | 15 (15%) | 0           | 2  |
| 42  | DV    | 99/101 (98%)  | 80 (81%)  | 9 (9%)   | 10 (10%) | 0           | 6  |
| 43  | BW    | 111/113 (98%) | 81 (73%)  | 22 (20%) | 8 (7%)   | 1           | 9  |
| 43  | DW    | 111/113 (98%) | 82 (74%)  | 19 (17%) | 10 (9%)  | 0           | 7  |
| 44  | BX    | 91/96 (95%)   | 69 (76%)  | 16 (18%) | 6 (7%)   | 1           | 11 |
| 44  | DX    | 91/96 (95%)   | 76 (84%)  | 11 (12%) | 4 (4%)   | 2           | 17 |

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| Mol | Chain | Analysed          | Favoured   | Allowed    | Outliers   | Percentiles |    |
|-----|-------|-------------------|------------|------------|------------|-------------|----|
| 45  | BY    | 99/110 (90%)      | 50 (50%)   | 22 (22%)   | 27 (27%)   | 0           | 0  |
| 45  | DY    | 100/110 (91%)     | 64 (64%)   | 11 (11%)   | 25 (25%)   | 0           | 0  |
| 46  | BZ    | 175/206 (85%)     | 114 (65%)  | 40 (23%)   | 21 (12%)   | 0           | 4  |
| 46  | DZ    | 175/206 (85%)     | 101 (58%)  | 46 (26%)   | 28 (16%)   | 0           | 2  |
| 47  | B0    | 82/85 (96%)       | 64 (78%)   | 13 (16%)   | 5 (6%)     | 1           | 12 |
| 47  | D0    | 82/85 (96%)       | 67 (82%)   | 8 (10%)    | 7 (8%)     | 0           | 7  |
| 48  | B1    | 92/98 (94%)       | 68 (74%)   | 13 (14%)   | 11 (12%)   | 0           | 4  |
| 48  | D1    | 92/98 (94%)       | 69 (75%)   | 12 (13%)   | 11 (12%)   | 0           | 4  |
| 49  | B2    | 69/72 (96%)       | 49 (71%)   | 15 (22%)   | 5 (7%)     | 1           | 9  |
| 49  | D2    | 69/72 (96%)       | 57 (83%)   | 5 (7%)     | 7 (10%)    | 0           | 6  |
| 50  | B3    | 58/60 (97%)       | 48 (83%)   | 3 (5%)     | 7 (12%)    | 0           | 4  |
| 50  | D3    | 58/60 (97%)       | 46 (79%)   | 7 (12%)    | 5 (9%)     | 0           | 7  |
| 51  | B4    | 29/71 (41%)       | 17 (59%)   | 8 (28%)    | 4 (14%)    | 0           | 3  |
| 51  | D4    | 38/71 (54%)       | 21 (55%)   | 12 (32%)   | 5 (13%)    | 0           | 3  |
| 52  | B5    | 57/60 (95%)       | 46 (81%)   | 6 (10%)    | 5 (9%)     | 0           | 7  |
| 52  | D5    | 57/60 (95%)       | 46 (81%)   | 5 (9%)     | 6 (10%)    | 0           | 5  |
| 53  | B6    | 43/54 (80%)       | 17 (40%)   | 14 (33%)   | 12 (28%)   | 0           | 0  |
| 53  | D6    | 43/54 (80%)       | 18 (42%)   | 15 (35%)   | 10 (23%)   | 0           | 0  |
| 54  | B7    | 47/49 (96%)       | 38 (81%)   | 5 (11%)    | 4 (8%)     | 0           | 7  |
| 54  | D7    | 47/49 (96%)       | 43 (92%)   | 3 (6%)     | 1 (2%)     | 5           | 31 |
| 55  | B8    | 62/65 (95%)       | 42 (68%)   | 14 (23%)   | 6 (10%)    | 0           | 6  |
| 55  | D8    | 62/65 (95%)       | 41 (66%)   | 14 (23%)   | 7 (11%)    | 0           | 4  |
| 56  | B9    | 34/37 (92%)       | 23 (68%)   | 10 (29%)   | 1 (3%)     | 3           | 25 |
| 56  | D9    | 34/37 (92%)       | 27 (79%)   | 6 (18%)    | 1 (3%)     | 3           | 25 |
| All | All   | 11730/12586 (93%) | 8097 (69%) | 2283 (20%) | 1350 (12%) | 0           | 4  |

All (1350) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | AB    | 15  | VAL  |
| 2   | AB    | 195 | ASP  |
| 2   | AB    | 238 | LEU  |
| 3   | AC    | 18  | TRP  |
| 3   | AC    | 20  | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | AC    | 47  | LEU  |
| 3   | AC    | 61  | ALA  |
| 3   | AC    | 62  | ASP  |
| 3   | AC    | 154 | SER  |
| 3   | AC    | 207 | VAL  |
| 4   | AD    | 3   | ARG  |
| 4   | AD    | 109 | GLY  |
| 4   | AD    | 171 | GLY  |
| 4   | AD    | 178 | VAL  |
| 4   | AD    | 192 | GLU  |
| 5   | AE    | 6   | PHE  |
| 5   | AE    | 27  | ARG  |
| 5   | AE    | 85  | GLY  |
| 5   | AE    | 140 | ARG  |
| 5   | AE    | 146 | ALA  |
| 6   | AF    | 42  | GLU  |
| 6   | AF    | 62  | TRP  |
| 7   | AG    | 7   | ALA  |
| 7   | AG    | 41  | ARG  |
| 7   | AG    | 42  | ILE  |
| 7   | AG    | 58  | PRO  |
| 8   | AH    | 41  | ARG  |
| 8   | AH    | 133 | LEU  |
| 9   | AI    | 56  | LEU  |
| 9   | AI    | 89  | ASN  |
| 10  | AJ    | 32  | ALA  |
| 10  | AJ    | 36  | GLY  |
| 10  | AJ    | 51  | ARG  |
| 10  | AJ    | 59  | SER  |
| 12  | AL    | 8   | ASN  |
| 12  | AL    | 22  | SER  |
| 12  | AL    | 23  | LYS  |
| 12  | AL    | 42  | THR  |
| 12  | AL    | 47  | LYS  |
| 12  | AL    | 62  | SER  |
| 12  | AL    | 64  | TYR  |
| 12  | AL    | 65  | GLU  |
| 12  | AL    | 76  | ASN  |
| 12  | AL    | 80  | HIS  |
| 13  | AM    | 12  | ASN  |
| 13  | AM    | 66  | LEU  |
| 13  | AM    | 83  | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 13  | AM    | 95  | GLY  |
| 13  | AM    | 100 | GLY  |
| 13  | AM    | 104 | ARG  |
| 13  | AM    | 113 | PRO  |
| 13  | AM    | 117 | VAL  |
| 13  | AM    | 125 | ARG  |
| 14  | AN    | 14  | PRO  |
| 14  | AN    | 16  | PHE  |
| 14  | AN    | 23  | ARG  |
| 14  | AN    | 24  | CYS  |
| 16  | AP    | 67  | THR  |
| 17  | AQ    | 34  | LYS  |
| 17  | AQ    | 53  | LEU  |
| 17  | AQ    | 80  | GLY  |
| 18  | AR    | 20  | ALA  |
| 18  | AR    | 37  | VAL  |
| 19  | AS    | 28  | LYS  |
| 19  | AS    | 29  | ARG  |
| 19  | AS    | 61  | TYR  |
| 19  | AS    | 62  | ILE  |
| 20  | AT    | 49  | ALA  |
| 21  | AU    | 3   | LYS  |
| 21  | AU    | 7   | ARG  |
| 27  | BC    | 35  | ALA  |
| 27  | BC    | 55  | ASP  |
| 27  | BC    | 58  | VAL  |
| 27  | BC    | 74  | VAL  |
| 27  | BC    | 108 | MET  |
| 27  | BC    | 153 | ILE  |
| 27  | BC    | 171 | ILE  |
| 27  | BC    | 173 | ALA  |
| 27  | BC    | 174 | PRO  |
| 27  | BC    | 182 | PRO  |
| 27  | BC    | 209 | LEU  |
| 27  | BC    | 220 | PRO  |
| 28  | BD    | 25  | THR  |
| 28  | BD    | 169 | GLU  |
| 28  | BD    | 181 | GLU  |
| 28  | BD    | 211 | ARG  |
| 28  | BD    | 271 | ILE  |
| 29  | BE    | 4   | ILE  |
| 29  | BE    | 38  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 29  | BE    | 69  | LYS  |
| 29  | BE    | 71  | GLY  |
| 29  | BE    | 72  | VAL  |
| 29  | BE    | 73  | GLU  |
| 29  | BE    | 75  | VAL  |
| 29  | BE    | 76  | ARG  |
| 29  | BE    | 77  | ILE  |
| 29  | BE    | 130 | GLY  |
| 29  | BE    | 173 | VAL  |
| 29  | BE    | 187 | ALA  |
| 29  | BE    | 201 | THR  |
| 30  | BF    | 14  | PRO  |
| 30  | BF    | 20  | LEU  |
| 30  | BF    | 21  | ALA  |
| 30  | BF    | 54  | ARG  |
| 30  | BF    | 115 | ALA  |
| 30  | BF    | 126 | VAL  |
| 30  | BF    | 127 | GLU  |
| 30  | BF    | 132 | VAL  |
| 30  | BF    | 166 | ALA  |
| 31  | BG    | 52  | ILE  |
| 31  | BG    | 55  | LYS  |
| 31  | BG    | 82  | LEU  |
| 31  | BG    | 86  | MET  |
| 31  | BG    | 87  | PRO  |
| 31  | BG    | 114 | ILE  |
| 31  | BG    | 115 | ARG  |
| 32  | BH    | 55  | PRO  |
| 32  | BH    | 83  | TYR  |
| 32  | BH    | 98  | LEU  |
| 32  | BH    | 156 | ALA  |
| 32  | BH    | 159 | GLU  |
| 33  | BI    | 42  | SER  |
| 33  | BI    | 120 | ILE  |
| 33  | BI    | 122 | GLU  |
| 34  | BN    | 13  | TRP  |
| 34  | BN    | 47  | ALA  |
| 34  | BN    | 57  | ALA  |
| 34  | BN    | 58  | ASP  |
| 34  | BN    | 63  | THR  |
| 34  | BN    | 134 | ARG  |
| 34  | BN    | 136 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 35  | BO    | 5   | GLN  |
| 35  | BO    | 48  | PRO  |
| 35  | BO    | 115 | VAL  |
| 35  | BO    | 116 | SER  |
| 35  | BO    | 120 | GLU  |
| 36  | BP    | 10  | PRO  |
| 36  | BP    | 17  | LYS  |
| 36  | BP    | 19  | VAL  |
| 36  | BP    | 35  | HIS  |
| 36  | BP    | 47  | ASP  |
| 36  | BP    | 56  | SER  |
| 36  | BP    | 57  | THR  |
| 36  | BP    | 94  | GLU  |
| 36  | BP    | 108 | LYS  |
| 36  | BP    | 110 | TYR  |
| 36  | BP    | 111 | ARG  |
| 36  | BP    | 147 | LEU  |
| 37  | BQ    | 2   | LEU  |
| 37  | BQ    | 47  | ILE  |
| 37  | BQ    | 134 | ARG  |
| 37  | BQ    | 135 | ASP  |
| 38  | BR    | 8   | ARG  |
| 38  | BR    | 12  | ARG  |
| 38  | BR    | 107 | ASP  |
| 38  | BR    | 117 | VAL  |
| 39  | BS    | 19  | LYS  |
| 39  | BS    | 23  | ARG  |
| 39  | BS    | 57  | LYS  |
| 39  | BS    | 58  | LEU  |
| 39  | BS    | 67  | ARG  |
| 39  | BS    | 83  | LYS  |
| 39  | BS    | 88  | ASP  |
| 39  | BS    | 89  | ARG  |
| 39  | BS    | 90  | GLY  |
| 39  | BS    | 97  | ARG  |
| 39  | BS    | 102 | ALA  |
| 39  | BS    | 103 | GLU  |
| 40  | BT    | 17  | THR  |
| 40  | BT    | 24  | PRO  |
| 40  | BT    | 28  | VAL  |
| 40  | BT    | 29  | ARG  |
| 40  | BT    | 32  | TYR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 40  | BT    | 36  | GLU  |
| 40  | BT    | 58  | ASN  |
| 40  | BT    | 80  | SER  |
| 40  | BT    | 88  | ILE  |
| 40  | BT    | 94  | ALA  |
| 40  | BT    | 107 | ASP  |
| 40  | BT    | 115 | ARG  |
| 41  | BU    | 8   | VAL  |
| 41  | BU    | 26  | GLY  |
| 41  | BU    | 86  | ALA  |
| 42  | BV    | 16  | PRO  |
| 42  | BV    | 19  | LYS  |
| 42  | BV    | 35  | LEU  |
| 42  | BV    | 46  | VAL  |
| 42  | BV    | 79  | VAL  |
| 43  | BW    | 6   | ILE  |
| 43  | BW    | 111 | HIS  |
| 44  | BX    | 12  | VAL  |
| 45  | BY    | 3   | VAL  |
| 45  | BY    | 7   | VAL  |
| 45  | BY    | 17  | SER  |
| 45  | BY    | 44  | ILE  |
| 45  | BY    | 53  | PRO  |
| 45  | BY    | 56  | PRO  |
| 45  | BY    | 77  | PRO  |
| 45  | BY    | 78  | ALA  |
| 45  | BY    | 82  | PRO  |
| 45  | BY    | 90  | LEU  |
| 45  | BY    | 101 | LYS  |
| 46  | BZ    | 16  | SER  |
| 46  | BZ    | 38  | TYR  |
| 46  | BZ    | 93  | ASP  |
| 46  | BZ    | 152 | ALA  |
| 46  | BZ    | 158 | PRO  |
| 47  | B0    | 55  | ARG  |
| 48  | B1    | 26  | ARG  |
| 48  | B1    | 52  | ARG  |
| 48  | B1    | 56  | GLN  |
| 48  | B1    | 85  | LEU  |
| 49  | B2    | 43  | GLN  |
| 49  | B2    | 44  | LEU  |
| 49  | B2    | 47  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 50  | B3    | 38  | GLU  |
| 50  | B3    | 39  | ASP  |
| 50  | B3    | 52  | HIS  |
| 52  | B5    | 57  | VAL  |
| 53  | B6    | 16  | CYS  |
| 53  | B6    | 28  | ARG  |
| 53  | B6    | 44  | ARG  |
| 54  | B7    | 22  | MET  |
| 55  | B8    | 47  | LYS  |
| 2   | CB    | 15  | VAL  |
| 2   | CB    | 77  | ALA  |
| 2   | CB    | 169 | LYS  |
| 2   | CB    | 195 | ASP  |
| 2   | CB    | 204 | ASN  |
| 2   | CB    | 216 | SER  |
| 2   | CB    | 236 | TYR  |
| 2   | CB    | 237 | ALA  |
| 2   | CB    | 239 | VAL  |
| 3   | CC    | 29  | TYR  |
| 3   | CC    | 47  | LEU  |
| 3   | CC    | 121 | ALA  |
| 3   | CC    | 154 | SER  |
| 3   | CC    | 189 | ALA  |
| 4   | CD    | 4   | TYR  |
| 4   | CD    | 9   | CYS  |
| 4   | CD    | 10  | ARG  |
| 4   | CD    | 14  | ARG  |
| 4   | CD    | 24  | GLU  |
| 4   | CD    | 30  | LYS  |
| 4   | CD    | 81  | GLU  |
| 4   | CD    | 93  | PHE  |
| 5   | CE    | 6   | PHE  |
| 5   | CE    | 73  | ASN  |
| 5   | CE    | 153 | LYS  |
| 7   | CG    | 111 | ARG  |
| 7   | CG    | 116 | ALA  |
| 7   | CG    | 154 | TYR  |
| 8   | CH    | 105 | ARG  |
| 9   | CI    | 117 | HIS  |
| 10  | CJ    | 32  | ALA  |
| 10  | CJ    | 57  | LYS  |
| 10  | CJ    | 59  | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 12  | CL    | 47  | LYS  |
| 12  | CL    | 51  | ALA  |
| 12  | CL    | 120 | TYR  |
| 13  | CM    | 4   | ILE  |
| 13  | CM    | 12  | ASN  |
| 13  | CM    | 28  | ALA  |
| 13  | CM    | 60  | VAL  |
| 13  | CM    | 67  | GLU  |
| 13  | CM    | 101 | GLN  |
| 13  | CM    | 116 | THR  |
| 13  | CM    | 118 | ALA  |
| 13  | CM    | 122 | LYS  |
| 14  | CN    | 14  | PRO  |
| 14  | CN    | 16  | PHE  |
| 14  | CN    | 29  | ARG  |
| 14  | CN    | 60  | SER  |
| 15  | CO    | 62  | GLN  |
| 17  | CQ    | 34  | LYS  |
| 18  | CR    | 20  | ALA  |
| 18  | CR    | 41  | LYS  |
| 18  | CR    | 87  | ARG  |
| 19  | CS    | 9   | VAL  |
| 19  | CS    | 10  | PHE  |
| 19  | CS    | 29  | ARG  |
| 19  | CS    | 80  | TYR  |
| 20  | CT    | 50  | GLU  |
| 20  | CT    | 97  | ALA  |
| 21  | CU    | 3   | LYS  |
| 21  | CU    | 25  | LYS  |
| 27  | DC    | 35  | ALA  |
| 27  | DC    | 38  | ASP  |
| 27  | DC    | 46  | LYS  |
| 27  | DC    | 58  | VAL  |
| 27  | DC    | 108 | MET  |
| 27  | DC    | 133 | PRO  |
| 27  | DC    | 140 | PRO  |
| 27  | DC    | 142 | ALA  |
| 27  | DC    | 148 | ASN  |
| 27  | DC    | 153 | ILE  |
| 27  | DC    | 156 | ILE  |
| 27  | DC    | 167 | LYS  |
| 27  | DC    | 173 | ALA  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 27  | DC    | 174 | PRO  |
| 27  | DC    | 182 | PRO  |
| 27  | DC    | 220 | PRO  |
| 28  | DD    | 10  | THR  |
| 28  | DD    | 25  | THR  |
| 28  | DD    | 33  | LEU  |
| 28  | DD    | 225 | ALA  |
| 28  | DD    | 239 | ARG  |
| 28  | DD    | 267 | SER  |
| 28  | DD    | 271 | ILE  |
| 29  | DE    | 4   | ILE  |
| 29  | DE    | 18  | ASP  |
| 29  | DE    | 53  | PRO  |
| 29  | DE    | 54  | GLN  |
| 29  | DE    | 56  | PRO  |
| 29  | DE    | 59  | VAL  |
| 29  | DE    | 60  | ASN  |
| 29  | DE    | 71  | GLY  |
| 29  | DE    | 73  | GLU  |
| 29  | DE    | 75  | VAL  |
| 29  | DE    | 77  | ILE  |
| 29  | DE    | 84  | PHE  |
| 29  | DE    | 89  | ASP  |
| 29  | DE    | 118 | LYS  |
| 29  | DE    | 132 | HIS  |
| 30  | DF    | 24  | LEU  |
| 30  | DF    | 73  | ALA  |
| 30  | DF    | 89  | VAL  |
| 30  | DF    | 128 | ALA  |
| 30  | DF    | 132 | VAL  |
| 30  | DF    | 134 | GLY  |
| 31  | DG    | 14  | GLU  |
| 31  | DG    | 96  | ARG  |
| 32  | DH    | 10  | PRO  |
| 32  | DH    | 12  | PRO  |
| 32  | DH    | 16  | SER  |
| 32  | DH    | 17  | VAL  |
| 32  | DH    | 20  | ALA  |
| 32  | DH    | 27  | LYS  |
| 32  | DH    | 83  | TYR  |
| 32  | DH    | 86  | GLU  |
| 32  | DH    | 92  | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 32  | DH    | 138 | LYS  |
| 32  | DH    | 153 | LYS  |
| 32  | DH    | 154 | PRO  |
| 32  | DH    | 155 | SER  |
| 32  | DH    | 156 | ALA  |
| 32  | DH    | 167 | GLU  |
| 32  | DH    | 169 | VAL  |
| 33  | DI    | 13  | GLY  |
| 33  | DI    | 15  | VAL  |
| 33  | DI    | 77  | LEU  |
| 33  | DI    | 78  | THR  |
| 33  | DI    | 79  | ILE  |
| 33  | DI    | 115 | ALA  |
| 33  | DI    | 134 | PRO  |
| 34  | DN    | 57  | ALA  |
| 34  | DN    | 58  | ASP  |
| 34  | DN    | 132 | ALA  |
| 36  | DP    | 10  | PRO  |
| 36  | DP    | 22  | GLY  |
| 36  | DP    | 35  | HIS  |
| 36  | DP    | 47  | ASP  |
| 36  | DP    | 56  | SER  |
| 36  | DP    | 57  | THR  |
| 36  | DP    | 94  | GLU  |
| 36  | DP    | 108 | LYS  |
| 36  | DP    | 110 | TYR  |
| 36  | DP    | 111 | ARG  |
| 36  | DP    | 147 | LEU  |
| 37  | DQ    | 2   | LEU  |
| 37  | DQ    | 6   | ARG  |
| 37  | DQ    | 134 | ARG  |
| 37  | DQ    | 135 | ASP  |
| 37  | DQ    | 138 | ASP  |
| 38  | DR    | 3   | HIS  |
| 38  | DR    | 4   | LEU  |
| 38  | DR    | 82  | GLU  |
| 38  | DR    | 107 | ASP  |
| 39  | DS    | 11  | LYS  |
| 39  | DS    | 14  | VAL  |
| 39  | DS    | 19  | LYS  |
| 39  | DS    | 61  | ASN  |
| 39  | DS    | 88  | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 39  | DS    | 89  | ARG  |
| 39  | DS    | 107 | GLU  |
| 40  | DT    | 17  | THR  |
| 40  | DT    | 24  | PRO  |
| 40  | DT    | 29  | ARG  |
| 40  | DT    | 30  | VAL  |
| 40  | DT    | 41  | ARG  |
| 40  | DT    | 80  | SER  |
| 40  | DT    | 82  | LEU  |
| 40  | DT    | 85  | LYS  |
| 40  | DT    | 88  | ILE  |
| 40  | DT    | 107 | ASP  |
| 40  | DT    | 115 | ARG  |
| 42  | DV    | 45  | THR  |
| 42  | DV    | 49  | THR  |
| 42  | DV    | 79  | VAL  |
| 45  | DY    | 5   | MET  |
| 45  | DY    | 11  | ASP  |
| 45  | DY    | 20  | TYR  |
| 45  | DY    | 45  | VAL  |
| 45  | DY    | 49  | VAL  |
| 45  | DY    | 50  | ARG  |
| 45  | DY    | 57  | GLN  |
| 45  | DY    | 63  | LYS  |
| 45  | DY    | 77  | PRO  |
| 45  | DY    | 78  | ALA  |
| 45  | DY    | 80  | GLY  |
| 46  | DZ    | 20  | ARG  |
| 46  | DZ    | 32  | HIS  |
| 46  | DZ    | 41  | LEU  |
| 46  | DZ    | 49  | ARG  |
| 46  | DZ    | 65  | GLN  |
| 46  | DZ    | 81  | ARG  |
| 46  | DZ    | 105 | VAL  |
| 46  | DZ    | 108 | PRO  |
| 46  | DZ    | 146 | ILE  |
| 46  | DZ    | 152 | ALA  |
| 46  | DZ    | 159 | PRO  |
| 47  | D0    | 55  | ARG  |
| 47  | D0    | 74  | ARG  |
| 48  | D1    | 24  | ALA  |
| 48  | D1    | 31  | GLY  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 48  | D1    | 58  | ILE  |
| 48  | D1    | 83  | GLU  |
| 48  | D1    | 85  | LEU  |
| 49  | D2    | 43  | GLN  |
| 49  | D2    | 44  | LEU  |
| 49  | D2    | 47  | ASN  |
| 51  | D4    | 20  | ASN  |
| 51  | D4    | 26  | SER  |
| 52  | D5    | 34  | PRO  |
| 52  | D5    | 57  | VAL  |
| 53  | D6    | 28  | ARG  |
| 55  | D8    | 3   | LYS  |
| 55  | D8    | 61  | LEU  |
| 2   | AB    | 122 | PHE  |
| 2   | AB    | 150 | SER  |
| 2   | AB    | 154 | LEU  |
| 2   | AB    | 165 | VAL  |
| 2   | AB    | 173 | ALA  |
| 2   | AB    | 174 | VAL  |
| 2   | AB    | 189 | ASP  |
| 2   | AB    | 239 | VAL  |
| 3   | AC    | 4   | LYS  |
| 3   | AC    | 15  | THR  |
| 3   | AC    | 45  | LYS  |
| 3   | AC    | 145 | GLY  |
| 3   | AC    | 156 | ARG  |
| 3   | AC    | 157 | ILE  |
| 4   | AD    | 4   | TYR  |
| 4   | AD    | 5   | ILE  |
| 4   | AD    | 7   | PRO  |
| 4   | AD    | 10  | ARG  |
| 4   | AD    | 39  | PRO  |
| 4   | AD    | 101 | LEU  |
| 4   | AD    | 193 | ASP  |
| 5   | AE    | 139 | LEU  |
| 6   | AF    | 29  | ALA  |
| 6   | AF    | 38  | GLU  |
| 7   | AG    | 33  | ASP  |
| 7   | AG    | 45  | ASP  |
| 9   | AI    | 100 | GLY  |
| 9   | AI    | 121 | ARG  |
| 11  | AK    | 12  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 12  | AL    | 18  | VAL  |
| 13  | AM    | 6   | GLY  |
| 14  | AN    | 22  | THR  |
| 16  | AP    | 43  | LYS  |
| 18  | AR    | 38  | GLU  |
| 19  | AS    | 30  | LEU  |
| 19  | AS    | 80  | TYR  |
| 20  | AT    | 48  | LYS  |
| 20  | AT    | 63  | ILE  |
| 20  | AT    | 103 | GLY  |
| 21  | AU    | 25  | LYS  |
| 27  | BC    | 20  | TYR  |
| 27  | BC    | 78  | ALA  |
| 27  | BC    | 125 | SER  |
| 27  | BC    | 133 | PRO  |
| 27  | BC    | 156 | ILE  |
| 27  | BC    | 170 | ALA  |
| 27  | BC    | 184 | LYS  |
| 27  | BC    | 198 | ALA  |
| 27  | BC    | 216 | THR  |
| 28  | BD    | 26  | LYS  |
| 29  | BE    | 2   | LYS  |
| 29  | BE    | 87  | GLU  |
| 29  | BE    | 178 | GLU  |
| 30  | BF    | 86  | GLY  |
| 30  | BF    | 89  | VAL  |
| 30  | BF    | 134 | GLY  |
| 31  | BG    | 10  | LYS  |
| 31  | BG    | 14  | GLU  |
| 31  | BG    | 47  | LYS  |
| 31  | BG    | 49  | ASP  |
| 31  | BG    | 110 | ALA  |
| 31  | BG    | 117 | PHE  |
| 31  | BG    | 129 | GLY  |
| 32  | BH    | 21  | PRO  |
| 32  | BH    | 45  | VAL  |
| 32  | BH    | 85  | LYS  |
| 32  | BH    | 92  | ILE  |
| 32  | BH    | 155 | SER  |
| 32  | BH    | 164 | TYR  |
| 32  | BH    | 170 | ARG  |
| 33  | BI    | 137 | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 34  | BN    | 42  | TRP  |
| 34  | BN    | 98  | VAL  |
| 34  | BN    | 135 | PRO  |
| 35  | BO    | 89  | ASN  |
| 35  | BO    | 117 | LEU  |
| 36  | BP    | 5   | ASP  |
| 36  | BP    | 6   | LEU  |
| 36  | BP    | 15  | ARG  |
| 36  | BP    | 16  | ARG  |
| 36  | BP    | 29  | LYS  |
| 36  | BP    | 34  | GLY  |
| 36  | BP    | 58  | THR  |
| 36  | BP    | 64  | LYS  |
| 36  | BP    | 90  | ARG  |
| 36  | BP    | 116 | GLY  |
| 36  | BP    | 119 | GLU  |
| 36  | BP    | 141 | ALA  |
| 36  | BP    | 146 | VAL  |
| 37  | BQ    | 59  | ARG  |
| 37  | BQ    | 60  | ARG  |
| 37  | BQ    | 111 | GLU  |
| 38  | BR    | 7   | GLY  |
| 38  | BR    | 10  | LEU  |
| 38  | BR    | 14  | SER  |
| 38  | BR    | 69  | ASP  |
| 38  | BR    | 82  | GLU  |
| 39  | BS    | 14  | VAL  |
| 39  | BS    | 18  | ILE  |
| 39  | BS    | 59  | LYS  |
| 39  | BS    | 66  | ALA  |
| 39  | BS    | 85  | VAL  |
| 39  | BS    | 93  | LYS  |
| 39  | BS    | 96  | GLY  |
| 39  | BS    | 104 | GLY  |
| 40  | BT    | 55  | ASN  |
| 41  | BU    | 46  | ALA  |
| 42  | BV    | 18  | LEU  |
| 42  | BV    | 48  | GLY  |
| 42  | BV    | 53  | GLU  |
| 43  | BW    | 12  | ILE  |
| 43  | BW    | 43  | GLY  |
| 43  | BW    | 112 | GLY  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 45  | BY    | 18  | GLY  |
| 45  | BY    | 29  | GLU  |
| 45  | BY    | 48  | ALA  |
| 45  | BY    | 99  | CYS  |
| 46  | BZ    | 45  | ASP  |
| 46  | BZ    | 53  | ILE  |
| 46  | BZ    | 64  | GLY  |
| 46  | BZ    | 111 | VAL  |
| 46  | BZ    | 166 | SER  |
| 46  | BZ    | 168 | GLU  |
| 48  | B1    | 28  | GLY  |
| 48  | B1    | 53  | VAL  |
| 48  | B1    | 58  | ILE  |
| 48  | B1    | 84  | GLY  |
| 49  | B2    | 49  | LYS  |
| 49  | B2    | 70  | GLN  |
| 52  | B5    | 34  | PRO  |
| 53  | B6    | 17  | LYS  |
| 53  | B6    | 41  | PRO  |
| 53  | B6    | 52  | VAL  |
| 54  | B7    | 31  | LEU  |
| 55  | B8    | 14  | VAL  |
| 55  | B8    | 17  | THR  |
| 55  | B8    | 34  | TRP  |
| 2   | CB    | 9   | GLU  |
| 2   | CB    | 18  | GLY  |
| 2   | CB    | 168 | THR  |
| 2   | CB    | 194 | PRO  |
| 2   | CB    | 209 | ARG  |
| 3   | CC    | 15  | THR  |
| 3   | CC    | 61  | ALA  |
| 3   | CC    | 156 | ARG  |
| 3   | CC    | 181 | ASN  |
| 3   | CC    | 190 | ARG  |
| 3   | CC    | 207 | VAL  |
| 4   | CD    | 3   | ARG  |
| 4   | CD    | 5   | ILE  |
| 4   | CD    | 26  | CYS  |
| 4   | CD    | 166 | LYS  |
| 5   | CE    | 16  | THR  |
| 5   | CE    | 17  | ALA  |
| 5   | CE    | 146 | ALA  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | CE    | 154 | GLY  |
| 6   | CF    | 40  | VAL  |
| 7   | CG    | 147 | ALA  |
| 8   | CH    | 50  | ARG  |
| 9   | CI    | 78  | LYS  |
| 9   | CI    | 100 | GLY  |
| 9   | CI    | 127 | LYS  |
| 10  | CJ    | 23  | ILE  |
| 10  | CJ    | 27  | ALA  |
| 10  | CJ    | 39  | PRO  |
| 12  | CL    | 6   | THR  |
| 12  | CL    | 28  | LYS  |
| 12  | CL    | 52  | LEU  |
| 12  | CL    | 65  | GLU  |
| 13  | CM    | 6   | GLY  |
| 13  | CM    | 106 | ASN  |
| 14  | CN    | 59  | ALA  |
| 15  | CO    | 76  | GLU  |
| 15  | CO    | 88  | ARG  |
| 17  | CQ    | 94  | ASN  |
| 18  | CR    | 32  | ARG  |
| 19  | CS    | 14  | HIS  |
| 19  | CS    | 26  | GLY  |
| 19  | CS    | 30  | LEU  |
| 20  | CT    | 51  | GLU  |
| 20  | CT    | 84  | LEU  |
| 20  | CT    | 99  | LEU  |
| 27  | DC    | 20  | TYR  |
| 27  | DC    | 55  | ASP  |
| 27  | DC    | 63  | SER  |
| 27  | DC    | 78  | ALA  |
| 27  | DC    | 120 | MET  |
| 27  | DC    | 128 | GLY  |
| 27  | DC    | 179 | SER  |
| 27  | DC    | 183 | GLU  |
| 27  | DC    | 217 | THR  |
| 27  | DC    | 222 | VAL  |
| 28  | DD    | 24  | ILE  |
| 28  | DD    | 27  | THR  |
| 28  | DD    | 32  | SER  |
| 28  | DD    | 169 | GLU  |
| 29  | DE    | 2   | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 29  | DE    | 29  | GLY  |
| 29  | DE    | 35  | GLN  |
| 29  | DE    | 57  | LYS  |
| 29  | DE    | 76  | ARG  |
| 29  | DE    | 82  | ARG  |
| 29  | DE    | 162 | ALA  |
| 30  | DF    | 181 | LEU  |
| 31  | DG    | 4   | ASP  |
| 31  | DG    | 5   | VAL  |
| 31  | DG    | 24  | GLY  |
| 31  | DG    | 97  | ASP  |
| 31  | DG    | 110 | ALA  |
| 31  | DG    | 124 | SER  |
| 31  | DG    | 137 | GLU  |
| 31  | DG    | 150 | ASP  |
| 32  | DH    | 21  | PRO  |
| 32  | DH    | 87  | LEU  |
| 32  | DH    | 90  | LYS  |
| 32  | DH    | 126 | PRO  |
| 32  | DH    | 151 | ILE  |
| 33  | DI    | 9   | LEU  |
| 33  | DI    | 36  | ALA  |
| 33  | DI    | 102 | SER  |
| 33  | DI    | 104 | GLN  |
| 34  | DN    | 42  | TRP  |
| 34  | DN    | 68  | GLU  |
| 35  | DO    | 27  | GLY  |
| 35  | DO    | 48  | PRO  |
| 35  | DO    | 120 | GLU  |
| 36  | DP    | 5   | ASP  |
| 36  | DP    | 6   | LEU  |
| 36  | DP    | 12  | ALA  |
| 36  | DP    | 16  | ARG  |
| 36  | DP    | 17  | LYS  |
| 36  | DP    | 29  | LYS  |
| 36  | DP    | 34  | GLY  |
| 36  | DP    | 64  | LYS  |
| 36  | DP    | 90  | ARG  |
| 36  | DP    | 116 | GLY  |
| 36  | DP    | 119 | GLU  |
| 36  | DP    | 141 | ALA  |
| 36  | DP    | 146 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 37  | DQ    | 5   | ARG  |
| 37  | DQ    | 57  | HIS  |
| 37  | DQ    | 60  | ARG  |
| 37  | DQ    | 78  | PRO  |
| 38  | DR    | 78  | LYS  |
| 39  | DS    | 4   | LEU  |
| 39  | DS    | 12  | PHE  |
| 39  | DS    | 57  | LYS  |
| 39  | DS    | 96  | GLY  |
| 39  | DS    | 109 | GLY  |
| 40  | DT    | 33  | LYS  |
| 40  | DT    | 55  | ASN  |
| 40  | DT    | 58  | ASN  |
| 40  | DT    | 94  | ALA  |
| 40  | DT    | 131 | ALA  |
| 41  | DU    | 9   | VAL  |
| 41  | DU    | 25  | TRP  |
| 41  | DU    | 54  | LYS  |
| 41  | DU    | 58  | ARG  |
| 41  | DU    | 90  | VAL  |
| 42  | DV    | 48  | GLY  |
| 42  | DV    | 50  | PRO  |
| 42  | DV    | 53  | GLU  |
| 43  | DW    | 63  | ASP  |
| 43  | DW    | 111 | HIS  |
| 44  | DX    | 4   | ALA  |
| 44  | DX    | 22  | ALA  |
| 45  | DY    | 41  | GLY  |
| 45  | DY    | 47  | LYS  |
| 45  | DY    | 58  | GLY  |
| 45  | DY    | 91  | GLU  |
| 45  | DY    | 98  | VAL  |
| 45  | DY    | 102 | CYS  |
| 46  | DZ    | 52  | SER  |
| 46  | DZ    | 138 | GLU  |
| 47  | D0    | 64  | ASP  |
| 48  | D1    | 28  | GLY  |
| 48  | D1    | 52  | ARG  |
| 48  | D1    | 84  | GLY  |
| 49  | D2    | 68  | ARG  |
| 49  | D2    | 70  | GLN  |
| 53  | D6    | 16  | CYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 53  | D6    | 19  | ARG  |
| 53  | D6    | 25  | LYS  |
| 53  | D6    | 26  | ASN  |
| 53  | D6    | 52  | VAL  |
| 55  | D8    | 31  | HIS  |
| 55  | D8    | 33  | ASN  |
| 55  | D8    | 34  | TRP  |
| 55  | D8    | 64  | TYR  |
| 56  | D9    | 25  | VAL  |
| 2   | AB    | 194 | PRO  |
| 2   | AB    | 222 | ILE  |
| 3   | AC    | 29  | TYR  |
| 4   | AD    | 24  | GLU  |
| 4   | AD    | 138 | TYR  |
| 5   | AE    | 73  | ASN  |
| 6   | AF    | 69  | GLU  |
| 7   | AG    | 52  | GLU  |
| 7   | AG    | 53  | LYS  |
| 8   | AH    | 49  | GLU  |
| 9   | AI    | 33  | PHE  |
| 9   | AI    | 78  | LYS  |
| 9   | AI    | 85  | LEU  |
| 11  | AK    | 127 | LYS  |
| 12  | AL    | 27  | LEU  |
| 12  | AL    | 87  | GLY  |
| 13  | AM    | 29  | ARG  |
| 13  | AM    | 90  | LEU  |
| 14  | AN    | 29  | ARG  |
| 14  | AN    | 60  | SER  |
| 18  | AR    | 87  | ARG  |
| 20  | AT    | 97  | ALA  |
| 21  | AU    | 9   | ARG  |
| 27  | BC    | 128 | GLY  |
| 27  | BC    | 140 | PRO  |
| 27  | BC    | 188 | ASN  |
| 28  | BD    | 32  | SER  |
| 28  | BD    | 33  | LEU  |
| 28  | BD    | 34  | VAL  |
| 28  | BD    | 122 | ASP  |
| 28  | BD    | 159 | ALA  |
| 28  | BD    | 202 | LYS  |
| 28  | BD    | 210 | GLY  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 28  | BD    | 239 | ARG  |
| 28  | BD    | 244 | ARG  |
| 28  | BD    | 257 | LEU  |
| 29  | BE    | 52  | LEU  |
| 29  | BE    | 61  | ARG  |
| 29  | BE    | 202 | LYS  |
| 30  | BF    | 19  | GLU  |
| 30  | BF    | 102 | PRO  |
| 31  | BG    | 28  | VAL  |
| 31  | BG    | 96  | ARG  |
| 31  | BG    | 126 | ASP  |
| 31  | BG    | 151 | ALA  |
| 31  | BG    | 171 | ALA  |
| 32  | BH    | 14  | GLY  |
| 32  | BH    | 63  | SER  |
| 32  | BH    | 154 | PRO  |
| 33  | BI    | 14  | ASP  |
| 34  | BN    | 8   | GLN  |
| 34  | BN    | 16  | ILE  |
| 34  | BN    | 17  | ASP  |
| 34  | BN    | 68  | GLU  |
| 35  | BO    | 64  | ARG  |
| 36  | BP    | 67  | MET  |
| 37  | BQ    | 14  | ARG  |
| 38  | BR    | 6   | SER  |
| 39  | BS    | 12  | PHE  |
| 39  | BS    | 61  | ASN  |
| 39  | BS    | 62  | LYS  |
| 40  | BT    | 20  | PRO  |
| 40  | BT    | 129 | ARG  |
| 41  | BU    | 25  | TRP  |
| 41  | BU    | 87  | GLY  |
| 41  | BU    | 92  | ARG  |
| 41  | BU    | 112 | ARG  |
| 42  | BV    | 2   | PHE  |
| 42  | BV    | 78  | LYS  |
| 43  | BW    | 49  | LYS  |
| 43  | BW    | 63  | ASP  |
| 44  | BX    | 4   | ALA  |
| 44  | BX    | 11  | PRO  |
| 45  | BY    | 35  | TYR  |
| 46  | BZ    | 30  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 46  | BZ    | 136 | PHE  |
| 46  | BZ    | 163 | LEU  |
| 46  | BZ    | 165 | VAL  |
| 46  | BZ    | 177 | PRO  |
| 47  | B0    | 20  | ARG  |
| 47  | B0    | 75  | LEU  |
| 51  | B4    | 52  | SER  |
| 51  | B4    | 54  | LYS  |
| 52  | B5    | 36  | CYS  |
| 53  | B6    | 20  | ASN  |
| 53  | B6    | 31  | PRO  |
| 54  | B7    | 17  | GLY  |
| 55  | B8    | 56  | GLU  |
| 2   | CB    | 87  | ARG  |
| 2   | CB    | 106 | LYS  |
| 2   | CB    | 143 | GLU  |
| 2   | CB    | 173 | ALA  |
| 2   | CB    | 189 | ASP  |
| 2   | CB    | 217 | ARG  |
| 2   | CB    | 240 | GLN  |
| 3   | CC    | 20  | SER  |
| 3   | CC    | 81  | GLY  |
| 4   | CD    | 13  | ARG  |
| 4   | CD    | 125 | HIS  |
| 5   | CE    | 37  | ARG  |
| 5   | CE    | 106 | PRO  |
| 6   | CF    | 42  | GLU  |
| 6   | CF    | 53  | ALA  |
| 6   | CF    | 78  | GLU  |
| 8   | CH    | 2   | LEU  |
| 8   | CH    | 34  | GLU  |
| 9   | CI    | 12  | GLU  |
| 9   | CI    | 34  | ASN  |
| 9   | CI    | 61  | ALA  |
| 9   | CI    | 92  | TYR  |
| 9   | CI    | 107 | ARG  |
| 10  | CJ    | 36  | GLY  |
| 12  | CL    | 23  | LYS  |
| 13  | CM    | 14  | ARG  |
| 13  | CM    | 30  | ALA  |
| 13  | CM    | 59  | TYR  |
| 13  | CM    | 100 | GLY  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 13  | CM    | 107 | ALA  |
| 16  | CP    | 58  | TYR  |
| 16  | CP    | 83  | GLU  |
| 17  | CQ    | 49  | GLU  |
| 17  | CQ    | 64  | PRO  |
| 18  | CR    | 70  | ILE  |
| 19  | CS    | 6   | LYS  |
| 19  | CS    | 13  | ASP  |
| 19  | CS    | 28  | LYS  |
| 20  | CT    | 39  | LYS  |
| 20  | CT    | 83  | ARG  |
| 20  | CT    | 96  | GLY  |
| 27  | DC    | 89  | ALA  |
| 27  | DC    | 151 | GLU  |
| 27  | DC    | 170 | ALA  |
| 27  | DC    | 175 | VAL  |
| 27  | DC    | 188 | ASN  |
| 27  | DC    | 209 | LEU  |
| 28  | DD    | 3   | VAL  |
| 28  | DD    | 58  | HIS  |
| 28  | DD    | 191 | ALA  |
| 28  | DD    | 238 | GLY  |
| 28  | DD    | 272 | ALA  |
| 29  | DE    | 44  | TYR  |
| 29  | DE    | 66  | HIS  |
| 31  | DG    | 48  | GLU  |
| 31  | DG    | 113 | ARG  |
| 31  | DG    | 115 | ARG  |
| 31  | DG    | 143 | GLU  |
| 32  | DH    | 168 | PRO  |
| 33  | DI    | 39  | ALA  |
| 33  | DI    | 87  | LYS  |
| 33  | DI    | 98  | ALA  |
| 33  | DI    | 109 | ILE  |
| 33  | DI    | 110 | ASP  |
| 33  | DI    | 113 | ARG  |
| 33  | DI    | 131 | LYS  |
| 34  | DN    | 8   | GLN  |
| 34  | DN    | 127 | ASP  |
| 34  | DN    | 133 | GLN  |
| 35  | DO    | 5   | GLN  |
| 36  | DP    | 15  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 36  | DP    | 42  | SER  |
| 36  | DP    | 53  | GLY  |
| 36  | DP    | 67  | MET  |
| 37  | DQ    | 59  | ARG  |
| 38  | DR    | 17  | ARG  |
| 38  | DR    | 102 | GLU  |
| 39  | DS    | 20  | ARG  |
| 40  | DT    | 28  | VAL  |
| 40  | DT    | 97  | ALA  |
| 40  | DT    | 116 | ALA  |
| 40  | DT    | 136 | GLN  |
| 42  | DV    | 54  | GLY  |
| 43  | DW    | 6   | ILE  |
| 43  | DW    | 11  | ARG  |
| 43  | DW    | 35  | ILE  |
| 44  | DX    | 40  | LYS  |
| 45  | DY    | 48  | ALA  |
| 45  | DY    | 92  | ASN  |
| 46  | DZ    | 48  | PHE  |
| 46  | DZ    | 80  | ARG  |
| 46  | DZ    | 110 | GLY  |
| 46  | DZ    | 157 | LEU  |
| 46  | DZ    | 166 | SER  |
| 47  | D0    | 13  | GLY  |
| 47  | D0    | 83  | PRO  |
| 48  | D1    | 65  | SER  |
| 51  | D4    | 28  | LYS  |
| 51  | D4    | 36  | CYS  |
| 52  | D5    | 33  | CYS  |
| 53  | D6    | 44  | ARG  |
| 2   | AB    | 83  | MET  |
| 2   | AB    | 130 | ARG  |
| 3   | AC    | 14  | ILE  |
| 3   | AC    | 91  | LEU  |
| 3   | AC    | 113 | ALA  |
| 3   | AC    | 181 | ASN  |
| 4   | AD    | 9   | CYS  |
| 4   | AD    | 102 | ASP  |
| 4   | AD    | 159 | ARG  |
| 5   | AE    | 74  | GLY  |
| 5   | AE    | 121 | LYS  |
| 5   | AE    | 138 | ALA  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | AF    | 27  | GLN  |
| 7   | AG    | 96  | GLN  |
| 8   | AH    | 8   | ASP  |
| 10  | AJ    | 57  | LYS  |
| 11  | AK    | 27  | ASN  |
| 11  | AK    | 117 | ASN  |
| 12  | AL    | 102 | ARG  |
| 12  | AL    | 127 | GLU  |
| 13  | AM    | 67  | GLU  |
| 13  | AM    | 120 | LYS  |
| 15  | AO    | 16  | ALA  |
| 16  | AP    | 72  | ARG  |
| 17  | AQ    | 14  | LYS  |
| 17  | AQ    | 87  | LYS  |
| 27  | BC    | 66  | HIS  |
| 27  | BC    | 68  | LEU  |
| 27  | BC    | 183 | GLU  |
| 27  | BC    | 197 | GLU  |
| 27  | BC    | 213 | TYR  |
| 27  | BC    | 217 | THR  |
| 28  | BD    | 3   | VAL  |
| 28  | BD    | 58  | HIS  |
| 28  | BD    | 74  | GLY  |
| 28  | BD    | 156 | ALA  |
| 28  | BD    | 268 | ARG  |
| 29  | BE    | 45  | THR  |
| 29  | BE    | 90  | THR  |
| 30  | BF    | 25  | PRO  |
| 30  | BF    | 26  | ALA  |
| 30  | BF    | 90  | PHE  |
| 30  | BF    | 182 | ASN  |
| 31  | BG    | 24  | GLY  |
| 32  | BH    | 71  | LEU  |
| 32  | BH    | 84  | SER  |
| 32  | BH    | 158 | HIS  |
| 32  | BH    | 168 | PRO  |
| 33  | BI    | 85  | GLU  |
| 33  | BI    | 117 | GLU  |
| 33  | BI    | 119 | PRO  |
| 34  | BN    | 9   | VAL  |
| 34  | BN    | 88  | GLU  |
| 34  | BN    | 127 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 36  | BP    | 4   | SER  |
| 36  | BP    | 42  | SER  |
| 36  | BP    | 48  | PRO  |
| 36  | BP    | 104 | GLY  |
| 36  | BP    | 106 | LEU  |
| 38  | BR    | 44  | LEU  |
| 39  | BS    | 74  | ALA  |
| 39  | BS    | 94  | TYR  |
| 39  | BS    | 108 | GLY  |
| 40  | BT    | 131 | ALA  |
| 40  | BT    | 132 | LYS  |
| 41  | BU    | 116 | ALA  |
| 42  | BV    | 3   | ALA  |
| 45  | BY    | 39  | VAL  |
| 45  | BY    | 50  | ARG  |
| 45  | BY    | 81  | LYS  |
| 46  | BZ    | 112 | ARG  |
| 47  | B0    | 47  | PRO  |
| 51  | B4    | 45  | GLY  |
| 51  | B4    | 61  | VAL  |
| 52  | B5    | 33  | CYS  |
| 53  | B6    | 46  | HIS  |
| 53  | B6    | 49  | HIS  |
| 54  | B7    | 2   | LYS  |
| 55  | B8    | 61  | LEU  |
| 2   | CB    | 130 | ARG  |
| 2   | CB    | 196 | LEU  |
| 2   | CB    | 220 | ASP  |
| 2   | CB    | 221 | LEU  |
| 3   | CC    | 145 | GLY  |
| 4   | CD    | 31  | CYS  |
| 4   | CD    | 167 | GLY  |
| 5   | CE    | 11  | ILE  |
| 5   | CE    | 12  | LEU  |
| 5   | CE    | 85  | GLY  |
| 5   | CE    | 107 | ARG  |
| 7   | CG    | 146 | GLU  |
| 9   | CI    | 89  | ASN  |
| 10  | CJ    | 58  | ASP  |
| 10  | CJ    | 66  | ARG  |
| 12  | CL    | 48  | PRO  |
| 12  | CL    | 115 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 13  | CM    | 21  | TYR  |
| 13  | CM    | 45  | VAL  |
| 13  | CM    | 49  | THR  |
| 13  | CM    | 68  | GLY  |
| 14  | CN    | 24  | CYS  |
| 17  | CQ    | 30  | PRO  |
| 17  | CQ    | 78  | GLU  |
| 18  | CR    | 31  | LEU  |
| 19  | CS    | 17  | GLU  |
| 20  | CT    | 13  | LEU  |
| 20  | CT    | 46  | GLU  |
| 20  | CT    | 71  | THR  |
| 27  | DC    | 52  | ARG  |
| 27  | DC    | 79  | LYS  |
| 27  | DC    | 122 | ALA  |
| 27  | DC    | 125 | SER  |
| 27  | DC    | 132 | GLY  |
| 27  | DC    | 162 | GLU  |
| 27  | DC    | 164 | ARG  |
| 27  | DC    | 184 | LYS  |
| 27  | DC    | 197 | GLU  |
| 27  | DC    | 205 | LYS  |
| 27  | DC    | 213 | TYR  |
| 27  | DC    | 215 | THR  |
| 28  | DD    | 263 | ARG  |
| 29  | DE    | 52  | LEU  |
| 30  | DF    | 25  | PRO  |
| 30  | DF    | 47  | GLY  |
| 31  | DG    | 36  | LYS  |
| 31  | DG    | 86  | MET  |
| 31  | DG    | 116 | ASP  |
| 31  | DG    | 181 | ARG  |
| 32  | DH    | 81  | GLU  |
| 32  | DH    | 152 | ARG  |
| 33  | DI    | 10  | GLU  |
| 33  | DI    | 12  | LEU  |
| 33  | DI    | 18  | VAL  |
| 33  | DI    | 100 | ALA  |
| 33  | DI    | 118 | LYS  |
| 33  | DI    | 133 | HIS  |
| 34  | DN    | 135 | PRO  |
| 36  | DP    | 4   | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 36  | DP    | 48  | PRO  |
| 36  | DP    | 104 | GLY  |
| 36  | DP    | 106 | LEU  |
| 37  | DQ    | 54  | MET  |
| 38  | DR    | 106 | GLY  |
| 39  | DS    | 75  | GLU  |
| 39  | DS    | 97  | ARG  |
| 40  | DT    | 132 | LYS  |
| 41  | DU    | 32  | PHE  |
| 41  | DU    | 77  | SER  |
| 41  | DU    | 99  | ALA  |
| 41  | DU    | 112 | ARG  |
| 42  | DV    | 36  | PRO  |
| 43  | DW    | 44  | ALA  |
| 43  | DW    | 49  | LYS  |
| 45  | DY    | 39  | VAL  |
| 46  | DZ    | 42  | VAL  |
| 46  | DZ    | 118 | GLN  |
| 47  | D0    | 47  | PRO  |
| 49  | D2    | 17  | SER  |
| 50  | D3    | 39  | ASP  |
| 50  | D3    | 57  | GLU  |
| 52  | D5    | 4   | HIS  |
| 52  | D5    | 51  | TYR  |
| 53  | D6    | 33  | LYS  |
| 2   | AB    | 167 | PRO  |
| 3   | AC    | 12  | LEU  |
| 3   | AC    | 119 | ARG  |
| 3   | AC    | 189 | ALA  |
| 4   | AD    | 208 | SER  |
| 5   | AE    | 152 | ARG  |
| 7   | AG    | 108 | ALA  |
| 7   | AG    | 112 | PRO  |
| 8   | AH    | 2   | LEU  |
| 10  | AJ    | 39  | PRO  |
| 11  | AK    | 49  | GLY  |
| 11  | AK    | 61  | ALA  |
| 12  | AL    | 19  | ARG  |
| 12  | AL    | 46  | LYS  |
| 13  | AM    | 48  | LEU  |
| 13  | AM    | 61  | GLU  |
| 13  | AM    | 91  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 16  | AP    | 38  | TYR  |
| 17  | AQ    | 94  | ASN  |
| 18  | AR    | 80  | PRO  |
| 20  | AT    | 28  | ALA  |
| 27  | BC    | 38  | ASP  |
| 27  | BC    | 50  | ASP  |
| 27  | BC    | 142 | ALA  |
| 27  | BC    | 205 | LYS  |
| 27  | BC    | 222 | VAL  |
| 28  | BD    | 28  | GLU  |
| 28  | BD    | 232 | PRO  |
| 28  | BD    | 237 | GLU  |
| 28  | BD    | 241 | PRO  |
| 28  | BD    | 242 | ARG  |
| 31  | BG    | 4   | ASP  |
| 31  | BG    | 68  | PRO  |
| 32  | BH    | 54  | ARG  |
| 33  | BI    | 97  | ILE  |
| 34  | BN    | 4   | TYR  |
| 34  | BN    | 64  | GLY  |
| 34  | BN    | 94  | HIS  |
| 36  | BP    | 7   | ARG  |
| 36  | BP    | 43  | GLY  |
| 37  | BQ    | 115 | MET  |
| 38  | BR    | 102 | GLU  |
| 40  | BT    | 68  | TYR  |
| 41  | BU    | 111 | GLU  |
| 42  | BV    | 15  | GLU  |
| 42  | BV    | 23  | GLU  |
| 42  | BV    | 50  | PRO  |
| 43  | BW    | 54  | ALA  |
| 44  | BX    | 38  | GLU  |
| 45  | BY    | 9   | LYS  |
| 45  | BY    | 96  | ILE  |
| 45  | BY    | 100 | ALA  |
| 47  | B0    | 50  | ASN  |
| 50  | B3    | 59  | VAL  |
| 53  | B6    | 33  | LYS  |
| 53  | B6    | 34  | LEU  |
| 2   | CB    | 122 | PHE  |
| 2   | CB    | 167 | PRO  |
| 3   | CC    | 66  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | CC    | 103 | VAL  |
| 3   | CC    | 129 | ALA  |
| 4   | CD    | 95  | GLY  |
| 4   | CD    | 200 | GLU  |
| 5   | CE    | 21  | ALA  |
| 7   | CG    | 7   | ALA  |
| 9   | CI    | 31  | GLN  |
| 10  | CJ    | 17  | ASP  |
| 10  | CJ    | 54  | PHE  |
| 11  | CK    | 27  | ASN  |
| 12  | CL    | 108 | ALA  |
| 13  | CM    | 3   | ARG  |
| 13  | CM    | 70  | LEU  |
| 13  | CM    | 121 | LYS  |
| 15  | CO    | 33  | THR  |
| 16  | CP    | 56  | ALA  |
| 19  | CS    | 5   | LEU  |
| 19  | CS    | 44  | MET  |
| 27  | DC    | 64  | LEU  |
| 28  | DD    | 12  | SER  |
| 28  | DD    | 241 | PRO  |
| 28  | DD    | 244 | ARG  |
| 29  | DE    | 39  | PRO  |
| 29  | DE    | 45  | THR  |
| 29  | DE    | 61  | ARG  |
| 30  | DF    | 8   | GLN  |
| 31  | DG    | 3   | LEU  |
| 31  | DG    | 6   | ALA  |
| 31  | DG    | 117 | PHE  |
| 32  | DH    | 110 | SER  |
| 33  | DI    | 33  | ARG  |
| 33  | DI    | 145 | VAL  |
| 36  | DP    | 7   | ARG  |
| 36  | DP    | 13  | ASN  |
| 36  | DP    | 43  | GLY  |
| 37  | DQ    | 28  | ALA  |
| 38  | DR    | 93  | GLY  |
| 39  | DS    | 21  | THR  |
| 41  | DU    | 68  | ALA  |
| 42  | DV    | 30  | GLY  |
| 43  | DW    | 14  | PRO  |
| 43  | DW    | 65  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 45  | DY    | 55  | TYR  |
| 46  | DZ    | 30  | ASN  |
| 46  | DZ    | 54  | HIS  |
| 46  | DZ    | 64  | GLY  |
| 46  | DZ    | 78  | LYS  |
| 47  | D0    | 41  | ARG  |
| 48  | D1    | 53  | VAL  |
| 51  | D4    | 35  | VAL  |
| 53  | D6    | 46  | HIS  |
| 54  | D7    | 44  | PRO  |
| 55  | D8    | 35  | GLN  |
| 2   | AB    | 158 | LEU  |
| 2   | AB    | 202 | PRO  |
| 3   | AC    | 3   | ASN  |
| 4   | AD    | 73  | ARG  |
| 12  | AL    | 48  | PRO  |
| 12  | AL    | 118 | SER  |
| 18  | AR    | 39  | VAL  |
| 20  | AT    | 68  | LYS  |
| 27  | BC    | 64  | LEU  |
| 27  | BC    | 143 | GLY  |
| 27  | BC    | 145 | VAL  |
| 27  | BC    | 175 | VAL  |
| 28  | BD    | 243 | GLY  |
| 30  | BF    | 183 | VAL  |
| 32  | BH    | 160 | LYS  |
| 33  | BI    | 65  | ALA  |
| 33  | BI    | 121 | LYS  |
| 33  | BI    | 132 | PRO  |
| 33  | BI    | 133 | HIS  |
| 33  | BI    | 134 | PRO  |
| 34  | BN    | 59  | LYS  |
| 34  | BN    | 112 | LEU  |
| 36  | BP    | 107 | LYS  |
| 37  | BQ    | 46  | GLN  |
| 39  | BS    | 107 | GLU  |
| 44  | BX    | 10  | ALA  |
| 45  | BY    | 55  | TYR  |
| 45  | BY    | 74  | PRO  |
| 48  | B1    | 30  | VAL  |
| 48  | B1    | 51  | VAL  |
| 50  | B3    | 2   | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 50  | B3    | 51  | ALA  |
| 52  | B5    | 5   | PRO  |
| 56  | B9    | 28  | GLU  |
| 6   | CF    | 30  | LEU  |
| 9   | CI    | 121 | ARG  |
| 15  | CO    | 61  | GLY  |
| 18  | CR    | 51  | LEU  |
| 28  | DD    | 234 | GLY  |
| 29  | DE    | 32  | PRO  |
| 29  | DE    | 72  | VAL  |
| 29  | DE    | 186 | GLY  |
| 31  | DG    | 82  | LEU  |
| 31  | DG    | 84  | LYS  |
| 31  | DG    | 85  | GLY  |
| 31  | DG    | 112 | PRO  |
| 32  | DH    | 55  | PRO  |
| 32  | DH    | 111 | HIS  |
| 33  | DI    | 82  | ARG  |
| 35  | DO    | 26  | LYS  |
| 36  | DP    | 27  | HIS  |
| 36  | DP    | 107 | LYS  |
| 38  | DR    | 2   | ARG  |
| 40  | DT    | 117 | ASP  |
| 43  | DW    | 110 | LYS  |
| 46  | DZ    | 12  | GLY  |
| 46  | DZ    | 46  | LYS  |
| 49  | D2    | 41  | ILE  |
| 6   | AF    | 37  | VAL  |
| 27  | BC    | 22  | ILE  |
| 27  | BC    | 48  | GLY  |
| 27  | BC    | 90  | GLY  |
| 28  | BD    | 234 | GLY  |
| 32  | BH    | 169 | VAL  |
| 33  | BI    | 144 | VAL  |
| 45  | BY    | 31  | LEU  |
| 45  | BY    | 75  | ILE  |
| 7   | CG    | 14  | PRO  |
| 8   | CH    | 75  | ARG  |
| 9   | CI    | 90  | PRO  |
| 9   | CI    | 97  | LYS  |
| 11  | CK    | 95  | ILE  |
| 20  | CT    | 98  | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 27  | DC    | 62  | VAL  |
| 27  | DC    | 145 | VAL  |
| 45  | DY    | 3   | VAL  |
| 48  | D1    | 30  | VAL  |
| 50  | D3    | 50  | VAL  |
| 52  | D5    | 50  | GLY  |
| 2   | AB    | 125 | PRO  |
| 2   | AB    | 228 | GLY  |
| 4   | AD    | 44  | GLY  |
| 4   | AD    | 56  | VAL  |
| 5   | AE    | 96  | PRO  |
| 9   | AI    | 44  | VAL  |
| 27  | BC    | 65  | PRO  |
| 29  | BE    | 22  | PRO  |
| 32  | BH    | 24  | VAL  |
| 32  | BH    | 151 | ILE  |
| 36  | BP    | 8   | PRO  |
| 37  | BQ    | 27  | VAL  |
| 41  | BU    | 90  | VAL  |
| 42  | BV    | 47  | VAL  |
| 46  | BZ    | 134 | PRO  |
| 46  | BZ    | 141 | VAL  |
| 48  | B1    | 55  | GLY  |
| 2   | CB    | 202 | PRO  |
| 14  | CN    | 51  | GLY  |
| 15  | CO    | 87  | ILE  |
| 27  | DC    | 74  | VAL  |
| 29  | DE    | 130 | GLY  |
| 30  | DF    | 30  | PRO  |
| 32  | DH    | 7   | LEU  |
| 34  | DN    | 129 | PRO  |
| 36  | DP    | 8   | PRO  |
| 45  | DY    | 56  | PRO  |
| 45  | DY    | 96  | ILE  |
| 46  | DZ    | 39  | VAL  |
| 50  | D3    | 13  | ILE  |
| 18  | AR    | 27  | GLY  |
| 27  | BC    | 152 | ILE  |
| 27  | BC    | 200 | LYS  |
| 28  | BD    | 24  | ILE  |
| 28  | BD    | 121 | PRO  |
| 28  | BD    | 249 | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 41  | BU    | 100 | VAL  |
| 44  | BX    | 84  | ALA  |
| 45  | BY    | 27  | VAL  |
| 46  | BZ    | 47  | VAL  |
| 2   | CB    | 158 | LEU  |
| 12  | CL    | 63  | GLY  |
| 18  | CR    | 50  | ILE  |
| 27  | DC    | 200 | LYS  |
| 34  | DN    | 60  | ILE  |
| 36  | DP    | 63  | PRO  |
| 9   | AI    | 97  | LYS  |
| 10  | AJ    | 53  | PRO  |
| 12  | AL    | 43  | VAL  |
| 13  | AM    | 7   | VAL  |
| 27  | BC    | 49  | ILE  |
| 32  | BH    | 76  | VAL  |
| 33  | BI    | 131 | LYS  |
| 36  | BP    | 63  | PRO  |
| 39  | BS    | 22  | GLY  |
| 50  | B3    | 13  | ILE  |
| 2   | CB    | 174 | VAL  |
| 3   | CC    | 120 | VAL  |
| 8   | CH    | 106 | GLY  |
| 29  | DE    | 86  | PRO  |
| 39  | DS    | 82  | ILE  |
| 42  | DV    | 28  | GLU  |
| 44  | DX    | 39  | ILE  |
| 45  | DY    | 52  | SER  |
| 50  | D3    | 27  | GLY  |
| 53  | D6    | 31  | PRO  |
| 2   | AB    | 230 | VAL  |
| 30  | BF    | 171 | PRO  |
| 46  | BZ    | 115 | GLY  |
| 9   | CI    | 123 | PRO  |
| 10  | CJ    | 93  | GLY  |
| 27  | DC    | 90  | GLY  |
| 27  | DC    | 143 | GLY  |
| 28  | DD    | 28  | GLU  |
| 28  | DD    | 35  | LYS  |
| 34  | DN    | 9   | VAL  |
| 46  | DZ    | 82  | ARG  |
| 28  | BD    | 245 | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 28  | DD    | 245 | 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 X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 2   | AB    | 202/220 (92%)  | 159 (79%) | 43 (21%) | 1           | 6  |
| 2   | CB    | 202/220 (92%)  | 147 (73%) | 55 (27%) | 0           | 3  |
| 3   | AC    | 160/188 (85%)  | 126 (79%) | 34 (21%) | 1           | 6  |
| 3   | CC    | 160/188 (85%)  | 130 (81%) | 30 (19%) | 1           | 9  |
| 4   | AD    | 180/181 (99%)  | 150 (83%) | 30 (17%) | 2           | 13 |
| 4   | CD    | 180/181 (99%)  | 152 (84%) | 28 (16%) | 2           | 16 |
| 5   | AE    | 115/123 (94%)  | 93 (81%)  | 22 (19%) | 1           | 8  |
| 5   | CE    | 115/123 (94%)  | 86 (75%)  | 29 (25%) | 0           | 4  |
| 6   | AF    | 90/90 (100%)   | 72 (80%)  | 18 (20%) | 1           | 7  |
| 6   | CF    | 90/90 (100%)   | 75 (83%)  | 15 (17%) | 2           | 13 |
| 7   | AG    | 126/127 (99%)  | 100 (79%) | 26 (21%) | 1           | 7  |
| 7   | CG    | 126/127 (99%)  | 101 (80%) | 25 (20%) | 1           | 8  |
| 8   | AH    | 119/119 (100%) | 97 (82%)  | 22 (18%) | 1           | 9  |
| 8   | CH    | 119/119 (100%) | 83 (70%)  | 36 (30%) | 0           | 2  |
| 9   | AI    | 98/99 (99%)    | 79 (81%)  | 19 (19%) | 1           | 8  |
| 9   | CI    | 98/99 (99%)    | 76 (78%)  | 22 (22%) | 1           | 5  |
| 10  | AJ    | 88/92 (96%)    | 65 (74%)  | 23 (26%) | 0           | 3  |
| 10  | CJ    | 88/92 (96%)    | 67 (76%)  | 21 (24%) | 1           | 4  |
| 11  | AK    | 90/99 (91%)    | 74 (82%)  | 16 (18%) | 2           | 10 |
| 11  | CK    | 90/99 (91%)    | 67 (74%)  | 23 (26%) | 0           | 3  |
| 12  | AL    | 104/109 (95%)  | 79 (76%)  | 25 (24%) | 1           | 4  |
| 12  | CL    | 104/109 (95%)  | 80 (77%)  | 24 (23%) | 1           | 5  |
| 13  | AM    | 99/101 (98%)   | 77 (78%)  | 22 (22%) | 1           | 5  |

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| Mol | Chain | Analysed      | Rotameric | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|-------------|----|
| 13  | CM    | 100/101 (99%) | 85 (85%)  | 15 (15%) | 3           | 17 |
| 14  | AN    | 49/50 (98%)   | 41 (84%)  | 8 (16%)  | 2           | 14 |
| 14  | CN    | 49/50 (98%)   | 37 (76%)  | 12 (24%) | 1           | 4  |
| 15  | AO    | 79/80 (99%)   | 64 (81%)  | 15 (19%) | 1           | 8  |
| 15  | CO    | 79/80 (99%)   | 66 (84%)  | 13 (16%) | 2           | 14 |
| 16  | AP    | 72/74 (97%)   | 57 (79%)  | 15 (21%) | 1           | 6  |
| 16  | CP    | 72/74 (97%)   | 56 (78%)  | 16 (22%) | 1           | 5  |
| 17  | AQ    | 94/97 (97%)   | 84 (89%)  | 10 (11%) | 6           | 28 |
| 17  | CQ    | 94/97 (97%)   | 77 (82%)  | 17 (18%) | 2           | 10 |
| 18  | AR    | 61/77 (79%)   | 47 (77%)  | 14 (23%) | 1           | 5  |
| 18  | CR    | 61/77 (79%)   | 49 (80%)  | 12 (20%) | 1           | 8  |
| 19  | AS    | 69/80 (86%)   | 49 (71%)  | 20 (29%) | 0           | 2  |
| 19  | CS    | 69/80 (86%)   | 46 (67%)  | 23 (33%) | 0           | 2  |
| 20  | AT    | 76/82 (93%)   | 52 (68%)  | 24 (32%) | 0           | 2  |
| 20  | CT    | 76/82 (93%)   | 50 (66%)  | 26 (34%) | 0           | 2  |
| 21  | AU    | 19/22 (86%)   | 17 (90%)  | 2 (10%)  | 6           | 28 |
| 21  | CU    | 19/22 (86%)   | 12 (63%)  | 7 (37%)  | 0           | 1  |
| 27  | BC    | 61/181 (34%)  | 49 (80%)  | 12 (20%) | 1           | 8  |
| 27  | DC    | 61/181 (34%)  | 54 (88%)  | 7 (12%)  | 5           | 25 |
| 28  | BD    | 213/218 (98%) | 157 (74%) | 56 (26%) | 0           | 3  |
| 28  | DD    | 213/218 (98%) | 178 (84%) | 35 (16%) | 2           | 14 |
| 29  | BE    | 165/166 (99%) | 124 (75%) | 41 (25%) | 1           | 4  |
| 29  | DE    | 165/166 (99%) | 137 (83%) | 28 (17%) | 2           | 12 |
| 30  | BF    | 165/166 (99%) | 124 (75%) | 41 (25%) | 1           | 4  |
| 30  | DF    | 161/166 (97%) | 133 (83%) | 28 (17%) | 2           | 11 |
| 31  | BG    | 155/156 (99%) | 116 (75%) | 39 (25%) | 0           | 4  |
| 31  | DG    | 155/156 (99%) | 137 (88%) | 18 (12%) | 5           | 25 |
| 32  | BH    | 132/148 (89%) | 110 (83%) | 22 (17%) | 2           | 13 |
| 32  | DH    | 140/148 (95%) | 113 (81%) | 27 (19%) | 1           | 8  |
| 33  | BI    | 122/124 (98%) | 95 (78%)  | 27 (22%) | 1           | 6  |
| 33  | DI    | 122/124 (98%) | 96 (79%)  | 26 (21%) | 1           | 6  |

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| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 34  | BN    | 117/119 (98%)  | 87 (74%)  | 30 (26%) | 0           | 3  |
| 34  | DN    | 117/119 (98%)  | 99 (85%)  | 18 (15%) | 2           | 16 |
| 35  | BO    | 100/100 (100%) | 77 (77%)  | 23 (23%) | 1           | 5  |
| 35  | DO    | 100/100 (100%) | 88 (88%)  | 12 (12%) | 5           | 23 |
| 36  | BP    | 116/116 (100%) | 85 (73%)  | 31 (27%) | 0           | 3  |
| 36  | DP    | 116/116 (100%) | 86 (74%)  | 30 (26%) | 0           | 3  |
| 37  | BQ    | 111/111 (100%) | 79 (71%)  | 32 (29%) | 0           | 2  |
| 37  | DQ    | 111/111 (100%) | 92 (83%)  | 19 (17%) | 2           | 12 |
| 38  | BR    | 100/101 (99%)  | 67 (67%)  | 33 (33%) | 0           | 2  |
| 38  | DR    | 101/101 (100%) | 86 (85%)  | 15 (15%) | 3           | 17 |
| 39  | BS    | 77/88 (88%)    | 52 (68%)  | 25 (32%) | 0           | 2  |
| 39  | DS    | 87/88 (99%)    | 74 (85%)  | 13 (15%) | 3           | 17 |
| 40  | BT    | 120/127 (94%)  | 88 (73%)  | 32 (27%) | 0           | 3  |
| 40  | DT    | 120/127 (94%)  | 88 (73%)  | 32 (27%) | 0           | 3  |
| 41  | BU    | 93/94 (99%)    | 68 (73%)  | 25 (27%) | 0           | 3  |
| 41  | DU    | 92/94 (98%)    | 78 (85%)  | 14 (15%) | 3           | 17 |
| 42  | BV    | 82/82 (100%)   | 54 (66%)  | 28 (34%) | 0           | 2  |
| 42  | DV    | 82/82 (100%)   | 61 (74%)  | 21 (26%) | 0           | 3  |
| 43  | BW    | 91/92 (99%)    | 66 (72%)  | 25 (28%) | 0           | 3  |
| 43  | DW    | 91/92 (99%)    | 83 (91%)  | 8 (9%)   | 9           | 33 |
| 44  | BX    | 74/78 (95%)    | 56 (76%)  | 18 (24%) | 1           | 4  |
| 44  | DX    | 74/78 (95%)    | 61 (82%)  | 13 (18%) | 2           | 11 |
| 45  | BY    | 84/91 (92%)    | 64 (76%)  | 20 (24%) | 1           | 4  |
| 45  | DY    | 85/91 (93%)    | 66 (78%)  | 19 (22%) | 1           | 5  |
| 46  | BZ    | 155/179 (87%)  | 122 (79%) | 33 (21%) | 1           | 6  |
| 46  | DZ    | 155/179 (87%)  | 137 (88%) | 18 (12%) | 5           | 25 |
| 47  | B0    | 66/67 (98%)    | 57 (86%)  | 9 (14%)  | 3           | 20 |
| 47  | D0    | 66/67 (98%)    | 56 (85%)  | 10 (15%) | 3           | 17 |
| 48  | B1    | 78/83 (94%)    | 59 (76%)  | 19 (24%) | 1           | 4  |
| 48  | D1    | 78/83 (94%)    | 60 (77%)  | 18 (23%) | 1           | 5  |
| 49  | B2    | 66/67 (98%)    | 50 (76%)  | 16 (24%) | 1           | 4  |

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| Mol | Chain | Analysed         | Rotameric  | Outliers   | Percentiles |    |
|-----|-------|------------------|------------|------------|-------------|----|
| 49  | D2    | 66/67 (98%)      | 54 (82%)   | 12 (18%)   | 2           | 10 |
| 50  | B3    | 51/52 (98%)      | 38 (74%)   | 13 (26%)   | 0           | 3  |
| 50  | D3    | 51/52 (98%)      | 47 (92%)   | 4 (8%)     | 11          | 37 |
| 51  | B4    | 27/63 (43%)      | 17 (63%)   | 10 (37%)   | 0           | 1  |
| 51  | D4    | 35/63 (56%)      | 32 (91%)   | 3 (9%)     | 10          | 34 |
| 52  | B5    | 51/52 (98%)      | 40 (78%)   | 11 (22%)   | 1           | 6  |
| 52  | D5    | 51/52 (98%)      | 43 (84%)   | 8 (16%)    | 2           | 15 |
| 53  | B6    | 43/52 (83%)      | 31 (72%)   | 12 (28%)   | 0           | 3  |
| 53  | D6    | 43/52 (83%)      | 32 (74%)   | 11 (26%)   | 0           | 3  |
| 54  | B7    | 41/42 (98%)      | 32 (78%)   | 9 (22%)    | 1           | 6  |
| 54  | D7    | 41/42 (98%)      | 36 (88%)   | 5 (12%)    | 5           | 23 |
| 55  | B8    | 53/55 (96%)      | 38 (72%)   | 15 (28%)   | 0           | 3  |
| 55  | D8    | 53/55 (96%)      | 46 (87%)   | 7 (13%)    | 4           | 21 |
| 56  | B9    | 33/34 (97%)      | 28 (85%)   | 5 (15%)    | 3           | 17 |
| 56  | D9    | 33/34 (97%)      | 29 (88%)   | 4 (12%)    | 5           | 23 |
| All | All   | 9688/10428 (93%) | 7636 (79%) | 2052 (21%) | 1           | 6  |

All (2052) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | AB    | 15  | VAL  |
| 2   | AB    | 17  | PHE  |
| 2   | AB    | 20  | GLU  |
| 2   | AB    | 22  | LYS  |
| 2   | AB    | 23  | ARG  |
| 2   | AB    | 32  | ILE  |
| 2   | AB    | 36  | ARG  |
| 2   | AB    | 37  | ASN  |
| 2   | AB    | 44  | LEU  |
| 2   | AB    | 45  | GLN  |
| 2   | AB    | 58  | ILE  |
| 2   | AB    | 69  | LEU  |
| 2   | AB    | 74  | LYS  |
| 2   | AB    | 75  | LYS  |
| 2   | AB    | 76  | GLN  |
| 2   | AB    | 80  | ILE  |
| 2   | AB    | 87  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | AB    | 94  | ASN  |
| 2   | AB    | 101 | MET  |
| 2   | AB    | 108 | ILE  |
| 2   | AB    | 111 | ARG  |
| 2   | AB    | 113 | HIS  |
| 2   | AB    | 116 | GLU  |
| 2   | AB    | 119 | GLU  |
| 2   | AB    | 130 | ARG  |
| 2   | AB    | 136 | VAL  |
| 2   | AB    | 140 | HIS  |
| 2   | AB    | 145 | LEU  |
| 2   | AB    | 155 | LEU  |
| 2   | AB    | 158 | LEU  |
| 2   | AB    | 164 | VAL  |
| 2   | AB    | 172 | ILE  |
| 2   | AB    | 174 | VAL  |
| 2   | AB    | 187 | LEU  |
| 2   | AB    | 196 | LEU  |
| 2   | AB    | 204 | ASN  |
| 2   | AB    | 208 | ILE  |
| 2   | AB    | 212 | GLN  |
| 2   | AB    | 219 | VAL  |
| 2   | AB    | 221 | LEU  |
| 2   | AB    | 223 | ILE  |
| 2   | AB    | 233 | SER  |
| 2   | AB    | 235 | SER  |
| 3   | AC    | 5   | ILE  |
| 3   | AC    | 12  | LEU  |
| 3   | AC    | 16  | ARG  |
| 3   | AC    | 18  | TRP  |
| 3   | AC    | 22  | TRP  |
| 3   | AC    | 29  | TYR  |
| 3   | AC    | 30  | ARG  |
| 3   | AC    | 34  | LEU  |
| 3   | AC    | 39  | ILE  |
| 3   | AC    | 42  | LEU  |
| 3   | AC    | 55  | VAL  |
| 3   | AC    | 58  | GLU  |
| 3   | AC    | 64  | VAL  |
| 3   | AC    | 76  | VAL  |
| 3   | AC    | 94  | LEU  |
| 3   | AC    | 102 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | AC    | 106 | VAL  |
| 3   | AC    | 116 | VAL  |
| 3   | AC    | 131 | ARG  |
| 3   | AC    | 134 | ILE  |
| 3   | AC    | 140 | ARG  |
| 3   | AC    | 141 | VAL  |
| 3   | AC    | 152 | ILE  |
| 3   | AC    | 156 | ARG  |
| 3   | AC    | 164 | ARG  |
| 3   | AC    | 165 | THR  |
| 3   | AC    | 175 | LEU  |
| 3   | AC    | 178 | LEU  |
| 3   | AC    | 188 | LEU  |
| 3   | AC    | 190 | ARG  |
| 3   | AC    | 192 | THR  |
| 3   | AC    | 195 | VAL  |
| 3   | AC    | 198 | VAL  |
| 3   | AC    | 202 | ILE  |
| 4   | AD    | 3   | ARG  |
| 4   | AD    | 5   | ILE  |
| 4   | AD    | 9   | CYS  |
| 4   | AD    | 10  | ARG  |
| 4   | AD    | 11  | LEU  |
| 4   | AD    | 13  | ARG  |
| 4   | AD    | 15  | GLU  |
| 4   | AD    | 26  | CYS  |
| 4   | AD    | 36  | ARG  |
| 4   | AD    | 38  | TYR  |
| 4   | AD    | 45  | GLN  |
| 4   | AD    | 49  | ARG  |
| 4   | AD    | 50  | ARG  |
| 4   | AD    | 59  | ARG  |
| 4   | AD    | 66  | ARG  |
| 4   | AD    | 70  | ILE  |
| 4   | AD    | 78  | LEU  |
| 4   | AD    | 94  | LEU  |
| 4   | AD    | 99  | SER  |
| 4   | AD    | 104 | VAL  |
| 4   | AD    | 106 | TYR  |
| 4   | AD    | 110 | PHE  |
| 4   | AD    | 132 | ARG  |
| 4   | AD    | 133 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | AD    | 135 | LEU  |
| 4   | AD    | 139 | ARG  |
| 4   | AD    | 146 | ILE  |
| 4   | AD    | 150 | GLU  |
| 4   | AD    | 155 | LEU  |
| 4   | AD    | 178 | VAL  |
| 5   | AE    | 12  | LEU  |
| 5   | AE    | 13  | ILE  |
| 5   | AE    | 16  | THR  |
| 5   | AE    | 20  | GLN  |
| 5   | AE    | 41  | VAL  |
| 5   | AE    | 51  | VAL  |
| 5   | AE    | 55  | VAL  |
| 5   | AE    | 64  | ARG  |
| 5   | AE    | 69  | VAL  |
| 5   | AE    | 76  | ILE  |
| 5   | AE    | 79  | GLU  |
| 5   | AE    | 80  | ILE  |
| 5   | AE    | 90  | VAL  |
| 5   | AE    | 91  | LEU  |
| 5   | AE    | 101 | ILE  |
| 5   | AE    | 105 | VAL  |
| 5   | AE    | 116 | THR  |
| 5   | AE    | 119 | LEU  |
| 5   | AE    | 120 | THR  |
| 5   | AE    | 121 | LYS  |
| 5   | AE    | 131 | ILE  |
| 5   | AE    | 137 | GLU  |
| 6   | AF    | 7   | ASN  |
| 6   | AF    | 19  | LEU  |
| 6   | AF    | 21  | LEU  |
| 6   | AF    | 24  | GLU  |
| 6   | AF    | 25  | ILE  |
| 6   | AF    | 37  | VAL  |
| 6   | AF    | 40  | VAL  |
| 6   | AF    | 43  | LEU  |
| 6   | AF    | 45  | LEU  |
| 6   | AF    | 52  | ILE  |
| 6   | AF    | 64  | GLN  |
| 6   | AF    | 69  | GLU  |
| 6   | AF    | 75  | LEU  |
| 6   | AF    | 77  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | AF    | 82  | ARG  |
| 6   | AF    | 83  | ASP  |
| 6   | AF    | 92  | LYS  |
| 6   | AF    | 100 | ASN  |
| 7   | AG    | 4   | ARG  |
| 7   | AG    | 10  | ARG  |
| 7   | AG    | 11  | GLN  |
| 7   | AG    | 15  | ASP  |
| 7   | AG    | 16  | LEU  |
| 7   | AG    | 22  | LEU  |
| 7   | AG    | 23  | VAL  |
| 7   | AG    | 27  | ILE  |
| 7   | AG    | 30  | ILE  |
| 7   | AG    | 57  | GLU  |
| 7   | AG    | 60  | LYS  |
| 7   | AG    | 66  | VAL  |
| 7   | AG    | 73  | MET  |
| 7   | AG    | 79  | ARG  |
| 7   | AG    | 80  | VAL  |
| 7   | AG    | 97  | GLN  |
| 7   | AG    | 104 | LEU  |
| 7   | AG    | 106 | GLN  |
| 7   | AG    | 113 | GLU  |
| 7   | AG    | 114 | ARG  |
| 7   | AG    | 120 | ILE  |
| 7   | AG    | 124 | LEU  |
| 7   | AG    | 140 | ASP  |
| 7   | AG    | 141 | VAL  |
| 7   | AG    | 142 | GLU  |
| 7   | AG    | 155 | ARG  |
| 8   | AH    | 1   | MET  |
| 8   | AH    | 3   | THR  |
| 8   | AH    | 19  | VAL  |
| 8   | AH    | 25  | ASP  |
| 8   | AH    | 26  | VAL  |
| 8   | AH    | 51  | VAL  |
| 8   | AH    | 52  | ASP  |
| 8   | AH    | 64  | LYS  |
| 8   | AH    | 75  | ARG  |
| 8   | AH    | 77  | GLU  |
| 8   | AH    | 84  | ARG  |
| 8   | AH    | 85  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8   | AH    | 86  | ILE  |
| 8   | AH    | 91  | ARG  |
| 8   | AH    | 102 | ARG  |
| 8   | AH    | 103 | VAL  |
| 8   | AH    | 104 | ARG  |
| 8   | AH    | 109 | ILE  |
| 8   | AH    | 119 | LEU  |
| 8   | AH    | 122 | ARG  |
| 8   | AH    | 127 | LEU  |
| 8   | AH    | 129 | VAL  |
| 9   | AI    | 4   | TYR  |
| 9   | AI    | 10  | ARG  |
| 9   | AI    | 51  | ARG  |
| 9   | AI    | 56  | LEU  |
| 9   | AI    | 59  | PHE  |
| 9   | AI    | 78  | LYS  |
| 9   | AI    | 85  | LEU  |
| 9   | AI    | 88  | TYR  |
| 9   | AI    | 89  | ASN  |
| 9   | AI    | 91  | ASP  |
| 9   | AI    | 95  | LYS  |
| 9   | AI    | 99  | LEU  |
| 9   | AI    | 102 | LEU  |
| 9   | AI    | 104 | ARG  |
| 9   | AI    | 108 | VAL  |
| 9   | AI    | 114 | TYR  |
| 9   | AI    | 118 | LYS  |
| 9   | AI    | 124 | GLN  |
| 9   | AI    | 126 | SER  |
| 10  | AJ    | 13  | HIS  |
| 10  | AJ    | 16  | LEU  |
| 10  | AJ    | 23  | ILE  |
| 10  | AJ    | 40  | LEU  |
| 10  | AJ    | 45  | ARG  |
| 10  | AJ    | 47  | PHE  |
| 10  | AJ    | 50  | ILE  |
| 10  | AJ    | 54  | PHE  |
| 10  | AJ    | 60  | ARG  |
| 10  | AJ    | 62  | HIS  |
| 10  | AJ    | 63  | PHE  |
| 10  | AJ    | 67  | THR  |
| 10  | AJ    | 70  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10  | AJ    | 74  | ILE  |
| 10  | AJ    | 76  | ASN  |
| 10  | AJ    | 80  | LYS  |
| 10  | AJ    | 85  | LEU  |
| 10  | AJ    | 86  | MET  |
| 10  | AJ    | 89  | ASP  |
| 10  | AJ    | 90  | LEU  |
| 10  | AJ    | 95  | GLU  |
| 10  | AJ    | 96  | ILE  |
| 10  | AJ    | 100 | THR  |
| 11  | AK    | 29  | ILE  |
| 11  | AK    | 30  | VAL  |
| 11  | AK    | 32  | ILE  |
| 11  | AK    | 33  | THR  |
| 11  | AK    | 47  | VAL  |
| 11  | AK    | 51  | LYS  |
| 11  | AK    | 53  | SER  |
| 11  | AK    | 63  | LEU  |
| 11  | AK    | 78  | GLN  |
| 11  | AK    | 82  | VAL  |
| 11  | AK    | 84  | VAL  |
| 11  | AK    | 98  | LEU  |
| 11  | AK    | 103 | LEU  |
| 11  | AK    | 109 | VAL  |
| 11  | AK    | 114 | VAL  |
| 11  | AK    | 124 | LYS  |
| 12  | AL    | 6   | THR  |
| 12  | AL    | 10  | LEU  |
| 12  | AL    | 11  | VAL  |
| 12  | AL    | 17  | LYS  |
| 12  | AL    | 24  | VAL  |
| 12  | AL    | 28  | LYS  |
| 12  | AL    | 31  | PRO  |
| 12  | AL    | 38  | THR  |
| 12  | AL    | 44  | THR  |
| 12  | AL    | 52  | LEU  |
| 12  | AL    | 60  | LEU  |
| 12  | AL    | 62  | SER  |
| 12  | AL    | 65  | GLU  |
| 12  | AL    | 66  | VAL  |
| 12  | AL    | 70  | ILE  |
| 12  | AL    | 73  | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 12  | AL    | 80  | HIS  |
| 12  | AL    | 81  | SER  |
| 12  | AL    | 83  | VAL  |
| 12  | AL    | 84  | LEU  |
| 12  | AL    | 85  | ILE  |
| 12  | AL    | 89  | ARG  |
| 12  | AL    | 116 | SER  |
| 12  | AL    | 122 | THR  |
| 12  | AL    | 126 | LYS  |
| 13  | AM    | 7   | VAL  |
| 13  | AM    | 17  | VAL  |
| 13  | AM    | 20  | THR  |
| 13  | AM    | 25  | ILE  |
| 13  | AM    | 39  | ILE  |
| 13  | AM    | 46  | LYS  |
| 13  | AM    | 48  | LEU  |
| 13  | AM    | 49  | THR  |
| 13  | AM    | 50  | GLU  |
| 13  | AM    | 53  | VAL  |
| 13  | AM    | 56  | LEU  |
| 13  | AM    | 63  | THR  |
| 13  | AM    | 69  | GLU  |
| 13  | AM    | 77  | ASN  |
| 13  | AM    | 88  | ARG  |
| 13  | AM    | 92  | HIS  |
| 13  | AM    | 93  | ARG  |
| 13  | AM    | 96  | LEU  |
| 13  | AM    | 102 | ARG  |
| 13  | AM    | 108 | ARG  |
| 13  | AM    | 115 | LYS  |
| 13  | AM    | 116 | THR  |
| 14  | AN    | 3   | ARG  |
| 14  | AN    | 16  | PHE  |
| 14  | AN    | 18  | VAL  |
| 14  | AN    | 32  | SER  |
| 14  | AN    | 33  | VAL  |
| 14  | AN    | 44  | LEU  |
| 14  | AN    | 45  | ARG  |
| 14  | AN    | 50  | LYS  |
| 15  | AO    | 3   | ILE  |
| 15  | AO    | 5   | LYS  |
| 15  | AO    | 24  | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 15  | AO    | 31  | LEU  |
| 15  | AO    | 39  | LEU  |
| 15  | AO    | 41  | GLU  |
| 15  | AO    | 45  | VAL  |
| 15  | AO    | 47  | LYS  |
| 15  | AO    | 48  | LYS  |
| 15  | AO    | 52  | SER  |
| 15  | AO    | 64  | ARG  |
| 15  | AO    | 65  | ARG  |
| 15  | AO    | 68  | ARG  |
| 15  | AO    | 82  | ILE  |
| 15  | AO    | 83  | GLU  |
| 16  | AP    | 2   | VAL  |
| 16  | AP    | 11  | SER  |
| 16  | AP    | 20  | VAL  |
| 16  | AP    | 21  | VAL  |
| 16  | AP    | 27  | LYS  |
| 16  | AP    | 28  | ARG  |
| 16  | AP    | 32  | TYR  |
| 16  | AP    | 33  | ILE  |
| 16  | AP    | 40  | ASP  |
| 16  | AP    | 45  | THR  |
| 16  | AP    | 53  | VAL  |
| 16  | AP    | 61  | SER  |
| 16  | AP    | 67  | THR  |
| 16  | AP    | 71  | ARG  |
| 16  | AP    | 82  | GLN  |
| 17  | AQ    | 38  | ARG  |
| 17  | AQ    | 49  | GLU  |
| 17  | AQ    | 53  | LEU  |
| 17  | AQ    | 57  | VAL  |
| 17  | AQ    | 60  | ILE  |
| 17  | AQ    | 68  | ARG  |
| 17  | AQ    | 74  | LEU  |
| 17  | AQ    | 77  | VAL  |
| 17  | AQ    | 89  | LEU  |
| 17  | AQ    | 96  | GLU  |
| 18  | AR    | 31  | LEU  |
| 18  | AR    | 32  | ARG  |
| 18  | AR    | 35  | ARG  |
| 18  | AR    | 37  | VAL  |
| 18  | AR    | 39  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 18  | AR    | 41  | LYS  |
| 18  | AR    | 51  | LEU  |
| 18  | AR    | 58  | LEU  |
| 18  | AR    | 66  | LEU  |
| 18  | AR    | 69  | THR  |
| 18  | AR    | 70  | ILE  |
| 18  | AR    | 76  | LEU  |
| 18  | AR    | 83  | GLU  |
| 18  | AR    | 87  | ARG  |
| 19  | AS    | 5   | LEU  |
| 19  | AS    | 6   | LYS  |
| 19  | AS    | 7   | LYS  |
| 19  | AS    | 10  | PHE  |
| 19  | AS    | 11  | VAL  |
| 19  | AS    | 13  | ASP  |
| 19  | AS    | 14  | HIS  |
| 19  | AS    | 16  | LEU  |
| 19  | AS    | 27  | GLU  |
| 19  | AS    | 28  | LYS  |
| 19  | AS    | 29  | ARG  |
| 19  | AS    | 32  | LYS  |
| 19  | AS    | 33  | THR  |
| 19  | AS    | 37  | ARG  |
| 19  | AS    | 44  | MET  |
| 19  | AS    | 45  | VAL  |
| 19  | AS    | 49  | ILE  |
| 19  | AS    | 58  | VAL  |
| 19  | AS    | 70  | LYS  |
| 19  | AS    | 77  | THR  |
| 20  | AT    | 8   | ARG  |
| 20  | AT    | 22  | ARG  |
| 20  | AT    | 24  | LEU  |
| 20  | AT    | 26  | ASN  |
| 20  | AT    | 30  | LYS  |
| 20  | AT    | 33  | ILE  |
| 20  | AT    | 36  | LEU  |
| 20  | AT    | 37  | SER  |
| 20  | AT    | 50  | GLU  |
| 20  | AT    | 51  | GLU  |
| 20  | AT    | 53  | LEU  |
| 20  | AT    | 56  | MET  |
| 20  | AT    | 70  | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 20  | AT    | 72  | LEU  |
| 20  | AT    | 73  | HIS  |
| 20  | AT    | 81  | LYS  |
| 20  | AT    | 83  | ARG  |
| 20  | AT    | 84  | LEU  |
| 20  | AT    | 85  | MET  |
| 20  | AT    | 86  | ARG  |
| 20  | AT    | 89  | ARG  |
| 20  | AT    | 93  | GLU  |
| 20  | AT    | 100 | ILE  |
| 20  | AT    | 105 | SER  |
| 21  | AU    | 15  | ARG  |
| 21  | AU    | 25  | LYS  |
| 27  | BC    | 20  | TYR  |
| 27  | BC    | 22  | ILE  |
| 27  | BC    | 36  | LYS  |
| 27  | BC    | 43  | VAL  |
| 27  | BC    | 44  | HIS  |
| 27  | BC    | 47  | LEU  |
| 27  | BC    | 49  | ILE  |
| 27  | BC    | 56  | GLN  |
| 27  | BC    | 58  | VAL  |
| 27  | BC    | 64  | LEU  |
| 27  | BC    | 77  | ILE  |
| 27  | BC    | 94  | VAL  |
| 28  | BD    | 10  | THR  |
| 28  | BD    | 14  | ARG  |
| 28  | BD    | 18  | VAL  |
| 28  | BD    | 23  | GLU  |
| 28  | BD    | 24  | ILE  |
| 28  | BD    | 25  | THR  |
| 28  | BD    | 26  | LYS  |
| 28  | BD    | 28  | GLU  |
| 28  | BD    | 33  | LEU  |
| 28  | BD    | 43  | ARG  |
| 28  | BD    | 44  | ASN  |
| 28  | BD    | 48  | ARG  |
| 28  | BD    | 49  | ILE  |
| 28  | BD    | 61  | LEU  |
| 28  | BD    | 64  | ILE  |
| 28  | BD    | 65  | ILE  |
| 28  | BD    | 67  | PHE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 28  | BD    | 71  | ASP  |
| 28  | BD    | 79  | VAL  |
| 28  | BD    | 83  | GLU  |
| 28  | BD    | 88  | ARG  |
| 28  | BD    | 92  | ILE  |
| 28  | BD    | 94  | LEU  |
| 28  | BD    | 95  | LEU  |
| 28  | BD    | 102 | LYS  |
| 28  | BD    | 103 | ARG  |
| 28  | BD    | 105 | ILE  |
| 28  | BD    | 111 | LEU  |
| 28  | BD    | 113 | VAL  |
| 28  | BD    | 118 | VAL  |
| 28  | BD    | 125 | ILE  |
| 28  | BD    | 126 | GLN  |
| 28  | BD    | 138 | VAL  |
| 28  | BD    | 140 | THR  |
| 28  | BD    | 141 | VAL  |
| 28  | BD    | 154 | LYS  |
| 28  | BD    | 166 | GLN  |
| 28  | BD    | 168 | ARG  |
| 28  | BD    | 169 | GLU  |
| 28  | BD    | 173 | VAL  |
| 28  | BD    | 185 | VAL  |
| 28  | BD    | 192 | THR  |
| 28  | BD    | 193 | VAL  |
| 28  | BD    | 204 | ILE  |
| 28  | BD    | 211 | ARG  |
| 28  | BD    | 212 | SER  |
| 28  | BD    | 221 | VAL  |
| 28  | BD    | 222 | ARG  |
| 28  | BD    | 242 | ARG  |
| 28  | BD    | 257 | LEU  |
| 28  | BD    | 259 | THR  |
| 28  | BD    | 260 | ARG  |
| 28  | BD    | 266 | SER  |
| 28  | BD    | 268 | ARG  |
| 28  | BD    | 270 | ILE  |
| 28  | BD    | 271 | ILE  |
| 29  | BE    | 9   | VAL  |
| 29  | BE    | 17  | ASP  |
| 29  | BE    | 18  | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 29  | BE    | 33  | VAL  |
| 29  | BE    | 34  | VAL  |
| 29  | BE    | 40  | GLU  |
| 29  | BE    | 47  | VAL  |
| 29  | BE    | 48  | GLN  |
| 29  | BE    | 52  | LEU  |
| 29  | BE    | 54  | GLN  |
| 29  | BE    | 57  | LYS  |
| 29  | BE    | 59  | VAL  |
| 29  | BE    | 64  | LYS  |
| 29  | BE    | 66  | HIS  |
| 29  | BE    | 67  | PHE  |
| 29  | BE    | 73  | GLU  |
| 29  | BE    | 77  | ILE  |
| 29  | BE    | 78  | LEU  |
| 29  | BE    | 79  | ARG  |
| 29  | BE    | 81  | ILE  |
| 29  | BE    | 82  | ARG  |
| 29  | BE    | 89  | ASP  |
| 29  | BE    | 95  | ILE  |
| 29  | BE    | 102 | VAL  |
| 29  | BE    | 107 | THR  |
| 29  | BE    | 119 | ARG  |
| 29  | BE    | 121 | ASN  |
| 29  | BE    | 133 | LYS  |
| 29  | BE    | 134 | ILE  |
| 29  | BE    | 145 | LYS  |
| 29  | BE    | 165 | VAL  |
| 29  | BE    | 175 | VAL  |
| 29  | BE    | 176 | ILE  |
| 29  | BE    | 179 | GLU  |
| 29  | BE    | 181 | LEU  |
| 29  | BE    | 182 | LEU  |
| 29  | BE    | 184 | VAL  |
| 29  | BE    | 195 | LEU  |
| 29  | BE    | 197 | ILE  |
| 29  | BE    | 202 | LYS  |
| 29  | BE    | 203 | LYS  |
| 30  | BF    | 2   | LYS  |
| 30  | BF    | 4   | VAL  |
| 30  | BF    | 11  | VAL  |
| 30  | BF    | 33  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 30  | BF    | 36  | VAL  |
| 30  | BF    | 38  | ARG  |
| 30  | BF    | 43  | LYS  |
| 30  | BF    | 44  | ARG  |
| 30  | BF    | 51  | THR  |
| 30  | BF    | 52  | LYS  |
| 30  | BF    | 53  | THR  |
| 30  | BF    | 54  | ARG  |
| 30  | BF    | 64  | ILE  |
| 30  | BF    | 67  | GLN  |
| 30  | BF    | 68  | LYS  |
| 30  | BF    | 69  | HIS  |
| 30  | BF    | 72  | ARG  |
| 30  | BF    | 74  | ARG  |
| 30  | BF    | 78  | ILE  |
| 30  | BF    | 82  | ILE  |
| 30  | BF    | 89  | VAL  |
| 30  | BF    | 99  | TYR  |
| 30  | BF    | 100 | THR  |
| 30  | BF    | 106 | ARG  |
| 30  | BF    | 112 | MET  |
| 30  | BF    | 114 | VAL  |
| 30  | BF    | 116 | ASP  |
| 30  | BF    | 124 | LEU  |
| 30  | BF    | 125 | LEU  |
| 30  | BF    | 140 | LEU  |
| 30  | BF    | 151 | SER  |
| 30  | BF    | 155 | LEU  |
| 30  | BF    | 158 | THR  |
| 30  | BF    | 161 | GLU  |
| 30  | BF    | 164 | ARG  |
| 30  | BF    | 174 | VAL  |
| 30  | BF    | 175 | THR  |
| 30  | BF    | 181 | LEU  |
| 30  | BF    | 183 | VAL  |
| 30  | BF    | 192 | LEU  |
| 30  | BF    | 201 | VAL  |
| 31  | BG    | 4   | ASP  |
| 31  | BG    | 5   | VAL  |
| 31  | BG    | 16  | ARG  |
| 31  | BG    | 32  | PRO  |
| 31  | BG    | 37  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 31  | BG    | 39  | ILE  |
| 31  | BG    | 43  | LEU  |
| 31  | BG    | 48  | GLU  |
| 31  | BG    | 58  | GLN  |
| 31  | BG    | 59  | GLU  |
| 31  | BG    | 60  | LEU  |
| 31  | BG    | 63  | ILE  |
| 31  | BG    | 76  | SER  |
| 31  | BG    | 83  | ARG  |
| 31  | BG    | 86  | MET  |
| 31  | BG    | 87  | PRO  |
| 31  | BG    | 88  | ILE  |
| 31  | BG    | 90  | LEU  |
| 31  | BG    | 92  | VAL  |
| 31  | BG    | 96  | ARG  |
| 31  | BG    | 97  | ASP  |
| 31  | BG    | 99  | MET  |
| 31  | BG    | 101 | ILE  |
| 31  | BG    | 106 | LEU  |
| 31  | BG    | 128 | ARG  |
| 31  | BG    | 130 | ASN  |
| 31  | BG    | 132 | ASN  |
| 31  | BG    | 133 | LEU  |
| 31  | BG    | 139 | LEU  |
| 31  | BG    | 143 | GLU  |
| 31  | BG    | 144 | ILE  |
| 31  | BG    | 147 | ASP  |
| 31  | BG    | 149 | VAL  |
| 31  | BG    | 152 | LEU  |
| 31  | BG    | 153 | ARG  |
| 31  | BG    | 159 | VAL  |
| 31  | BG    | 162 | THR  |
| 31  | BG    | 166 | ASP  |
| 31  | BG    | 176 | LEU  |
| 32  | BH    | 13  | LYS  |
| 32  | BH    | 25  | LYS  |
| 32  | BH    | 34  | GLU  |
| 32  | BH    | 44  | VAL  |
| 32  | BH    | 46  | GLU  |
| 32  | BH    | 54  | ARG  |
| 32  | BH    | 61  | HIS  |
| 32  | BH    | 68  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 32  | BH    | 72  | ILE  |
| 32  | BH    | 86  | GLU  |
| 32  | BH    | 101 | ARG  |
| 32  | BH    | 109 | PHE  |
| 32  | BH    | 110 | SER  |
| 32  | BH    | 114 | VAL  |
| 32  | BH    | 116 | GLU  |
| 32  | BH    | 121 | ILE  |
| 32  | BH    | 139 | GLN  |
| 32  | BH    | 144 | VAL  |
| 32  | BH    | 151 | ILE  |
| 32  | BH    | 153 | LYS  |
| 32  | BH    | 163 | TYR  |
| 32  | BH    | 170 | ARG  |
| 33  | BI    | 2   | LYS  |
| 33  | BI    | 22  | LYS  |
| 33  | BI    | 37  | VAL  |
| 33  | BI    | 38  | LEU  |
| 33  | BI    | 47  | LEU  |
| 33  | BI    | 52  | ARG  |
| 33  | BI    | 64  | GLU  |
| 33  | BI    | 75  | LEU  |
| 33  | BI    | 76  | THR  |
| 33  | BI    | 77  | LEU  |
| 33  | BI    | 78  | THR  |
| 33  | BI    | 81  | VAL  |
| 33  | BI    | 85  | GLU  |
| 33  | BI    | 88  | ILE  |
| 33  | BI    | 92  | VAL  |
| 33  | BI    | 93  | THR  |
| 33  | BI    | 101 | LEU  |
| 33  | BI    | 109 | ILE  |
| 33  | BI    | 113 | ARG  |
| 33  | BI    | 114 | LEU  |
| 33  | BI    | 122 | GLU  |
| 33  | BI    | 125 | GLU  |
| 33  | BI    | 131 | LYS  |
| 33  | BI    | 133 | HIS  |
| 33  | BI    | 136 | VAL  |
| 33  | BI    | 138 | ILE  |
| 33  | BI    | 142 | VAL  |
| 34  | BN    | 1   | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 34  | BN    | 4   | TYR  |
| 34  | BN    | 9   | VAL  |
| 34  | BN    | 12  | ARG  |
| 34  | BN    | 15  | LEU  |
| 34  | BN    | 26  | LEU  |
| 34  | BN    | 28  | THR  |
| 34  | BN    | 34  | LEU  |
| 34  | BN    | 38  | HIS  |
| 34  | BN    | 39  | ARG  |
| 34  | BN    | 45  | ASN  |
| 34  | BN    | 48  | MET  |
| 34  | BN    | 58  | ASP  |
| 34  | BN    | 60  | ILE  |
| 34  | BN    | 62  | VAL  |
| 34  | BN    | 63  | THR  |
| 34  | BN    | 65  | LYS  |
| 34  | BN    | 66  | LYS  |
| 34  | BN    | 67  | LEU  |
| 34  | BN    | 68  | GLU  |
| 34  | BN    | 82  | LEU  |
| 34  | BN    | 87  | LEU  |
| 34  | BN    | 89  | LYS  |
| 34  | BN    | 93  | THR  |
| 34  | BN    | 99  | LEU  |
| 34  | BN    | 119 | ARG  |
| 34  | BN    | 120 | LEU  |
| 34  | BN    | 130 | HIS  |
| 34  | BN    | 134 | ARG  |
| 34  | BN    | 136 | GLU  |
| 35  | BO    | 3   | GLN  |
| 35  | BO    | 8   | LEU  |
| 35  | BO    | 10  | VAL  |
| 35  | BO    | 17  | ARG  |
| 35  | BO    | 22  | ILE  |
| 35  | BO    | 23  | ARG  |
| 35  | BO    | 24  | VAL  |
| 35  | BO    | 26  | LYS  |
| 35  | BO    | 28  | SER  |
| 35  | BO    | 32  | TYR  |
| 35  | BO    | 38  | VAL  |
| 35  | BO    | 47  | ILE  |
| 35  | BO    | 52  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 35  | BO    | 62  | VAL  |
| 35  | BO    | 69  | ILE  |
| 35  | BO    | 70  | LYS  |
| 35  | BO    | 73  | ASP  |
| 35  | BO    | 82  | ASN  |
| 35  | BO    | 85  | VAL  |
| 35  | BO    | 91  | LEU  |
| 35  | BO    | 94  | ARG  |
| 35  | BO    | 105 | GLU  |
| 35  | BO    | 117 | LEU  |
| 36  | BP    | 8   | PRO  |
| 36  | BP    | 10  | PRO  |
| 36  | BP    | 13  | ASN  |
| 36  | BP    | 14  | LYS  |
| 36  | BP    | 21  | ARG  |
| 36  | BP    | 25  | SER  |
| 36  | BP    | 27  | HIS  |
| 36  | BP    | 32  | THR  |
| 36  | BP    | 33  | ARG  |
| 36  | BP    | 50  | ARG  |
| 36  | BP    | 55  | ARG  |
| 36  | BP    | 59  | LEU  |
| 36  | BP    | 61  | ARG  |
| 36  | BP    | 67  | MET  |
| 36  | BP    | 75  | ILE  |
| 36  | BP    | 81  | GLN  |
| 36  | BP    | 85  | LEU  |
| 36  | BP    | 91  | PHE  |
| 36  | BP    | 98  | GLU  |
| 36  | BP    | 100 | LEU  |
| 36  | BP    | 110 | TYR  |
| 36  | BP    | 112 | LEU  |
| 36  | BP    | 114 | ILE  |
| 36  | BP    | 115 | LEU  |
| 36  | BP    | 117 | GLU  |
| 36  | BP    | 125 | VAL  |
| 36  | BP    | 136 | GLU  |
| 36  | BP    | 138 | LEU  |
| 36  | BP    | 144 | GLU  |
| 36  | BP    | 147 | LEU  |
| 36  | BP    | 148 | LEU  |
| 37  | BQ    | 2   | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 37  | BQ    | 3   | MET  |
| 37  | BQ    | 10  | ARG  |
| 37  | BQ    | 14  | ARG  |
| 37  | BQ    | 16  | ARG  |
| 37  | BQ    | 17  | LEU  |
| 37  | BQ    | 22  | LYS  |
| 37  | BQ    | 35  | VAL  |
| 37  | BQ    | 42  | ILE  |
| 37  | BQ    | 43  | THR  |
| 37  | BQ    | 45  | GLN  |
| 37  | BQ    | 47  | ILE  |
| 37  | BQ    | 51  | ARG  |
| 37  | BQ    | 54  | MET  |
| 37  | BQ    | 55  | VAL  |
| 37  | BQ    | 56  | ARG  |
| 37  | BQ    | 59  | ARG  |
| 37  | BQ    | 65  | PHE  |
| 37  | BQ    | 66  | ILE  |
| 37  | BQ    | 75  | THR  |
| 37  | BQ    | 76  | LYS  |
| 37  | BQ    | 79  | LEU  |
| 37  | BQ    | 81  | VAL  |
| 37  | BQ    | 82  | ARG  |
| 37  | BQ    | 96  | VAL  |
| 37  | BQ    | 109 | VAL  |
| 37  | BQ    | 110 | THR  |
| 37  | BQ    | 112 | GLU  |
| 37  | BQ    | 118 | LEU  |
| 37  | BQ    | 134 | ARG  |
| 37  | BQ    | 138 | ASP  |
| 37  | BQ    | 139 | GLU  |
| 38  | BR    | 2   | ARG  |
| 38  | BR    | 5   | LYS  |
| 38  | BR    | 9   | LYS  |
| 38  | BR    | 10  | LEU  |
| 38  | BR    | 13  | HIS  |
| 38  | BR    | 14  | SER  |
| 38  | BR    | 18  | LEU  |
| 38  | BR    | 28  | LEU  |
| 38  | BR    | 29  | LEU  |
| 38  | BR    | 33  | ARG  |
| 38  | BR    | 34  | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 38  | BR    | 35  | THR  |
| 38  | BR    | 37  | THR  |
| 38  | BR    | 45  | ARG  |
| 38  | BR    | 47  | PHE  |
| 38  | BR    | 51  | LEU  |
| 38  | BR    | 56  | LYS  |
| 38  | BR    | 57  | ARG  |
| 38  | BR    | 60  | LEU  |
| 38  | BR    | 67  | LEU  |
| 38  | BR    | 73  | VAL  |
| 38  | BR    | 75  | LEU  |
| 38  | BR    | 76  | VAL  |
| 38  | BR    | 77  | ARG  |
| 38  | BR    | 79  | LEU  |
| 38  | BR    | 80  | PHE  |
| 38  | BR    | 81  | ASP  |
| 38  | BR    | 83  | ILE  |
| 38  | BR    | 94  | TYR  |
| 38  | BR    | 104 | ARG  |
| 38  | BR    | 111 | LEU  |
| 38  | BR    | 113 | LEU  |
| 38  | BR    | 114 | VAL  |
| 39  | BS    | 11  | LYS  |
| 39  | BS    | 12  | PHE  |
| 39  | BS    | 14  | VAL  |
| 39  | BS    | 15  | ARG  |
| 39  | BS    | 16  | ASN  |
| 39  | BS    | 18  | ILE  |
| 39  | BS    | 20  | ARG  |
| 39  | BS    | 32  | LEU  |
| 39  | BS    | 33  | LYS  |
| 39  | BS    | 35  | ILE  |
| 39  | BS    | 39  | ILE  |
| 39  | BS    | 42  | ASP  |
| 39  | BS    | 50  | SER  |
| 39  | BS    | 56  | LEU  |
| 39  | BS    | 57  | LYS  |
| 39  | BS    | 69  | VAL  |
| 39  | BS    | 73  | LEU  |
| 39  | BS    | 89  | ARG  |
| 39  | BS    | 92  | TYR  |
| 39  | BS    | 97  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 39  | BS    | 99  | LYS  |
| 39  | BS    | 101 | LEU  |
| 39  | BS    | 103 | GLU  |
| 39  | BS    | 106 | ARG  |
| 39  | BS    | 107 | GLU  |
| 40  | BT    | 3   | ARG  |
| 40  | BT    | 6   | LEU  |
| 40  | BT    | 11  | GLU  |
| 40  | BT    | 19  | LEU  |
| 40  | BT    | 21  | GLU  |
| 40  | BT    | 23  | ARG  |
| 40  | BT    | 27  | THR  |
| 40  | BT    | 29  | ARG  |
| 40  | BT    | 31  | SER  |
| 40  | BT    | 34  | VAL  |
| 40  | BT    | 42  | ILE  |
| 40  | BT    | 50  | ILE  |
| 40  | BT    | 51  | ARG  |
| 40  | BT    | 53  | ARG  |
| 40  | BT    | 54  | ARG  |
| 40  | BT    | 55  | ASN  |
| 40  | BT    | 59  | THR  |
| 40  | BT    | 63  | VAL  |
| 40  | BT    | 74  | ARG  |
| 40  | BT    | 75  | ILE  |
| 40  | BT    | 84  | GLN  |
| 40  | BT    | 86  | ILE  |
| 40  | BT    | 89  | VAL  |
| 40  | BT    | 90  | GLN  |
| 40  | BT    | 96  | ARG  |
| 40  | BT    | 99  | LEU  |
| 40  | BT    | 107 | ASP  |
| 40  | BT    | 113 | LYS  |
| 40  | BT    | 114 | LEU  |
| 40  | BT    | 119 | LYS  |
| 40  | BT    | 121 | ILE  |
| 40  | BT    | 128 | GLU  |
| 41  | BU    | 8   | VAL  |
| 41  | BU    | 11  | ARG  |
| 41  | BU    | 14  | HIS  |
| 41  | BU    | 15  | LYS  |
| 41  | BU    | 16  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 41  | BU    | 17  | ILE  |
| 41  | BU    | 20  | LEU  |
| 41  | BU    | 30  | LYS  |
| 41  | BU    | 31  | SER  |
| 41  | BU    | 33  | ARG  |
| 41  | BU    | 34  | LYS  |
| 41  | BU    | 37  | GLU  |
| 41  | BU    | 52  | ARG  |
| 41  | BU    | 60  | LEU  |
| 41  | BU    | 69  | CYS  |
| 41  | BU    | 74  | LEU  |
| 41  | BU    | 80  | ILE  |
| 41  | BU    | 83  | LEU  |
| 41  | BU    | 88  | ILE  |
| 41  | BU    | 89  | GLU  |
| 41  | BU    | 90  | VAL  |
| 41  | BU    | 92  | ARG  |
| 41  | BU    | 102 | GLU  |
| 41  | BU    | 104 | GLN  |
| 41  | BU    | 105 | VAL  |
| 42  | BV    | 1   | MET  |
| 42  | BV    | 4   | ILE  |
| 42  | BV    | 5   | VAL  |
| 42  | BV    | 10  | LYS  |
| 42  | BV    | 18  | LEU  |
| 42  | BV    | 19  | LYS  |
| 42  | BV    | 20  | LEU  |
| 42  | BV    | 26  | ASP  |
| 42  | BV    | 35  | LEU  |
| 42  | BV    | 37  | VAL  |
| 42  | BV    | 38  | LEU  |
| 42  | BV    | 39  | LEU  |
| 42  | BV    | 40  | LEU  |
| 42  | BV    | 46  | VAL  |
| 42  | BV    | 47  | VAL  |
| 42  | BV    | 49  | THR  |
| 42  | BV    | 52  | VAL  |
| 42  | BV    | 57  | VAL  |
| 42  | BV    | 61  | VAL  |
| 42  | BV    | 62  | LEU  |
| 42  | BV    | 68  | LYS  |
| 42  | BV    | 78  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 42  | BV    | 80  | GLN  |
| 42  | BV    | 82  | ARG  |
| 42  | BV    | 91  | TYR  |
| 42  | BV    | 94  | LEU  |
| 42  | BV    | 95  | LEU  |
| 42  | BV    | 99  | ILE  |
| 43  | BW    | 1   | MET  |
| 43  | BW    | 8   | ARG  |
| 43  | BW    | 9   | TYR  |
| 43  | BW    | 11  | ARG  |
| 43  | BW    | 16  | LYS  |
| 43  | BW    | 17  | VAL  |
| 43  | BW    | 20  | VAL  |
| 43  | BW    | 24  | ILE  |
| 43  | BW    | 27  | LYS  |
| 43  | BW    | 36  | LEU  |
| 43  | BW    | 39  | THR  |
| 43  | BW    | 41  | LYS  |
| 43  | BW    | 45  | TYR  |
| 43  | BW    | 51  | LEU  |
| 43  | BW    | 53  | SER  |
| 43  | BW    | 59  | VAL  |
| 43  | BW    | 70  | TYR  |
| 43  | BW    | 76  | VAL  |
| 43  | BW    | 92  | ARG  |
| 43  | BW    | 96  | ILE  |
| 43  | BW    | 99  | ARG  |
| 43  | BW    | 100 | THR  |
| 43  | BW    | 103 | ILE  |
| 43  | BW    | 105 | VAL  |
| 43  | BW    | 107 | LEU  |
| 44  | BX    | 12  | VAL  |
| 44  | BX    | 14  | SER  |
| 44  | BX    | 27  | THR  |
| 44  | BX    | 35  | THR  |
| 44  | BX    | 37  | THR  |
| 44  | BX    | 39  | ILE  |
| 44  | BX    | 43  | VAL  |
| 44  | BX    | 51  | VAL  |
| 44  | BX    | 52  | VAL  |
| 44  | BX    | 57  | LEU  |
| 44  | BX    | 63  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 44  | BX    | 64  | LYS  |
| 44  | BX    | 68  | ARG  |
| 44  | BX    | 70  | LEU  |
| 44  | BX    | 80  | ILE  |
| 44  | BX    | 81  | VAL  |
| 44  | BX    | 83  | VAL  |
| 44  | BX    | 89  | ILE  |
| 45  | BY    | 6   | HIS  |
| 45  | BY    | 7   | VAL  |
| 45  | BY    | 15  | VAL  |
| 45  | BY    | 19  | LYS  |
| 45  | BY    | 28  | LYS  |
| 45  | BY    | 30  | VAL  |
| 45  | BY    | 31  | LEU  |
| 45  | BY    | 37  | VAL  |
| 45  | BY    | 40  | GLU  |
| 45  | BY    | 42  | VAL  |
| 45  | BY    | 47  | LYS  |
| 45  | BY    | 62  | GLU  |
| 45  | BY    | 67  | LEU  |
| 45  | BY    | 76  | CYS  |
| 45  | BY    | 83  | THR  |
| 45  | BY    | 84  | ARG  |
| 45  | BY    | 89  | PHE  |
| 45  | BY    | 91  | GLU  |
| 45  | BY    | 96  | ILE  |
| 45  | BY    | 98  | VAL  |
| 46  | BZ    | 3   | TYR  |
| 46  | BZ    | 9   | TYR  |
| 46  | BZ    | 11  | GLU  |
| 46  | BZ    | 23  | LYS  |
| 46  | BZ    | 24  | LEU  |
| 46  | BZ    | 38  | TYR  |
| 46  | BZ    | 39  | VAL  |
| 46  | BZ    | 41  | LEU  |
| 46  | BZ    | 53  | ILE  |
| 46  | BZ    | 72  | ARG  |
| 46  | BZ    | 74  | VAL  |
| 46  | BZ    | 75  | ASN  |
| 46  | BZ    | 76  | LEU  |
| 46  | BZ    | 79  | ARG  |
| 46  | BZ    | 82  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 46  | BZ    | 85  | HIS  |
| 46  | BZ    | 86  | VAL  |
| 46  | BZ    | 116 | VAL  |
| 46  | BZ    | 119 | GLU  |
| 46  | BZ    | 121 | HIS  |
| 46  | BZ    | 128 | VAL  |
| 46  | BZ    | 129 | SER  |
| 46  | BZ    | 131 | ARG  |
| 46  | BZ    | 138 | GLU  |
| 46  | BZ    | 140 | ASP  |
| 46  | BZ    | 145 | GLU  |
| 46  | BZ    | 150 | LEU  |
| 46  | BZ    | 151 | HIS  |
| 46  | BZ    | 157 | LEU  |
| 46  | BZ    | 163 | LEU  |
| 46  | BZ    | 166 | SER  |
| 46  | BZ    | 168 | GLU  |
| 46  | BZ    | 174 | VAL  |
| 47  | B0    | 5   | LYS  |
| 47  | B0    | 10  | THR  |
| 47  | B0    | 14  | ARG  |
| 47  | B0    | 40  | GLN  |
| 47  | B0    | 43  | THR  |
| 47  | B0    | 53  | MET  |
| 47  | B0    | 62  | LEU  |
| 47  | B0    | 70  | GLN  |
| 47  | B0    | 84  | LEU  |
| 48  | B1    | 5   | CYS  |
| 48  | B1    | 21  | ARG  |
| 48  | B1    | 27  | GLU  |
| 48  | B1    | 30  | VAL  |
| 48  | B1    | 34  | THR  |
| 48  | B1    | 39  | LYS  |
| 48  | B1    | 40  | ARG  |
| 48  | B1    | 41  | ARG  |
| 48  | B1    | 45  | ASN  |
| 48  | B1    | 46  | LEU  |
| 48  | B1    | 53  | VAL  |
| 48  | B1    | 58  | ILE  |
| 48  | B1    | 59  | THR  |
| 48  | B1    | 61  | ARG  |
| 48  | B1    | 65  | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 48  | B1    | 67  | ILE  |
| 48  | B1    | 82  | LEU  |
| 48  | B1    | 91  | LYS  |
| 48  | B1    | 94  | LEU  |
| 49  | B2    | 8   | LYS  |
| 49  | B2    | 12  | GLU  |
| 49  | B2    | 17  | SER  |
| 49  | B2    | 32  | LEU  |
| 49  | B2    | 35  | LEU  |
| 49  | B2    | 41  | ILE  |
| 49  | B2    | 44  | LEU  |
| 49  | B2    | 50  | ILE  |
| 49  | B2    | 51  | ARG  |
| 49  | B2    | 52  | ASP  |
| 49  | B2    | 53  | LEU  |
| 49  | B2    | 59  | ARG  |
| 49  | B2    | 65  | ASN  |
| 49  | B2    | 68  | ARG  |
| 49  | B2    | 69  | ARG  |
| 49  | B2    | 70  | GLN  |
| 50  | B3    | 4   | LEU  |
| 50  | B3    | 8   | LEU  |
| 50  | B3    | 23  | LEU  |
| 50  | B3    | 26  | LEU  |
| 50  | B3    | 30  | ARG  |
| 50  | B3    | 36  | VAL  |
| 50  | B3    | 37  | LEU  |
| 50  | B3    | 38  | GLU  |
| 50  | B3    | 39  | ASP  |
| 50  | B3    | 50  | VAL  |
| 50  | B3    | 53  | LEU  |
| 50  | B3    | 56  | VAL  |
| 50  | B3    | 59  | VAL  |
| 51  | B4    | 36  | VAL  |
| 51  | B4    | 44  | CYS  |
| 51  | B4    | 48  | ILE  |
| 51  | B4    | 50  | THR  |
| 51  | B4    | 53  | THR  |
| 51  | B4    | 54  | LYS  |
| 51  | B4    | 56  | GLU  |
| 51  | B4    | 60  | GLU  |
| 51  | B4    | 61  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 51  | B4    | 63  | SER  |
| 52  | B5    | 3   | LYS  |
| 52  | B5    | 6   | VAL  |
| 52  | B5    | 8   | LYS  |
| 52  | B5    | 11  | THR  |
| 52  | B5    | 16  | ARG  |
| 52  | B5    | 19  | ARG  |
| 52  | B5    | 40  | LYS  |
| 52  | B5    | 45  | VAL  |
| 52  | B5    | 48  | GLU  |
| 52  | B5    | 55  | ARG  |
| 52  | B5    | 56  | LYS  |
| 53  | B6    | 10  | LEU  |
| 53  | B6    | 11  | LEU  |
| 53  | B6    | 12  | GLU  |
| 53  | B6    | 14  | THR  |
| 53  | B6    | 17  | LYS  |
| 53  | B6    | 18  | ARG  |
| 53  | B6    | 33  | LYS  |
| 53  | B6    | 36  | LEU  |
| 53  | B6    | 42  | TRP  |
| 53  | B6    | 43  | CYS  |
| 53  | B6    | 45  | LYS  |
| 53  | B6    | 47  | THR  |
| 54  | B7    | 1   | MET  |
| 54  | B7    | 4   | THR  |
| 54  | B7    | 9   | ARG  |
| 54  | B7    | 10  | ARG  |
| 54  | B7    | 15  | THR  |
| 54  | B7    | 24  | THR  |
| 54  | B7    | 41  | ARG  |
| 54  | B7    | 42  | LEU  |
| 54  | B7    | 43  | THR  |
| 55  | B8    | 4   | MET  |
| 55  | B8    | 14  | VAL  |
| 55  | B8    | 29  | LYS  |
| 55  | B8    | 30  | ARG  |
| 55  | B8    | 32  | LEU  |
| 55  | B8    | 33  | ASN  |
| 55  | B8    | 34  | TRP  |
| 55  | B8    | 36  | LYS  |
| 55  | B8    | 42  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 55  | B8    | 43  | GLN  |
| 55  | B8    | 49  | VAL  |
| 55  | B8    | 52  | LYS  |
| 55  | B8    | 59  | LYS  |
| 55  | B8    | 60  | LEU  |
| 55  | B8    | 61  | LEU  |
| 56  | B9    | 2   | LYS  |
| 56  | B9    | 25  | VAL  |
| 56  | B9    | 28  | GLU  |
| 56  | B9    | 29  | ASN  |
| 56  | B9    | 35  | ARG  |
| 2   | CB    | 8   | LYS  |
| 2   | CB    | 15  | VAL  |
| 2   | CB    | 16  | HIS  |
| 2   | CB    | 32  | ILE  |
| 2   | CB    | 36  | ARG  |
| 2   | CB    | 37  | ASN  |
| 2   | CB    | 39  | ILE  |
| 2   | CB    | 41  | ILE  |
| 2   | CB    | 42  | ILE  |
| 2   | CB    | 45  | GLN  |
| 2   | CB    | 48  | MET  |
| 2   | CB    | 53  | ARG  |
| 2   | CB    | 61  | LEU  |
| 2   | CB    | 64  | ARG  |
| 2   | CB    | 67  | THR  |
| 2   | CB    | 71  | VAL  |
| 2   | CB    | 74  | LYS  |
| 2   | CB    | 75  | LYS  |
| 2   | CB    | 80  | ILE  |
| 2   | CB    | 83  | MET  |
| 2   | CB    | 103 | THR  |
| 2   | CB    | 109 | SER  |
| 2   | CB    | 113 | HIS  |
| 2   | CB    | 115 | LEU  |
| 2   | CB    | 119 | GLU  |
| 2   | CB    | 121 | LEU  |
| 2   | CB    | 130 | ARG  |
| 2   | CB    | 140 | HIS  |
| 2   | CB    | 145 | LEU  |
| 2   | CB    | 150 | SER  |
| 2   | CB    | 155 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | CB    | 156 | LYS  |
| 2   | CB    | 158 | LEU  |
| 2   | CB    | 160 | ASP  |
| 2   | CB    | 162 | ILE  |
| 2   | CB    | 164 | VAL  |
| 2   | CB    | 172 | ILE  |
| 2   | CB    | 178 | ARG  |
| 2   | CB    | 180 | LEU  |
| 2   | CB    | 184 | VAL  |
| 2   | CB    | 187 | LEU  |
| 2   | CB    | 189 | ASP  |
| 2   | CB    | 191 | ASP  |
| 2   | CB    | 192 | SER  |
| 2   | CB    | 196 | LEU  |
| 2   | CB    | 201 | ILE  |
| 2   | CB    | 208 | ILE  |
| 2   | CB    | 211 | ILE  |
| 2   | CB    | 213 | LEU  |
| 2   | CB    | 214 | ILE  |
| 2   | CB    | 215 | LEU  |
| 2   | CB    | 223 | ILE  |
| 2   | CB    | 226 | ARG  |
| 2   | CB    | 238 | LEU  |
| 2   | CB    | 239 | VAL  |
| 3   | CC    | 3   | ASN  |
| 3   | CC    | 4   | LYS  |
| 3   | CC    | 5   | ILE  |
| 3   | CC    | 8   | ILE  |
| 3   | CC    | 12  | LEU  |
| 3   | CC    | 16  | ARG  |
| 3   | CC    | 17  | ASP  |
| 3   | CC    | 21  | ARG  |
| 3   | CC    | 29  | TYR  |
| 3   | CC    | 30  | ARG  |
| 3   | CC    | 31  | HIS  |
| 3   | CC    | 32  | LEU  |
| 3   | CC    | 34  | LEU  |
| 3   | CC    | 36  | ASP  |
| 3   | CC    | 56  | ASP  |
| 3   | CC    | 64  | VAL  |
| 3   | CC    | 69  | HIS  |
| 3   | CC    | 70  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | CC    | 97  | LYS  |
| 3   | CC    | 102 | ASN  |
| 3   | CC    | 140 | ARG  |
| 3   | CC    | 144 | SER  |
| 3   | CC    | 153 | VAL  |
| 3   | CC    | 165 | THR  |
| 3   | CC    | 166 | GLU  |
| 3   | CC    | 178 | LEU  |
| 3   | CC    | 192 | THR  |
| 3   | CC    | 196 | LEU  |
| 3   | CC    | 202 | ILE  |
| 3   | CC    | 204 | LEU  |
| 4   | CD    | 3   | ARG  |
| 4   | CD    | 8   | VAL  |
| 4   | CD    | 9   | CYS  |
| 4   | CD    | 10  | ARG  |
| 4   | CD    | 11  | LEU  |
| 4   | CD    | 13  | ARG  |
| 4   | CD    | 33  | MET  |
| 4   | CD    | 35  | ARG  |
| 4   | CD    | 36  | ARG  |
| 4   | CD    | 49  | ARG  |
| 4   | CD    | 58  | LEU  |
| 4   | CD    | 59  | ARG  |
| 4   | CD    | 61  | LYS  |
| 4   | CD    | 70  | ILE  |
| 4   | CD    | 73  | ARG  |
| 4   | CD    | 105 | VAL  |
| 4   | CD    | 108 | LEU  |
| 4   | CD    | 114 | ARG  |
| 4   | CD    | 118 | ARG  |
| 4   | CD    | 122 | ARG  |
| 4   | CD    | 135 | LEU  |
| 4   | CD    | 139 | ARG  |
| 4   | CD    | 146 | ILE  |
| 4   | CD    | 154 | ASN  |
| 4   | CD    | 158 | ILE  |
| 4   | CD    | 166 | LYS  |
| 4   | CD    | 182 | LYS  |
| 4   | CD    | 200 | GLU  |
| 5   | CE    | 16  | THR  |
| 5   | CE    | 18  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | CE    | 26  | PHE  |
| 5   | CE    | 31  | LEU  |
| 5   | CE    | 34  | VAL  |
| 5   | CE    | 41  | VAL  |
| 5   | CE    | 45  | PHE  |
| 5   | CE    | 51  | VAL  |
| 5   | CE    | 64  | ARG  |
| 5   | CE    | 68  | GLU  |
| 5   | CE    | 71  | LEU  |
| 5   | CE    | 72  | GLN  |
| 5   | CE    | 79  | GLU  |
| 5   | CE    | 80  | ILE  |
| 5   | CE    | 87  | SER  |
| 5   | CE    | 91  | LEU  |
| 5   | CE    | 100 | VAL  |
| 5   | CE    | 101 | ILE  |
| 5   | CE    | 110 | LEU  |
| 5   | CE    | 112 | LEU  |
| 5   | CE    | 116 | THR  |
| 5   | CE    | 126 | ARG  |
| 5   | CE    | 131 | ILE  |
| 5   | CE    | 136 | MET  |
| 5   | CE    | 143 | ARG  |
| 5   | CE    | 144 | THR  |
| 5   | CE    | 145 | LYS  |
| 5   | CE    | 147 | ASP  |
| 5   | CE    | 150 | ARG  |
| 6   | CF    | 1   | MET  |
| 6   | CF    | 10  | LEU  |
| 6   | CF    | 14  | LEU  |
| 6   | CF    | 25  | ILE  |
| 6   | CF    | 28  | ARG  |
| 6   | CF    | 37  | VAL  |
| 6   | CF    | 43  | LEU  |
| 6   | CF    | 46  | ARG  |
| 6   | CF    | 63  | TYR  |
| 6   | CF    | 64  | GLN  |
| 6   | CF    | 70  | ASP  |
| 6   | CF    | 72  | VAL  |
| 6   | CF    | 73  | ASN  |
| 6   | CF    | 82  | ARG  |
| 6   | CF    | 92  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | CG    | 9   | VAL  |
| 7   | CG    | 10  | ARG  |
| 7   | CG    | 17  | VAL  |
| 7   | CG    | 21  | VAL  |
| 7   | CG    | 30  | ILE  |
| 7   | CG    | 38  | LEU  |
| 7   | CG    | 45  | ASP  |
| 7   | CG    | 49  | ILE  |
| 7   | CG    | 50  | ILE  |
| 7   | CG    | 60  | LYS  |
| 7   | CG    | 61  | VAL  |
| 7   | CG    | 79  | ARG  |
| 7   | CG    | 90  | GLU  |
| 7   | CG    | 91  | VAL  |
| 7   | CG    | 104 | LEU  |
| 7   | CG    | 113 | GLU  |
| 7   | CG    | 114 | ARG  |
| 7   | CG    | 118 | VAL  |
| 7   | CG    | 124 | LEU  |
| 7   | CG    | 136 | LYS  |
| 7   | CG    | 137 | LYS  |
| 7   | CG    | 138 | LYS  |
| 7   | CG    | 140 | ASP  |
| 7   | CG    | 142 | GLU  |
| 7   | CG    | 156 | TRP  |
| 8   | CH    | 1   | MET  |
| 8   | CH    | 2   | LEU  |
| 8   | CH    | 3   | THR  |
| 8   | CH    | 8   | ASP  |
| 8   | CH    | 12  | ARG  |
| 8   | CH    | 17  | THR  |
| 8   | CH    | 19  | VAL  |
| 8   | CH    | 22  | GLU  |
| 8   | CH    | 24  | THR  |
| 8   | CH    | 26  | VAL  |
| 8   | CH    | 30  | ARG  |
| 8   | CH    | 37  | ARG  |
| 8   | CH    | 38  | ILE  |
| 8   | CH    | 39  | LEU  |
| 8   | CH    | 41  | ARG  |
| 8   | CH    | 45  | ILE  |
| 8   | CH    | 52  | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8   | CH    | 63  | LEU  |
| 8   | CH    | 68  | ARG  |
| 8   | CH    | 82  | HIS  |
| 8   | CH    | 83  | ILE  |
| 8   | CH    | 84  | ARG  |
| 8   | CH    | 85  | ARG  |
| 8   | CH    | 88  | LYS  |
| 8   | CH    | 91  | ARG  |
| 8   | CH    | 92  | ARG  |
| 8   | CH    | 102 | ARG  |
| 8   | CH    | 104 | ARG  |
| 8   | CH    | 105 | ARG  |
| 8   | CH    | 109 | ILE  |
| 8   | CH    | 111 | ILE  |
| 8   | CH    | 112 | LEU  |
| 8   | CH    | 118 | VAL  |
| 8   | CH    | 125 | ARG  |
| 8   | CH    | 127 | LEU  |
| 8   | CH    | 133 | LEU  |
| 9   | CI    | 4   | TYR  |
| 9   | CI    | 20  | ARG  |
| 9   | CI    | 27  | THR  |
| 9   | CI    | 31  | GLN  |
| 9   | CI    | 44  | VAL  |
| 9   | CI    | 56  | LEU  |
| 9   | CI    | 59  | PHE  |
| 9   | CI    | 64  | THR  |
| 9   | CI    | 71  | SER  |
| 9   | CI    | 78  | LYS  |
| 9   | CI    | 79  | LEU  |
| 9   | CI    | 89  | ASN  |
| 9   | CI    | 91  | ASP  |
| 9   | CI    | 95  | LYS  |
| 9   | CI    | 101 | PHE  |
| 9   | CI    | 102 | LEU  |
| 9   | CI    | 104 | ARG  |
| 9   | CI    | 112 | LYS  |
| 9   | CI    | 114 | TYR  |
| 9   | CI    | 124 | GLN  |
| 9   | CI    | 126 | SER  |
| 9   | CI    | 128 | ARG  |
| 10  | CJ    | 8   | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10  | CJ    | 13  | HIS  |
| 10  | CJ    | 16  | LEU  |
| 10  | CJ    | 43  | ARG  |
| 10  | CJ    | 44  | VAL  |
| 10  | CJ    | 45  | ARG  |
| 10  | CJ    | 47  | PHE  |
| 10  | CJ    | 50  | ILE  |
| 10  | CJ    | 54  | PHE  |
| 10  | CJ    | 57  | LYS  |
| 10  | CJ    | 62  | HIS  |
| 10  | CJ    | 63  | PHE  |
| 10  | CJ    | 67  | THR  |
| 10  | CJ    | 70  | ARG  |
| 10  | CJ    | 72  | VAL  |
| 10  | CJ    | 74  | ILE  |
| 10  | CJ    | 76  | ASN  |
| 10  | CJ    | 78  | ASN  |
| 10  | CJ    | 80  | LYS  |
| 10  | CJ    | 86  | MET  |
| 10  | CJ    | 96  | ILE  |
| 11  | CK    | 11  | LYS  |
| 11  | CK    | 14  | VAL  |
| 11  | CK    | 21  | ILE  |
| 11  | CK    | 28  | THR  |
| 11  | CK    | 29  | ILE  |
| 11  | CK    | 32  | ILE  |
| 11  | CK    | 47  | VAL  |
| 11  | CK    | 48  | ILE  |
| 11  | CK    | 51  | LYS  |
| 11  | CK    | 57  | THR  |
| 11  | CK    | 63  | LEU  |
| 11  | CK    | 82  | VAL  |
| 11  | CK    | 84  | VAL  |
| 11  | CK    | 91  | ARG  |
| 11  | CK    | 98  | LEU  |
| 11  | CK    | 103 | LEU  |
| 11  | CK    | 105 | VAL  |
| 11  | CK    | 108 | ILE  |
| 11  | CK    | 109 | VAL  |
| 11  | CK    | 114 | VAL  |
| 11  | CK    | 119 | CYS  |
| 11  | CK    | 125 | PHE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11  | CK    | 127 | LYS  |
| 12  | CL    | 6   | THR  |
| 12  | CL    | 7   | ILE  |
| 12  | CL    | 11  | VAL  |
| 12  | CL    | 24  | VAL  |
| 12  | CL    | 33  | ARG  |
| 12  | CL    | 42  | THR  |
| 12  | CL    | 43  | VAL  |
| 12  | CL    | 52  | LEU  |
| 12  | CL    | 54  | LYS  |
| 12  | CL    | 58  | VAL  |
| 12  | CL    | 60  | LEU  |
| 12  | CL    | 70  | ILE  |
| 12  | CL    | 73  | GLU  |
| 12  | CL    | 78  | GLN  |
| 12  | CL    | 79  | GLU  |
| 12  | CL    | 83  | VAL  |
| 12  | CL    | 84  | LEU  |
| 12  | CL    | 85  | ILE  |
| 12  | CL    | 89  | ARG  |
| 12  | CL    | 100 | ILE  |
| 12  | CL    | 102 | ARG  |
| 12  | CL    | 104 | VAL  |
| 12  | CL    | 115 | LYS  |
| 12  | CL    | 122 | THR  |
| 13  | CM    | 11  | ARG  |
| 13  | CM    | 56  | LEU  |
| 13  | CM    | 57  | ARG  |
| 13  | CM    | 64  | TRP  |
| 13  | CM    | 66  | LEU  |
| 13  | CM    | 67  | GLU  |
| 13  | CM    | 69  | GLU  |
| 13  | CM    | 70  | LEU  |
| 13  | CM    | 88  | ARG  |
| 13  | CM    | 108 | ARG  |
| 13  | CM    | 114 | ARG  |
| 13  | CM    | 117 | VAL  |
| 13  | CM    | 120 | LYS  |
| 13  | CM    | 125 | ARG  |
| 13  | CM    | 126 | LYS  |
| 14  | CN    | 6   | LEU  |
| 14  | CN    | 7   | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 14  | CN    | 26  | ARG  |
| 14  | CN    | 33  | VAL  |
| 14  | CN    | 35  | ARG  |
| 14  | CN    | 40  | CYS  |
| 14  | CN    | 41  | ARG  |
| 14  | CN    | 43  | CYS  |
| 14  | CN    | 44  | LEU  |
| 14  | CN    | 49  | HIS  |
| 14  | CN    | 50  | LYS  |
| 14  | CN    | 58  | LYS  |
| 15  | CO    | 3   | ILE  |
| 15  | CO    | 24  | SER  |
| 15  | CO    | 26  | GLU  |
| 15  | CO    | 31  | LEU  |
| 15  | CO    | 39  | LEU  |
| 15  | CO    | 41  | GLU  |
| 15  | CO    | 58  | MET  |
| 15  | CO    | 65  | ARG  |
| 15  | CO    | 82  | ILE  |
| 15  | CO    | 83  | GLU  |
| 15  | CO    | 84  | LYS  |
| 15  | CO    | 87  | ILE  |
| 15  | CO    | 88  | ARG  |
| 16  | CP    | 2   | VAL  |
| 16  | CP    | 8   | ARG  |
| 16  | CP    | 16  | HIS  |
| 16  | CP    | 21  | VAL  |
| 16  | CP    | 26  | ARG  |
| 16  | CP    | 32  | TYR  |
| 16  | CP    | 45  | THR  |
| 16  | CP    | 47  | ASP  |
| 16  | CP    | 49  | LEU  |
| 16  | CP    | 53  | VAL  |
| 16  | CP    | 58  | TYR  |
| 16  | CP    | 60  | LEU  |
| 16  | CP    | 61  | SER  |
| 16  | CP    | 67  | THR  |
| 16  | CP    | 69  | THR  |
| 16  | CP    | 82  | GLN  |
| 17  | CQ    | 7   | THR  |
| 17  | CQ    | 14  | LYS  |
| 17  | CQ    | 19  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 17  | CQ    | 21  | VAL  |
| 17  | CQ    | 35  | VAL  |
| 17  | CQ    | 42  | TYR  |
| 17  | CQ    | 52  | LYS  |
| 17  | CQ    | 53  | LEU  |
| 17  | CQ    | 55  | ASP  |
| 17  | CQ    | 57  | VAL  |
| 17  | CQ    | 59  | ILE  |
| 17  | CQ    | 60  | ILE  |
| 17  | CQ    | 68  | ARG  |
| 17  | CQ    | 73  | VAL  |
| 17  | CQ    | 74  | LEU  |
| 17  | CQ    | 87  | LYS  |
| 17  | CQ    | 89  | LEU  |
| 18  | CR    | 23  | LYS  |
| 18  | CR    | 29  | PHE  |
| 18  | CR    | 31  | LEU  |
| 18  | CR    | 32  | ARG  |
| 18  | CR    | 39  | VAL  |
| 18  | CR    | 44  | LEU  |
| 18  | CR    | 47  | THR  |
| 18  | CR    | 58  | LEU  |
| 18  | CR    | 61  | LYS  |
| 18  | CR    | 69  | THR  |
| 18  | CR    | 76  | LEU  |
| 18  | CR    | 83  | GLU  |
| 19  | CS    | 5   | LEU  |
| 19  | CS    | 6   | LYS  |
| 19  | CS    | 7   | LYS  |
| 19  | CS    | 9   | VAL  |
| 19  | CS    | 16  | LEU  |
| 19  | CS    | 19  | VAL  |
| 19  | CS    | 27  | GLU  |
| 19  | CS    | 29  | ARG  |
| 19  | CS    | 33  | THR  |
| 19  | CS    | 37  | ARG  |
| 19  | CS    | 39  | THR  |
| 19  | CS    | 44  | MET  |
| 19  | CS    | 45  | VAL  |
| 19  | CS    | 48  | THR  |
| 19  | CS    | 49  | ILE  |
| 19  | CS    | 58  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 19  | CS    | 60  | VAL  |
| 19  | CS    | 62  | ILE  |
| 19  | CS    | 64  | GLU  |
| 19  | CS    | 66  | MET  |
| 19  | CS    | 67  | VAL  |
| 19  | CS    | 71  | LEU  |
| 19  | CS    | 77  | THR  |
| 20  | CT    | 10  | LEU  |
| 20  | CT    | 13  | LEU  |
| 20  | CT    | 23  | ARG  |
| 20  | CT    | 24  | LEU  |
| 20  | CT    | 25  | ARG  |
| 20  | CT    | 26  | ASN  |
| 20  | CT    | 29  | LYS  |
| 20  | CT    | 30  | LYS  |
| 20  | CT    | 33  | ILE  |
| 20  | CT    | 36  | LEU  |
| 20  | CT    | 41  | ILE  |
| 20  | CT    | 48  | LYS  |
| 20  | CT    | 50  | GLU  |
| 20  | CT    | 51  | GLU  |
| 20  | CT    | 53  | LEU  |
| 20  | CT    | 55  | ILE  |
| 20  | CT    | 56  | MET  |
| 20  | CT    | 57  | ARG  |
| 20  | CT    | 62  | LEU  |
| 20  | CT    | 73  | HIS  |
| 20  | CT    | 75  | ASN  |
| 20  | CT    | 82  | SER  |
| 20  | CT    | 83  | ARG  |
| 20  | CT    | 84  | LEU  |
| 20  | CT    | 93  | GLU  |
| 20  | CT    | 100 | ILE  |
| 21  | CU    | 3   | LYS  |
| 21  | CU    | 7   | ARG  |
| 21  | CU    | 8   | THR  |
| 21  | CU    | 10  | ARG  |
| 21  | CU    | 12  | LYS  |
| 21  | CU    | 15  | ARG  |
| 21  | CU    | 25  | LYS  |
| 27  | DC    | 24  | GLU  |
| 27  | DC    | 36  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 27  | DC    | 56  | GLN  |
| 27  | DC    | 58  | VAL  |
| 27  | DC    | 64  | LEU  |
| 27  | DC    | 77  | ILE  |
| 27  | DC    | 94  | VAL  |
| 28  | DD    | 18  | VAL  |
| 28  | DD    | 24  | ILE  |
| 28  | DD    | 26  | LYS  |
| 28  | DD    | 28  | GLU  |
| 28  | DD    | 44  | ASN  |
| 28  | DD    | 46  | GLN  |
| 28  | DD    | 49  | ILE  |
| 28  | DD    | 61  | LEU  |
| 28  | DD    | 64  | ILE  |
| 28  | DD    | 65  | ILE  |
| 28  | DD    | 73  | VAL  |
| 28  | DD    | 92  | ILE  |
| 28  | DD    | 94  | LEU  |
| 28  | DD    | 99  | ASP  |
| 28  | DD    | 103 | ARG  |
| 28  | DD    | 111 | LEU  |
| 28  | DD    | 113 | VAL  |
| 28  | DD    | 122 | ASP  |
| 28  | DD    | 131 | LEU  |
| 28  | DD    | 138 | VAL  |
| 28  | DD    | 166 | GLN  |
| 28  | DD    | 173 | VAL  |
| 28  | DD    | 192 | THR  |
| 28  | DD    | 193 | VAL  |
| 28  | DD    | 211 | ARG  |
| 28  | DD    | 212 | SER  |
| 28  | DD    | 218 | ARG  |
| 28  | DD    | 221 | VAL  |
| 28  | DD    | 229 | VAL  |
| 28  | DD    | 253 | GLN  |
| 28  | DD    | 257 | LEU  |
| 28  | DD    | 259 | THR  |
| 28  | DD    | 260 | ARG  |
| 28  | DD    | 270 | ILE  |
| 28  | DD    | 271 | ILE  |
| 29  | DE    | 9   | VAL  |
| 29  | DE    | 16  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 29  | DE    | 18  | ASP  |
| 29  | DE    | 33  | VAL  |
| 29  | DE    | 40  | GLU  |
| 29  | DE    | 49  | LEU  |
| 29  | DE    | 52  | LEU  |
| 29  | DE    | 67  | PHE  |
| 29  | DE    | 76  | ARG  |
| 29  | DE    | 78  | LEU  |
| 29  | DE    | 82  | ARG  |
| 29  | DE    | 89  | ASP  |
| 29  | DE    | 95  | ILE  |
| 29  | DE    | 101 | ARG  |
| 29  | DE    | 118 | LYS  |
| 29  | DE    | 119 | ARG  |
| 29  | DE    | 121 | ASN  |
| 29  | DE    | 144 | ARG  |
| 29  | DE    | 154 | LYS  |
| 29  | DE    | 169 | ASN  |
| 29  | DE    | 173 | VAL  |
| 29  | DE    | 175 | VAL  |
| 29  | DE    | 179 | GLU  |
| 29  | DE    | 181 | LEU  |
| 29  | DE    | 184 | VAL  |
| 29  | DE    | 197 | ILE  |
| 29  | DE    | 202 | LYS  |
| 29  | DE    | 203 | LYS  |
| 30  | DF    | 6   | VAL  |
| 30  | DF    | 7   | TYR  |
| 30  | DF    | 25  | PRO  |
| 30  | DF    | 28  | ILE  |
| 30  | DF    | 33  | LEU  |
| 30  | DF    | 45  | ARG  |
| 30  | DF    | 48  | THR  |
| 30  | DF    | 57  | VAL  |
| 30  | DF    | 60  | SER  |
| 30  | DF    | 62  | ARG  |
| 30  | DF    | 67  | GLN  |
| 30  | DF    | 74  | ARG  |
| 30  | DF    | 78  | ILE  |
| 30  | DF    | 84  | VAL  |
| 30  | DF    | 95  | ARG  |
| 30  | DF    | 104 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 30  | DF    | 117 | ARG  |
| 30  | DF    | 127 | GLU  |
| 30  | DF    | 140 | LEU  |
| 30  | DF    | 158 | THR  |
| 30  | DF    | 165 | ARG  |
| 30  | DF    | 174 | VAL  |
| 30  | DF    | 181 | LEU  |
| 30  | DF    | 183 | VAL  |
| 30  | DF    | 191 | ARG  |
| 30  | DF    | 192 | LEU  |
| 30  | DF    | 203 | GLN  |
| 30  | DF    | 206 | ILE  |
| 31  | DG    | 16  | ARG  |
| 31  | DG    | 34  | LEU  |
| 31  | DG    | 45  | GLU  |
| 31  | DG    | 60  | LEU  |
| 31  | DG    | 67  | LYS  |
| 31  | DG    | 71  | THR  |
| 31  | DG    | 77  | ILE  |
| 31  | DG    | 79  | ASN  |
| 31  | DG    | 88  | ILE  |
| 31  | DG    | 90  | LEU  |
| 31  | DG    | 95  | ARG  |
| 31  | DG    | 108 | ASN  |
| 31  | DG    | 112 | PRO  |
| 31  | DG    | 115 | ARG  |
| 31  | DG    | 118 | ARG  |
| 31  | DG    | 147 | ASP  |
| 31  | DG    | 159 | VAL  |
| 31  | DG    | 174 | GLU  |
| 32  | DH    | 4   | ILE  |
| 32  | DH    | 7   | LEU  |
| 32  | DH    | 12  | PRO  |
| 32  | DH    | 32  | GLU  |
| 32  | DH    | 41  | MET  |
| 32  | DH    | 50  | VAL  |
| 32  | DH    | 59  | ARG  |
| 32  | DH    | 60  | ARG  |
| 32  | DH    | 70  | THR  |
| 32  | DH    | 77  | LYS  |
| 32  | DH    | 83  | TYR  |
| 32  | DH    | 85  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 32  | DH    | 86  | GLU  |
| 32  | DH    | 88  | LEU  |
| 32  | DH    | 89  | ILE  |
| 32  | DH    | 92  | ILE  |
| 32  | DH    | 104 | GLU  |
| 32  | DH    | 105 | LEU  |
| 32  | DH    | 124 | GLU  |
| 32  | DH    | 127 | GLU  |
| 32  | DH    | 132 | ARG  |
| 32  | DH    | 139 | GLN  |
| 32  | DH    | 143 | GLN  |
| 32  | DH    | 147 | ASN  |
| 32  | DH    | 153 | LYS  |
| 32  | DH    | 154 | PRO  |
| 32  | DH    | 155 | SER  |
| 33  | DI    | 1   | MET  |
| 33  | DI    | 6   | LEU  |
| 33  | DI    | 9   | LEU  |
| 33  | DI    | 10  | GLU  |
| 33  | DI    | 12  | LEU  |
| 33  | DI    | 38  | LEU  |
| 33  | DI    | 41  | GLU  |
| 33  | DI    | 57  | ARG  |
| 33  | DI    | 64  | GLU  |
| 33  | DI    | 67  | ARG  |
| 33  | DI    | 70  | GLU  |
| 33  | DI    | 71  | ILE  |
| 33  | DI    | 74  | ASN  |
| 33  | DI    | 77  | LEU  |
| 33  | DI    | 78  | THR  |
| 33  | DI    | 79  | ILE  |
| 33  | DI    | 85  | GLU  |
| 33  | DI    | 88  | ILE  |
| 33  | DI    | 110 | ASP  |
| 33  | DI    | 114 | LEU  |
| 33  | DI    | 118 | LYS  |
| 33  | DI    | 120 | ILE  |
| 33  | DI    | 126 | TYR  |
| 33  | DI    | 134 | PRO  |
| 33  | DI    | 135 | GLU  |
| 33  | DI    | 139 | GLN  |
| 34  | DN    | 4   | TYR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 34  | DN    | 15  | LEU  |
| 34  | DN    | 22  | THR  |
| 34  | DN    | 25  | ARG  |
| 34  | DN    | 48  | MET  |
| 34  | DN    | 55  | VAL  |
| 34  | DN    | 63  | THR  |
| 34  | DN    | 67  | LEU  |
| 34  | DN    | 68  | GLU  |
| 34  | DN    | 87  | LEU  |
| 34  | DN    | 89  | LYS  |
| 34  | DN    | 90  | MET  |
| 34  | DN    | 99  | LEU  |
| 34  | DN    | 101 | HIS  |
| 34  | DN    | 119 | ARG  |
| 34  | DN    | 120 | LEU  |
| 34  | DN    | 134 | ARG  |
| 34  | DN    | 136 | GLU  |
| 35  | DO    | 10  | VAL  |
| 35  | DO    | 24  | VAL  |
| 35  | DO    | 29  | ASN  |
| 35  | DO    | 47  | ILE  |
| 35  | DO    | 49  | ARG  |
| 35  | DO    | 58  | VAL  |
| 35  | DO    | 69  | ILE  |
| 35  | DO    | 73  | ASP  |
| 35  | DO    | 89  | ASN  |
| 35  | DO    | 94  | ARG  |
| 35  | DO    | 114 | ILE  |
| 35  | DO    | 117 | LEU  |
| 36  | DP    | 8   | PRO  |
| 36  | DP    | 9   | ASN  |
| 36  | DP    | 14  | LYS  |
| 36  | DP    | 19  | VAL  |
| 36  | DP    | 21  | ARG  |
| 36  | DP    | 27  | HIS  |
| 36  | DP    | 32  | THR  |
| 36  | DP    | 50  | ARG  |
| 36  | DP    | 55  | ARG  |
| 36  | DP    | 59  | LEU  |
| 36  | DP    | 60  | MET  |
| 36  | DP    | 61  | ARG  |
| 36  | DP    | 67  | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 36  | DP    | 75  | ILE  |
| 36  | DP    | 81  | GLN  |
| 36  | DP    | 85  | LEU  |
| 36  | DP    | 91  | PHE  |
| 36  | DP    | 98  | GLU  |
| 36  | DP    | 100 | LEU  |
| 36  | DP    | 110 | TYR  |
| 36  | DP    | 112 | LEU  |
| 36  | DP    | 114 | ILE  |
| 36  | DP    | 115 | LEU  |
| 36  | DP    | 117 | GLU  |
| 36  | DP    | 125 | VAL  |
| 36  | DP    | 136 | GLU  |
| 36  | DP    | 138 | LEU  |
| 36  | DP    | 144 | GLU  |
| 36  | DP    | 147 | LEU  |
| 36  | DP    | 148 | LEU  |
| 37  | DQ    | 1   | MET  |
| 37  | DQ    | 5   | ARG  |
| 37  | DQ    | 6   | ARG  |
| 37  | DQ    | 17  | LEU  |
| 37  | DQ    | 45  | GLN  |
| 37  | DQ    | 51  | ARG  |
| 37  | DQ    | 54  | MET  |
| 37  | DQ    | 55  | VAL  |
| 37  | DQ    | 66  | ILE  |
| 37  | DQ    | 75  | THR  |
| 37  | DQ    | 79  | LEU  |
| 37  | DQ    | 81  | VAL  |
| 37  | DQ    | 109 | VAL  |
| 37  | DQ    | 110 | THR  |
| 37  | DQ    | 111 | GLU  |
| 37  | DQ    | 131 | ILE  |
| 37  | DQ    | 134 | ARG  |
| 37  | DQ    | 135 | ASP  |
| 37  | DQ    | 138 | ASP  |
| 38  | DR    | 6   | SER  |
| 38  | DR    | 9   | LYS  |
| 38  | DR    | 10  | LEU  |
| 38  | DR    | 17  | ARG  |
| 38  | DR    | 18  | LEU  |
| 38  | DR    | 29  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 38  | DR    | 37  | THR  |
| 38  | DR    | 56  | LYS  |
| 38  | DR    | 60  | LEU  |
| 38  | DR    | 76  | VAL  |
| 38  | DR    | 79  | LEU  |
| 38  | DR    | 80  | PHE  |
| 38  | DR    | 94  | TYR  |
| 38  | DR    | 99  | LYS  |
| 38  | DR    | 104 | ARG  |
| 39  | DS    | 12  | PHE  |
| 39  | DS    | 17  | ARG  |
| 39  | DS    | 19  | LYS  |
| 39  | DS    | 20  | ARG  |
| 39  | DS    | 44  | LYS  |
| 39  | DS    | 52  | SER  |
| 39  | DS    | 56  | LEU  |
| 39  | DS    | 58  | LEU  |
| 39  | DS    | 69  | VAL  |
| 39  | DS    | 89  | ARG  |
| 39  | DS    | 101 | LEU  |
| 39  | DS    | 103 | GLU  |
| 39  | DS    | 106 | ARG  |
| 40  | DT    | 13  | ARG  |
| 40  | DT    | 15  | VAL  |
| 40  | DT    | 16  | ARG  |
| 40  | DT    | 19  | LEU  |
| 40  | DT    | 23  | ARG  |
| 40  | DT    | 27  | THR  |
| 40  | DT    | 29  | ARG  |
| 40  | DT    | 30  | VAL  |
| 40  | DT    | 32  | TYR  |
| 40  | DT    | 33  | LYS  |
| 40  | DT    | 38  | ASN  |
| 40  | DT    | 40  | THR  |
| 40  | DT    | 41  | ARG  |
| 40  | DT    | 42  | ILE  |
| 40  | DT    | 49  | VAL  |
| 40  | DT    | 50  | ILE  |
| 40  | DT    | 53  | ARG  |
| 40  | DT    | 59  | THR  |
| 40  | DT    | 65  | LYS  |
| 40  | DT    | 70  | VAL  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 40         | DT           | 78         | LEU         |
| 40         | DT           | 80         | SER         |
| 40         | DT           | 82         | LEU         |
| 40         | DT           | 83         | ILE         |
| 40         | DT           | 85         | LYS         |
| 40         | DT           | 89         | VAL         |
| 40         | DT           | 95         | ARG         |
| 40         | DT           | 99         | LEU         |
| 40         | DT           | 110        | ILE         |
| 40         | DT           | 113        | LYS         |
| 40         | DT           | 121        | ILE         |
| 40         | DT           | 128        | GLU         |
| 41         | DU           | 9          | VAL         |
| 41         | DU           | 14         | HIS         |
| 41         | DU           | 15         | LYS         |
| 41         | DU           | 20         | LEU         |
| 41         | DU           | 27         | LEU         |
| 41         | DU           | 31         | SER         |
| 41         | DU           | 44         | ASN         |
| 41         | DU           | 60         | LEU         |
| 41         | DU           | 78         | THR         |
| 41         | DU           | 79         | PHE         |
| 41         | DU           | 88         | ILE         |
| 41         | DU           | 92         | ARG         |
| 41         | DU           | 102        | GLU         |
| 41         | DU           | 104        | GLN         |
| 42         | DV           | 14         | VAL         |
| 42         | DV           | 19         | LYS         |
| 42         | DV           | 21         | ARG         |
| 42         | DV           | 24         | LYS         |
| 42         | DV           | 32         | THR         |
| 42         | DV           | 33         | VAL         |
| 42         | DV           | 35         | LEU         |
| 42         | DV           | 36         | PRO         |
| 42         | DV           | 38         | LEU         |
| 42         | DV           | 39         | LEU         |
| 42         | DV           | 44         | LYS         |
| 42         | DV           | 49         | THR         |
| 42         | DV           | 57         | VAL         |
| 42         | DV           | 64         | HIS         |
| 42         | DV           | 66         | ARG         |
| 42         | DV           | 69         | LYS         |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 42  | DV    | 71  | LEU  |
| 42  | DV    | 73  | SER  |
| 42  | DV    | 89  | GLN  |
| 42  | DV    | 95  | LEU  |
| 42  | DV    | 99  | ILE  |
| 43  | DW    | 11  | ARG  |
| 43  | DW    | 19  | LEU  |
| 43  | DW    | 60  | ASN  |
| 43  | DW    | 70  | TYR  |
| 43  | DW    | 76  | VAL  |
| 43  | DW    | 103 | ILE  |
| 43  | DW    | 106 | ILE  |
| 43  | DW    | 107 | LEU  |
| 44  | DX    | 3   | THR  |
| 44  | DX    | 12  | VAL  |
| 44  | DX    | 13  | LEU  |
| 44  | DX    | 25  | LYS  |
| 44  | DX    | 27  | THR  |
| 44  | DX    | 47  | PHE  |
| 44  | DX    | 49  | VAL  |
| 44  | DX    | 52  | VAL  |
| 44  | DX    | 57  | LEU  |
| 44  | DX    | 68  | ARG  |
| 44  | DX    | 76  | ARG  |
| 44  | DX    | 80  | ILE  |
| 44  | DX    | 83  | VAL  |
| 45  | DY    | 14  | LEU  |
| 45  | DY    | 26  | LYS  |
| 45  | DY    | 27  | VAL  |
| 45  | DY    | 40  | GLU  |
| 45  | DY    | 45  | VAL  |
| 45  | DY    | 51  | VAL  |
| 45  | DY    | 57  | GLN  |
| 45  | DY    | 61  | ILE  |
| 45  | DY    | 63  | LYS  |
| 45  | DY    | 71  | LYS  |
| 45  | DY    | 75  | ILE  |
| 45  | DY    | 77  | PRO  |
| 45  | DY    | 87  | LYS  |
| 45  | DY    | 89  | PHE  |
| 45  | DY    | 90  | LEU  |
| 45  | DY    | 95  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 45  | DY    | 96  | ILE  |
| 45  | DY    | 97  | ARG  |
| 45  | DY    | 98  | VAL  |
| 46  | DZ    | 3   | TYR  |
| 46  | DZ    | 9   | TYR  |
| 46  | DZ    | 11  | GLU  |
| 46  | DZ    | 14  | LYS  |
| 46  | DZ    | 31  | ARG  |
| 46  | DZ    | 42  | VAL  |
| 46  | DZ    | 47  | VAL  |
| 46  | DZ    | 53  | ILE  |
| 46  | DZ    | 71  | VAL  |
| 46  | DZ    | 81  | ARG  |
| 46  | DZ    | 88  | PHE  |
| 46  | DZ    | 99  | TYR  |
| 46  | DZ    | 121 | HIS  |
| 46  | DZ    | 131 | ARG  |
| 46  | DZ    | 140 | ASP  |
| 46  | DZ    | 144 | LEU  |
| 46  | DZ    | 146 | ILE  |
| 46  | DZ    | 150 | LEU  |
| 47  | D0    | 3   | HIS  |
| 47  | D0    | 5   | LYS  |
| 47  | D0    | 30  | VAL  |
| 47  | D0    | 53  | MET  |
| 47  | D0    | 55  | ARG  |
| 47  | D0    | 62  | LEU  |
| 47  | D0    | 70  | GLN  |
| 47  | D0    | 75  | LEU  |
| 47  | D0    | 80  | HIS  |
| 47  | D0    | 84  | LEU  |
| 48  | D1    | 11  | ARG  |
| 48  | D1    | 14  | VAL  |
| 48  | D1    | 35  | THR  |
| 48  | D1    | 39  | LYS  |
| 48  | D1    | 40  | ARG  |
| 48  | D1    | 41  | ARG  |
| 48  | D1    | 46  | LEU  |
| 48  | D1    | 51  | VAL  |
| 48  | D1    | 56  | GLN  |
| 48  | D1    | 58  | ILE  |
| 48  | D1    | 59  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 48  | D1    | 61  | ARG  |
| 48  | D1    | 67  | ILE  |
| 48  | D1    | 72  | GLU  |
| 48  | D1    | 82  | LEU  |
| 48  | D1    | 83  | GLU  |
| 48  | D1    | 89  | GLU  |
| 48  | D1    | 94  | LEU  |
| 49  | D2    | 2   | LYS  |
| 49  | D2    | 17  | SER  |
| 49  | D2    | 30  | ARG  |
| 49  | D2    | 34  | GLU  |
| 49  | D2    | 41  | ILE  |
| 49  | D2    | 44  | LEU  |
| 49  | D2    | 52  | ASP  |
| 49  | D2    | 53  | LEU  |
| 49  | D2    | 56  | GLN  |
| 49  | D2    | 65  | ASN  |
| 49  | D2    | 68  | ARG  |
| 49  | D2    | 70  | GLN  |
| 50  | D3    | 8   | LEU  |
| 50  | D3    | 17  | LYS  |
| 50  | D3    | 24  | LYS  |
| 50  | D3    | 37  | LEU  |
| 51  | D4    | 9   | LEU  |
| 51  | D4    | 22  | ILE  |
| 51  | D4    | 30  | GLU  |
| 52  | D5    | 4   | HIS  |
| 52  | D5    | 11  | THR  |
| 52  | D5    | 40  | LYS  |
| 52  | D5    | 48  | GLU  |
| 52  | D5    | 56  | LYS  |
| 52  | D5    | 57  | VAL  |
| 52  | D5    | 58  | LEU  |
| 52  | D5    | 60  | VAL  |
| 53  | D6    | 9   | LEU  |
| 53  | D6    | 10  | LEU  |
| 53  | D6    | 11  | LEU  |
| 53  | D6    | 12  | GLU  |
| 53  | D6    | 18  | ARG  |
| 53  | D6    | 19  | ARG  |
| 53  | D6    | 36  | LEU  |
| 53  | D6    | 42  | TRP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 53  | D6    | 44  | ARG  |
| 53  | D6    | 45  | LYS  |
| 53  | D6    | 46  | HIS  |
| 54  | D7    | 1   | MET  |
| 54  | D7    | 2   | LYS  |
| 54  | D7    | 4   | THR  |
| 54  | D7    | 41  | ARG  |
| 54  | D7    | 43  | THR  |
| 55  | D8    | 6   | THR  |
| 55  | D8    | 30  | ARG  |
| 55  | D8    | 32  | LEU  |
| 55  | D8    | 33  | ASN  |
| 55  | D8    | 41  | ILE  |
| 55  | D8    | 49  | VAL  |
| 55  | D8    | 61  | LEU  |
| 56  | D9    | 2   | LYS  |
| 56  | D9    | 25  | VAL  |
| 56  | D9    | 28  | GLU  |
| 56  | D9    | 33  | LYS  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (163) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | AB    | 76  | GLN  |
| 2   | AB    | 94  | ASN  |
| 2   | AB    | 204 | ASN  |
| 3   | AC    | 6   | HIS  |
| 3   | AC    | 31  | HIS  |
| 3   | AC    | 123 | GLN  |
| 4   | AD    | 42  | GLN  |
| 4   | AD    | 119 | GLN  |
| 4   | AD    | 160 | GLN  |
| 5   | AE    | 78  | HIS  |
| 6   | AF    | 73  | ASN  |
| 6   | AF    | 94  | GLN  |
| 6   | AF    | 100 | ASN  |
| 7   | AG    | 28  | ASN  |
| 7   | AG    | 68  | ASN  |
| 7   | AG    | 97  | GLN  |
| 7   | AG    | 109 | ASN  |
| 8   | AH    | 78  | GLN  |
| 8   | AH    | 82  | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9   | AI    | 3   | GLN  |
| 9   | AI    | 38  | GLN  |
| 10  | AJ    | 84  | GLN  |
| 11  | AK    | 26  | ASN  |
| 12  | AL    | 9   | GLN  |
| 13  | AM    | 92  | HIS  |
| 13  | AM    | 106 | ASN  |
| 15  | AO    | 46  | HIS  |
| 16  | AP    | 16  | HIS  |
| 19  | AS    | 65  | ASN  |
| 20  | AT    | 42  | GLN  |
| 28  | BD    | 129 | ASN  |
| 28  | BD    | 143 | HIS  |
| 28  | BD    | 201 | HIS  |
| 29  | BE    | 48  | GLN  |
| 29  | BE    | 132 | HIS  |
| 30  | BF    | 133 | ASN  |
| 30  | BF    | 169 | ASN  |
| 30  | BF    | 203 | GLN  |
| 31  | BG    | 27  | ASN  |
| 31  | BG    | 40  | ASN  |
| 31  | BG    | 41  | GLN  |
| 31  | BG    | 132 | ASN  |
| 32  | BH    | 111 | HIS  |
| 33  | BI    | 17  | GLN  |
| 33  | BI    | 104 | GLN  |
| 34  | BN    | 45  | ASN  |
| 36  | BP    | 84  | ASN  |
| 37  | BQ    | 12  | GLN  |
| 37  | BQ    | 13  | GLN  |
| 37  | BQ    | 89  | ASN  |
| 38  | BR    | 11  | ASN  |
| 38  | BR    | 13  | HIS  |
| 38  | BR    | 16  | HIS  |
| 38  | BR    | 24  | GLN  |
| 38  | BR    | 53  | HIS  |
| 41  | BU    | 14  | HIS  |
| 41  | BU    | 117 | GLN  |
| 42  | BV    | 11  | GLN  |
| 43  | BW    | 40  | ASN  |
| 43  | BW    | 111 | HIS  |
| 46  | BZ    | 73  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 47  | B0    | 12  | ASN  |
| 47  | B0    | 29  | GLN  |
| 47  | B0    | 70  | GLN  |
| 48  | B1    | 45  | ASN  |
| 49  | B2    | 56  | GLN  |
| 49  | B2    | 70  | GLN  |
| 49  | B2    | 71  | ASN  |
| 50  | B3    | 52  | HIS  |
| 55  | B8    | 43  | GLN  |
| 56  | B9    | 20  | HIS  |
| 2   | CB    | 78  | GLN  |
| 2   | CB    | 140 | HIS  |
| 2   | CB    | 204 | ASN  |
| 3   | CC    | 98  | ASN  |
| 3   | CC    | 108 | ASN  |
| 4   | CD    | 123 | HIS  |
| 5   | CE    | 78  | HIS  |
| 6   | CF    | 18  | GLN  |
| 6   | CF    | 73  | ASN  |
| 6   | CF    | 94  | GLN  |
| 7   | CG    | 68  | ASN  |
| 7   | CG    | 122 | HIS  |
| 7   | CG    | 148 | ASN  |
| 7   | CG    | 153 | HIS  |
| 8   | CH    | 82  | HIS  |
| 9   | CI    | 73  | GLN  |
| 10  | CJ    | 13  | HIS  |
| 10  | CJ    | 68  | HIS  |
| 10  | CJ    | 76  | ASN  |
| 10  | CJ    | 78  | ASN  |
| 10  | CJ    | 84  | GLN  |
| 11  | CK    | 26  | ASN  |
| 12  | CL    | 9   | GLN  |
| 13  | CM    | 40  | ASN  |
| 13  | CM    | 92  | HIS  |
| 15  | CO    | 62  | GLN  |
| 16  | CP    | 82  | GLN  |
| 18  | CR    | 36  | ASN  |
| 19  | CS    | 57  | HIS  |
| 19  | CS    | 69  | HIS  |
| 20  | CT    | 18  | GLN  |
| 20  | CT    | 90  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 28  | DD    | 87  | ASN  |
| 28  | DD    | 112 | GLN  |
| 28  | DD    | 115 | GLN  |
| 29  | DE    | 169 | ASN  |
| 29  | DE    | 180 | ASN  |
| 30  | DF    | 69  | HIS  |
| 30  | DF    | 75  | HIS  |
| 30  | DF    | 203 | GLN  |
| 31  | DG    | 58  | GLN  |
| 32  | DH    | 139 | GLN  |
| 32  | DH    | 143 | GLN  |
| 32  | DH    | 147 | ASN  |
| 32  | DH    | 158 | HIS  |
| 33  | DI    | 28  | ASN  |
| 33  | DI    | 74  | ASN  |
| 33  | DI    | 105 | HIS  |
| 33  | DI    | 139 | GLN  |
| 34  | DN    | 45  | ASN  |
| 34  | DN    | 133 | GLN  |
| 36  | DP    | 9   | ASN  |
| 36  | DP    | 84  | ASN  |
| 36  | DP    | 128 | HIS  |
| 37  | DQ    | 12  | GLN  |
| 37  | DQ    | 123 | HIS  |
| 38  | DR    | 13  | HIS  |
| 38  | DR    | 31  | HIS  |
| 39  | DS    | 34  | HIS  |
| 40  | DT    | 38  | ASN  |
| 40  | DT    | 43  | GLN  |
| 41  | DU    | 49  | HIS  |
| 41  | DU    | 71  | GLN  |
| 41  | DU    | 81  | HIS  |
| 41  | DU    | 94  | ASN  |
| 41  | DU    | 104 | GLN  |
| 42  | DV    | 11  | GLN  |
| 42  | DV    | 80  | GLN  |
| 42  | DV    | 87  | HIS  |
| 42  | DV    | 89  | GLN  |
| 43  | DW    | 40  | ASN  |
| 43  | DW    | 60  | ASN  |
| 43  | DW    | 61  | ASN  |
| 45  | DY    | 57  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 46  | DZ    | 34  | ASN  |
| 46  | DZ    | 54  | HIS  |
| 46  | DZ    | 65  | GLN  |
| 46  | DZ    | 73  | GLN  |
| 47  | D0    | 29  | GLN  |
| 47  | D0    | 70  | GLN  |
| 48  | D1    | 45  | ASN  |
| 48  | D1    | 47  | GLN  |
| 48  | D1    | 56  | GLN  |
| 49  | D2    | 9   | GLN  |
| 49  | D2    | 70  | GLN  |
| 50  | D3    | 19  | GLN  |
| 50  | D3    | 52  | HIS  |
| 51  | D4    | 20  | ASN  |
| 53  | D6    | 20  | ASN  |
| 53  | D6    | 32  | ASN  |
| 53  | D6    | 46  | HIS  |
| 55  | D8    | 35  | GLN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1   | AA    | 1503/1522 (98%) | 369 (24%)         | 109 (7%)        |
| 1   | CA    | 1503/1522 (98%) | 363 (24%)         | 115 (7%)        |
| 22  | AV    | 76/77 (98%)     | 26 (34%)          | 3 (3%)          |
| 22  | CV    | 76/77 (98%)     | 30 (39%)          | 4 (5%)          |
| 23  | AW    | 75/76 (98%)     | 22 (29%)          | 0               |
| 23  | AY    | 16/76 (21%)     | 5 (31%)           | 0               |
| 23  | CW    | 75/76 (98%)     | 26 (34%)          | 0               |
| 23  | CY    | 16/76 (21%)     | 8 (50%)           | 0               |
| 24  | AX    | 11/24 (45%)     | 4 (36%)           | 0               |
| 24  | CX    | 9/24 (37%)      | 4 (44%)           | 1 (11%)         |
| 25  | BA    | 2804/2915 (96%) | 810 (28%)         | 260 (9%)        |
| 25  | DA    | 2818/2915 (96%) | 814 (28%)         | 264 (9%)        |
| 26  | BB    | 118/122 (96%)   | 26 (22%)          | 5 (4%)          |
| 26  | DB    | 118/122 (96%)   | 25 (21%)          | 7 (5%)          |
| All | All   | 9218/9624 (95%) | 2532 (27%)        | 768 (8%)        |

All (2532) RNA backbone outliers are listed below:

| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | AA    | 6      | G    |
| 1   | AA    | 8      | A    |
| 1   | AA    | 9      | G    |
| 1   | AA    | 10     | A    |
| 1   | AA    | 13     | U    |
| 1   | AA    | 14     | U    |
| 1   | AA    | 28     | G    |
| 1   | AA    | 31     | G    |
| 1   | AA    | 32     | A    |
| 1   | AA    | 39     | G    |
| 1   | AA    | 48     | C    |
| 1   | AA    | 49     | U    |
| 1   | AA    | 50     | A    |
| 1   | AA    | 51     | A    |
| 1   | AA    | 52     | G    |
| 1   | AA    | 54     | C    |
| 1   | AA    | 60     | A    |
| 1   | AA    | 61     | G    |
| 1   | AA    | 64     | G    |
| 1   | AA    | 65     | U    |
| 1   | AA    | 66     | G    |
| 1   | AA    | 80     | G    |
| 1   | AA    | 81     | U    |
| 1   | AA    | 89     | C    |
| 1   | AA    | 90     | U    |
| 1   | AA    | 91     | C    |
| 1   | AA    | 101    | A    |
| 1   | AA    | 108    | G    |
| 1   | AA    | 109    | A    |
| 1   | AA    | 110    | C    |
| 1   | AA    | 115    | G    |
| 1   | AA    | 116    | A    |
| 1   | AA    | 120    | A    |
| 1   | AA    | 121    | C    |
| 1   | AA    | 122    | G    |
| 1   | AA    | 129(A) | G    |
| 1   | AA    | 130    | A    |
| 1   | AA    | 144    | G    |
| 1   | AA    | 146    | G    |
| 1   | AA    | 155    | C    |
| 1   | AA    | 159    | G    |
| 1   | AA    | 160    | A    |
| 1   | AA    | 163    | C    |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | AA    | 173    | U    |
| 1   | AA    | 174    | C    |
| 1   | AA    | 181    | G    |
| 1   | AA    | 182    | U    |
| 1   | AA    | 189(F) | U    |
| 1   | AA    | 189(G) | G    |
| 1   | AA    | 189(H) | G    |
| 1   | AA    | 195    | A    |
| 1   | AA    | 197    | A    |
| 1   | AA    | 198    | G    |
| 1   | AA    | 203    | U    |
| 1   | AA    | 204    | U    |
| 1   | AA    | 216    | G    |
| 1   | AA    | 242    | C    |
| 1   | AA    | 243    | A    |
| 1   | AA    | 244    | U    |
| 1   | AA    | 245    | C    |
| 1   | AA    | 247    | G    |
| 1   | AA    | 251    | G    |
| 1   | AA    | 252    | U    |
| 1   | AA    | 262    | A    |
| 1   | AA    | 267    | C    |
| 1   | AA    | 275    | G    |
| 1   | AA    | 279    | A    |
| 1   | AA    | 280    | C    |
| 1   | AA    | 281    | G    |
| 1   | AA    | 289    | G    |
| 1   | AA    | 301    | G    |
| 1   | AA    | 305    | G    |
| 1   | AA    | 306    | G    |
| 1   | AA    | 316    | G    |
| 1   | AA    | 319    | G    |
| 1   | AA    | 321    | A    |
| 1   | AA    | 328    | C    |
| 1   | AA    | 329    | A    |
| 1   | AA    | 330    | C    |
| 1   | AA    | 332    | G    |
| 1   | AA    | 343    | U    |
| 1   | AA    | 344    | A    |
| 1   | AA    | 345    | C    |
| 1   | AA    | 346    | G    |
| 1   | AA    | 351    | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AA    | 352 | C    |
| 1   | AA    | 353 | A    |
| 1   | AA    | 354 | G    |
| 1   | AA    | 366 | C    |
| 1   | AA    | 367 | U    |
| 1   | AA    | 368 | U    |
| 1   | AA    | 372 | C    |
| 1   | AA    | 384 | G    |
| 1   | AA    | 387 | U    |
| 1   | AA    | 388 | G    |
| 1   | AA    | 389 | A    |
| 1   | AA    | 390 | C    |
| 1   | AA    | 397 | A    |
| 1   | AA    | 398 | C    |
| 1   | AA    | 406 | G    |
| 1   | AA    | 412 | A    |
| 1   | AA    | 413 | G    |
| 1   | AA    | 414 | A    |
| 1   | AA    | 421 | U    |
| 1   | AA    | 422 | C    |
| 1   | AA    | 423 | G    |
| 1   | AA    | 424 | G    |
| 1   | AA    | 428 | G    |
| 1   | AA    | 429 | U    |
| 1   | AA    | 430 | A    |
| 1   | AA    | 435 | C    |
| 1   | AA    | 436 | C    |
| 1   | AA    | 438 | G    |
| 1   | AA    | 439 | A    |
| 1   | AA    | 442 | C    |
| 1   | AA    | 451 | A    |
| 1   | AA    | 452 | A    |
| 1   | AA    | 461 | A    |
| 1   | AA    | 470 | C    |
| 1   | AA    | 484 | G    |
| 1   | AA    | 485 | G    |
| 1   | AA    | 496 | A    |
| 1   | AA    | 498 | U    |
| 1   | AA    | 500 | G    |
| 1   | AA    | 508 | C    |
| 1   | AA    | 509 | A    |
| 1   | AA    | 510 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AA    | 511 | C    |
| 1   | AA    | 512 | U    |
| 1   | AA    | 517 | G    |
| 1   | AA    | 518 | C    |
| 1   | AA    | 519 | C    |
| 1   | AA    | 521 | G    |
| 1   | AA    | 527 | G    |
| 1   | AA    | 530 | G    |
| 1   | AA    | 531 | U    |
| 1   | AA    | 532 | A    |
| 1   | AA    | 533 | A    |
| 1   | AA    | 534 | U    |
| 1   | AA    | 536 | C    |
| 1   | AA    | 545 | C    |
| 1   | AA    | 547 | A    |
| 1   | AA    | 548 | G    |
| 1   | AA    | 559 | A    |
| 1   | AA    | 560 | U    |
| 1   | AA    | 561 | U    |
| 1   | AA    | 562 | C    |
| 1   | AA    | 563 | A    |
| 1   | AA    | 566 | G    |
| 1   | AA    | 567 | G    |
| 1   | AA    | 572 | A    |
| 1   | AA    | 573 | A    |
| 1   | AA    | 575 | G    |
| 1   | AA    | 576 | G    |
| 1   | AA    | 577 | G    |
| 1   | AA    | 579 | G    |
| 1   | AA    | 596 | C    |
| 1   | AA    | 605 | U    |
| 1   | AA    | 623 | C    |
| 1   | AA    | 630 | G    |
| 1   | AA    | 632 | A    |
| 1   | AA    | 633 | G    |
| 1   | AA    | 653 | A    |
| 1   | AA    | 665 | A    |
| 1   | AA    | 686 | U    |
| 1   | AA    | 688 | G    |
| 1   | AA    | 701 | C    |
| 1   | AA    | 702 | A    |
| 1   | AA    | 703 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AA    | 704 | A    |
| 1   | AA    | 721 | G    |
| 1   | AA    | 722 | A    |
| 1   | AA    | 723 | U    |
| 1   | AA    | 731 | G    |
| 1   | AA    | 733 | A    |
| 1   | AA    | 734 | G    |
| 1   | AA    | 748 | C    |
| 1   | AA    | 749 | C    |
| 1   | AA    | 752 | G    |
| 1   | AA    | 753 | A    |
| 1   | AA    | 755 | G    |
| 1   | AA    | 759 | A    |
| 1   | AA    | 773 | G    |
| 1   | AA    | 777 | A    |
| 1   | AA    | 787 | A    |
| 1   | AA    | 791 | G    |
| 1   | AA    | 793 | U    |
| 1   | AA    | 794 | A    |
| 1   | AA    | 815 | A    |
| 1   | AA    | 816 | A    |
| 1   | AA    | 817 | C    |
| 1   | AA    | 818 | G    |
| 1   | AA    | 819 | A    |
| 1   | AA    | 820 | U    |
| 1   | AA    | 821 | G    |
| 1   | AA    | 828 | A    |
| 1   | AA    | 839 | U    |
| 1   | AA    | 841 | U    |
| 1   | AA    | 848 | C    |
| 1   | AA    | 853 | G    |
| 1   | AA    | 859 | A    |
| 1   | AA    | 864 | A    |
| 1   | AA    | 871 | U    |
| 1   | AA    | 872 | A    |
| 1   | AA    | 873 | A    |
| 1   | AA    | 874 | G    |
| 1   | AA    | 885 | G    |
| 1   | AA    | 889 | A    |
| 1   | AA    | 890 | G    |
| 1   | AA    | 902 | G    |
| 1   | AA    | 913 | A    |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 1   | AA    | 914     | A    |
| 1   | AA    | 920     | U    |
| 1   | AA    | 926     | G    |
| 1   | AA    | 927     | G    |
| 1   | AA    | 932     | C    |
| 1   | AA    | 934     | C    |
| 1   | AA    | 935     | A    |
| 1   | AA    | 960     | U    |
| 1   | AA    | 961     | U    |
| 1   | AA    | 965     | A    |
| 1   | AA    | 966     | G    |
| 1   | AA    | 968     | A    |
| 1   | AA    | 969     | A    |
| 1   | AA    | 971     | G    |
| 1   | AA    | 974     | A    |
| 1   | AA    | 975     | A    |
| 1   | AA    | 976     | G    |
| 1   | AA    | 977     | A    |
| 1   | AA    | 980     | C    |
| 1   | AA    | 982     | U    |
| 1   | AA    | 991     | U    |
| 1   | AA    | 992     | U    |
| 1   | AA    | 993     | G    |
| 1   | AA    | 1001(A) | G    |
| 1   | AA    | 1005    | A    |
| 1   | AA    | 1006    | C    |
| 1   | AA    | 1027    | C    |
| 1   | AA    | 1028    | C    |
| 1   | AA    | 1029    | C    |
| 1   | AA    | 1030    | C    |
| 1   | AA    | 1030(A) | G    |
| 1   | AA    | 1030(B) | C    |
| 1   | AA    | 1031    | G    |
| 1   | AA    | 1042    | G    |
| 1   | AA    | 1044    | A    |
| 1   | AA    | 1048    | G    |
| 1   | AA    | 1049    | U    |
| 1   | AA    | 1050    | G    |
| 1   | AA    | 1053    | G    |
| 1   | AA    | 1054    | C    |
| 1   | AA    | 1064    | G    |
| 1   | AA    | 1065    | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | AA    | 1066 | C    |
| 1   | AA    | 1067 | A    |
| 1   | AA    | 1068 | G    |
| 1   | AA    | 1081 | G    |
| 1   | AA    | 1085 | U    |
| 1   | AA    | 1086 | U    |
| 1   | AA    | 1093 | A    |
| 1   | AA    | 1094 | G    |
| 1   | AA    | 1101 | A    |
| 1   | AA    | 1102 | A    |
| 1   | AA    | 1117 | G    |
| 1   | AA    | 1118 | C    |
| 1   | AA    | 1125 | U    |
| 1   | AA    | 1126 | U    |
| 1   | AA    | 1127 | G    |
| 1   | AA    | 1128 | C    |
| 1   | AA    | 1129 | C    |
| 1   | AA    | 1130 | A    |
| 1   | AA    | 1131 | G    |
| 1   | AA    | 1132 | C    |
| 1   | AA    | 1136 | U    |
| 1   | AA    | 1137 | C    |
| 1   | AA    | 1138 | G    |
| 1   | AA    | 1139 | G    |
| 1   | AA    | 1140 | C    |
| 1   | AA    | 1145 | C    |
| 1   | AA    | 1146 | A    |
| 1   | AA    | 1153 | C    |
| 1   | AA    | 1157 | A    |
| 1   | AA    | 1158 | C    |
| 1   | AA    | 1159 | U    |
| 1   | AA    | 1160 | G    |
| 1   | AA    | 1182 | G    |
| 1   | AA    | 1183 | A    |
| 1   | AA    | 1184 | G    |
| 1   | AA    | 1187 | G    |
| 1   | AA    | 1196 | U    |
| 1   | AA    | 1200 | C    |
| 1   | AA    | 1201 | A    |
| 1   | AA    | 1202 | G    |
| 1   | AA    | 1211 | U    |
| 1   | AA    | 1212 | U    |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 1   | AA    | 1213    | A    |
| 1   | AA    | 1215    | G    |
| 1   | AA    | 1224    | G    |
| 1   | AA    | 1225    | A    |
| 1   | AA    | 1226    | C    |
| 1   | AA    | 1227    | A    |
| 1   | AA    | 1239    | A    |
| 1   | AA    | 1240    | U    |
| 1   | AA    | 1241    | G    |
| 1   | AA    | 1255    | G    |
| 1   | AA    | 1256    | A    |
| 1   | AA    | 1257    | U    |
| 1   | AA    | 1267    | C    |
| 1   | AA    | 1270    | C    |
| 1   | AA    | 1273    | G    |
| 1   | AA    | 1274    | G    |
| 1   | AA    | 1280    | A    |
| 1   | AA    | 1282    | C    |
| 1   | AA    | 1286    | A    |
| 1   | AA    | 1287    | A    |
| 1   | AA    | 1297    | C    |
| 1   | AA    | 1298    | C    |
| 1   | AA    | 1300    | G    |
| 1   | AA    | 1301    | U    |
| 1   | AA    | 1303    | C    |
| 1   | AA    | 1305    | G    |
| 1   | AA    | 1312    | G    |
| 1   | AA    | 1317    | C    |
| 1   | AA    | 1319    | A    |
| 1   | AA    | 1320    | C    |
| 1   | AA    | 1322    | C    |
| 1   | AA    | 1331    | G    |
| 1   | AA    | 1334    | G    |
| 1   | AA    | 1335    | C    |
| 1   | AA    | 1336    | C    |
| 1   | AA    | 1337    | G    |
| 1   | AA    | 1346    | A    |
| 1   | AA    | 1347    | G    |
| 1   | AA    | 1363    | C    |
| 1   | AA    | 1363(A) | A    |
| 1   | AA    | 1364    | U    |
| 1   | AA    | 1365    | G    |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 1   | AA    | 1379    | G    |
| 1   | AA    | 1381    | U    |
| 1   | AA    | 1394    | A    |
| 1   | AA    | 1395    | C    |
| 1   | AA    | 1396    | A    |
| 1   | AA    | 1397    | C    |
| 1   | AA    | 1398    | A    |
| 1   | AA    | 1400    | C    |
| 1   | AA    | 1401    | G    |
| 1   | AA    | 1419    | G    |
| 1   | AA    | 1442    | G    |
| 1   | AA    | 1442(B) | A    |
| 1   | AA    | 1443    | G    |
| 1   | AA    | 1447    | A    |
| 1   | AA    | 1452    | C    |
| 1   | AA    | 1456    | G    |
| 1   | AA    | 1466    | C    |
| 1   | AA    | 1492    | A    |
| 1   | AA    | 1497    | G    |
| 1   | AA    | 1498    | U    |
| 1   | AA    | 1499    | A    |
| 1   | AA    | 1502    | A    |
| 1   | AA    | 1503    | A    |
| 1   | AA    | 1504    | G    |
| 1   | AA    | 1506    | U    |
| 1   | AA    | 1507    | A    |
| 1   | AA    | 1517    | G    |
| 1   | AA    | 1519    | A    |
| 1   | AA    | 1520    | G    |
| 1   | AA    | 1528    | U    |
| 1   | AA    | 1529    | G    |
| 1   | AA    | 1530    | G    |
| 22  | AV    | 4       | G    |
| 22  | AV    | 5       | G    |
| 22  | AV    | 8       | U    |
| 22  | AV    | 9       | G    |
| 22  | AV    | 16      | C    |
| 22  | AV    | 17      | C    |
| 22  | AV    | 18      | U    |
| 22  | AV    | 19      | G    |
| 22  | AV    | 20      | G    |
| 22  | AV    | 21      | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 22  | AV    | 22  | A    |
| 22  | AV    | 23  | G    |
| 22  | AV    | 34  | U    |
| 22  | AV    | 35  | C    |
| 22  | AV    | 36  | A    |
| 22  | AV    | 38  | A    |
| 22  | AV    | 43  | G    |
| 22  | AV    | 48  | U    |
| 22  | AV    | 49  | C    |
| 22  | AV    | 51  | U    |
| 22  | AV    | 54  | G    |
| 22  | AV    | 55  | U    |
| 22  | AV    | 62  | C    |
| 22  | AV    | 64  | G    |
| 22  | AV    | 71  | G    |
| 22  | AV    | 76  | C    |
| 23  | AW    | 6   | G    |
| 23  | AW    | 15  | G    |
| 23  | AW    | 16  | U    |
| 23  | AW    | 17  | C    |
| 23  | AW    | 18  | G    |
| 23  | AW    | 19  | G    |
| 23  | AW    | 21  | A    |
| 23  | AW    | 30  | G    |
| 23  | AW    | 33  | U    |
| 23  | AW    | 34  | G    |
| 23  | AW    | 37  | A    |
| 23  | AW    | 38  | A    |
| 23  | AW    | 39  | U    |
| 23  | AW    | 41  | C    |
| 23  | AW    | 42  | C    |
| 23  | AW    | 46  | G    |
| 23  | AW    | 47  | U    |
| 23  | AW    | 48  | C    |
| 23  | AW    | 57  | G    |
| 23  | AW    | 59  | U    |
| 23  | AW    | 61  | C    |
| 23  | AW    | 71  | G    |
| 24  | AX    | 12  | A    |
| 24  | AX    | 13  | A    |
| 24  | AX    | 14  | A    |
| 24  | AX    | 22  | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 23  | AY    | 29  | G    |
| 23  | AY    | 30  | G    |
| 23  | AY    | 32  | U    |
| 23  | AY    | 35  | A    |
| 23  | AY    | 43  | C    |
| 25  | BA    | 13  | A    |
| 25  | BA    | 14  | A    |
| 25  | BA    | 15  | G    |
| 25  | BA    | 28  | A    |
| 25  | BA    | 34  | C    |
| 25  | BA    | 35  | G    |
| 25  | BA    | 45  | C    |
| 25  | BA    | 49  | A    |
| 25  | BA    | 50  | U    |
| 25  | BA    | 51  | G    |
| 25  | BA    | 52  | A    |
| 25  | BA    | 55  | G    |
| 25  | BA    | 64  | A    |
| 25  | BA    | 69  | C    |
| 25  | BA    | 70  | G    |
| 25  | BA    | 71  | A    |
| 25  | BA    | 72  | U    |
| 25  | BA    | 73  | A    |
| 25  | BA    | 74  | A    |
| 25  | BA    | 75  | G    |
| 25  | BA    | 83  | G    |
| 25  | BA    | 84  | A    |
| 25  | BA    | 85  | G    |
| 25  | BA    | 90  | U    |
| 25  | BA    | 92  | A    |
| 25  | BA    | 94  | C    |
| 25  | BA    | 95  | G    |
| 25  | BA    | 99  | U    |
| 25  | BA    | 100 | G    |
| 25  | BA    | 102 | G    |
| 25  | BA    | 105 | C    |
| 25  | BA    | 118 | A    |
| 25  | BA    | 119 | A    |
| 25  | BA    | 120 | U    |
| 25  | BA    | 121 | G    |
| 25  | BA    | 126 | A    |
| 25  | BA    | 128 | C    |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 25  | BA    | 129    | C    |
| 25  | BA    | 131    | G    |
| 25  | BA    | 141    | A    |
| 25  | BA    | 142    | A    |
| 25  | BA    | 154    | G    |
| 25  | BA    | 154(A) | C    |
| 25  | BA    | 174    | C    |
| 25  | BA    | 175    | G    |
| 25  | BA    | 178    | G    |
| 25  | BA    | 182    | A    |
| 25  | BA    | 196    | A    |
| 25  | BA    | 199    | A    |
| 25  | BA    | 204    | A    |
| 25  | BA    | 205    | G    |
| 25  | BA    | 212    | G    |
| 25  | BA    | 216    | A    |
| 25  | BA    | 221    | A    |
| 25  | BA    | 222    | A    |
| 25  | BA    | 223    | A    |
| 25  | BA    | 227    | A    |
| 25  | BA    | 228    | A    |
| 25  | BA    | 229    | A    |
| 25  | BA    | 232    | G    |
| 25  | BA    | 233    | A    |
| 25  | BA    | 241    | A    |
| 25  | BA    | 242    | G    |
| 25  | BA    | 248    | G    |
| 25  | BA    | 249    | C    |
| 25  | BA    | 250    | G    |
| 25  | BA    | 252    | G    |
| 25  | BA    | 265    | A    |
| 25  | BA    | 266    | G    |
| 25  | BA    | 271(A) | A    |
| 25  | BA    | 271(J) | C    |
| 25  | BA    | 271(K) | U    |
| 25  | BA    | 271(L) | U    |
| 25  | BA    | 271(O) | C    |
| 25  | BA    | 271(Y) | U    |
| 25  | BA    | 272(A) | U    |
| 25  | BA    | 272(B) | G    |
| 25  | BA    | 272(H) | C    |
| 25  | BA    | 272(I) | U    |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 25  | BA    | 272(J) | C    |
| 25  | BA    | 274    | G    |
| 25  | BA    | 284    | U    |
| 25  | BA    | 286    | C    |
| 25  | BA    | 288    | C    |
| 25  | BA    | 292    | C    |
| 25  | BA    | 301    | G    |
| 25  | BA    | 310    | A    |
| 25  | BA    | 311    | A    |
| 25  | BA    | 312    | G    |
| 25  | BA    | 323    | G    |
| 25  | BA    | 324    | A    |
| 25  | BA    | 329    | G    |
| 25  | BA    | 330    | A    |
| 25  | BA    | 331    | A    |
| 25  | BA    | 332    | A    |
| 25  | BA    | 333    | G    |
| 25  | BA    | 345    | A    |
| 25  | BA    | 346    | A    |
| 25  | BA    | 352    | G    |
| 25  | BA    | 353    | G    |
| 25  | BA    | 355    | G    |
| 25  | BA    | 357    | A    |
| 25  | BA    | 362    | U    |
| 25  | BA    | 363(B) | G    |
| 25  | BA    | 363(E) | U    |
| 25  | BA    | 362(F) | A    |
| 25  | BA    | 364    | C    |
| 25  | BA    | 370    | G    |
| 25  | BA    | 371    | A    |
| 25  | BA    | 372    | G    |
| 25  | BA    | 386    | G    |
| 25  | BA    | 387    | U    |
| 25  | BA    | 388    | G    |
| 25  | BA    | 390    | A    |
| 25  | BA    | 391    | G    |
| 25  | BA    | 396    | G    |
| 25  | BA    | 404    | C    |
| 25  | BA    | 405    | U    |
| 25  | BA    | 406    | G    |
| 25  | BA    | 409    | C    |
| 25  | BA    | 411    | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 25  | BA    | 412 | A    |
| 25  | BA    | 415 | A    |
| 25  | BA    | 418 | G    |
| 25  | BA    | 428 | A    |
| 25  | BA    | 435 | C    |
| 25  | BA    | 443 | A    |
| 25  | BA    | 444 | C    |
| 25  | BA    | 446 | G    |
| 25  | BA    | 447 | A    |
| 25  | BA    | 448 | U    |
| 25  | BA    | 454 | A    |
| 25  | BA    | 455 | C    |
| 25  | BA    | 456 | C    |
| 25  | BA    | 457 | A    |
| 25  | BA    | 458 | G    |
| 25  | BA    | 470 | A    |
| 25  | BA    | 475 | U    |
| 25  | BA    | 480 | A    |
| 25  | BA    | 481 | G    |
| 25  | BA    | 482 | A    |
| 25  | BA    | 491 | G    |
| 25  | BA    | 494 | G    |
| 25  | BA    | 504 | U    |
| 25  | BA    | 505 | A    |
| 25  | BA    | 506 | G    |
| 25  | BA    | 507 | A    |
| 25  | BA    | 508 | G    |
| 25  | BA    | 509 | C    |
| 25  | BA    | 512 | G    |
| 25  | BA    | 528 | A    |
| 25  | BA    | 530 | G    |
| 25  | BA    | 531 | C    |
| 25  | BA    | 532 | A    |
| 25  | BA    | 533 | G    |
| 25  | BA    | 537 | C    |
| 25  | BA    | 549 | G    |
| 25  | BA    | 551 | G    |
| 25  | BA    | 561 | G    |
| 25  | BA    | 562 | U    |
| 25  | BA    | 563 | G    |
| 25  | BA    | 571 | A    |
| 25  | BA    | 572 | A    |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 25  | BA    | 573    | G    |
| 25  | BA    | 574    | C    |
| 25  | BA    | 575    | A    |
| 25  | BA    | 588    | U    |
| 25  | BA    | 593    | G    |
| 25  | BA    | 604    | G    |
| 25  | BA    | 607    | U    |
| 25  | BA    | 608    | A    |
| 25  | BA    | 614    | U    |
| 25  | BA    | 614(A) | U    |
| 25  | BA    | 614(C) | A    |
| 25  | BA    | 615    | G    |
| 25  | BA    | 616    | G    |
| 25  | BA    | 620    | G    |
| 25  | BA    | 621    | A    |
| 25  | BA    | 627    | A    |
| 25  | BA    | 628    | G    |
| 25  | BA    | 634    | C    |
| 25  | BA    | 637    | A    |
| 25  | BA    | 638    | G    |
| 25  | BA    | 645    | C    |
| 25  | BA    | 646    | A    |
| 25  | BA    | 668    | G    |
| 25  | BA    | 669    | G    |
| 25  | BA    | 670    | A    |
| 25  | BA    | 675    | A    |
| 25  | BA    | 686    | G    |
| 25  | BA    | 687    | C    |
| 25  | BA    | 705    | A    |
| 25  | BA    | 708    | C    |
| 25  | BA    | 717    | G    |
| 25  | BA    | 722    | A    |
| 25  | BA    | 726    | G    |
| 25  | BA    | 727    | A    |
| 25  | BA    | 728    | G    |
| 25  | BA    | 729    | G    |
| 25  | BA    | 730    | C    |
| 25  | BA    | 738    | G    |
| 25  | BA    | 739    | G    |
| 25  | BA    | 740    | U    |
| 25  | BA    | 747    | U    |
| 25  | BA    | 753    | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 25  | BA    | 762 | U    |
| 25  | BA    | 763 | G    |
| 25  | BA    | 765 | G    |
| 25  | BA    | 776 | G    |
| 25  | BA    | 777 | A    |
| 25  | BA    | 782 | A    |
| 25  | BA    | 784 | A    |
| 25  | BA    | 785 | G    |
| 25  | BA    | 788 | A    |
| 25  | BA    | 789 | A    |
| 25  | BA    | 790 | C    |
| 25  | BA    | 791 | C    |
| 25  | BA    | 792 | G    |
| 25  | BA    | 793 | A    |
| 25  | BA    | 800 | A    |
| 25  | BA    | 801 | G    |
| 25  | BA    | 802 | A    |
| 25  | BA    | 805 | G    |
| 25  | BA    | 811 | U    |
| 25  | BA    | 812 | C    |
| 25  | BA    | 819 | A    |
| 25  | BA    | 827 | U    |
| 25  | BA    | 828 | U    |
| 25  | BA    | 830 | G    |
| 25  | BA    | 831 | G    |
| 25  | BA    | 832 | G    |
| 25  | BA    | 845 | G    |
| 25  | BA    | 846 | C    |
| 25  | BA    | 847 | U    |
| 25  | BA    | 856 | C    |
| 25  | BA    | 857 | C    |
| 25  | BA    | 859 | G    |
| 25  | BA    | 860 | U    |
| 25  | BA    | 865 | C    |
| 25  | BA    | 866 | A    |
| 25  | BA    | 869 | G    |
| 25  | BA    | 886 | C    |
| 25  | BA    | 889 | C    |
| 25  | BA    | 890 | A    |
| 25  | BA    | 892 | G    |
| 25  | BA    | 896 | A    |
| 25  | BA    | 897 | C    |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 25  | BA    | 901    | A    |
| 25  | BA    | 904    | C    |
| 25  | BA    | 910    | A    |
| 25  | BA    | 913    | U    |
| 25  | BA    | 914    | C    |
| 25  | BA    | 917    | A    |
| 25  | BA    | 926    | A    |
| 25  | BA    | 930    | U    |
| 25  | BA    | 931    | G    |
| 25  | BA    | 932    | G    |
| 25  | BA    | 933    | A    |
| 25  | BA    | 941    | A    |
| 25  | BA    | 943    | U    |
| 25  | BA    | 945    | A    |
| 25  | BA    | 946    | G    |
| 25  | BA    | 959    | A    |
| 25  | BA    | 961    | C    |
| 25  | BA    | 962    | G    |
| 25  | BA    | 965    | C    |
| 25  | BA    | 973    | A    |
| 25  | BA    | 974    | G    |
| 25  | BA    | 975(A) | G    |
| 25  | BA    | 980    | A    |
| 25  | BA    | 983    | A    |
| 25  | BA    | 989    | G    |
| 25  | BA    | 991    | C    |
| 25  | BA    | 995    | C    |
| 25  | BA    | 996    | A    |
| 25  | BA    | 1005   | C    |
| 25  | BA    | 1008   | C    |
| 25  | BA    | 1009   | A    |
| 25  | BA    | 1011   | G    |
| 25  | BA    | 1012   | U    |
| 25  | BA    | 1013   | C    |
| 25  | BA    | 1015   | G    |
| 25  | BA    | 1017   | G    |
| 25  | BA    | 1020   | A    |
| 25  | BA    | 1022   | G    |
| 25  | BA    | 1023   | U    |
| 25  | BA    | 1025   | G    |
| 25  | BA    | 1026   | U    |
| 25  | BA    | 1039   | G    |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 25  | BA    | 1040    | C    |
| 25  | BA    | 1044    | G    |
| 25  | BA    | 1045    | A    |
| 25  | BA    | 1047    | G    |
| 25  | BA    | 1048    | A    |
| 25  | BA    | 1049    | C    |
| 25  | BA    | 1052    | C    |
| 25  | BA    | 1053    | C    |
| 25  | BA    | 1110    | G    |
| 25  | BA    | 1111    | A    |
| 25  | BA    | 1112    | G    |
| 25  | BA    | 1113    | U    |
| 25  | BA    | 1115    | G    |
| 25  | BA    | 1116    | C    |
| 25  | BA    | 1118    | C    |
| 25  | BA    | 1122    | G    |
| 25  | BA    | 1126    | A    |
| 25  | BA    | 1127    | A    |
| 25  | BA    | 1128    | A    |
| 25  | BA    | 1129    | A    |
| 25  | BA    | 1130    | U    |
| 25  | BA    | 1131    | G    |
| 25  | BA    | 1135    | C    |
| 25  | BA    | 1136    | G    |
| 25  | BA    | 1140    | C    |
| 25  | BA    | 1141    | U    |
| 25  | BA    | 1142    | U    |
| 25  | BA    | 1142(A) | A    |
| 25  | BA    | 1143    | A    |
| 25  | BA    | 1144    | G    |
| 25  | BA    | 1155    | A    |
| 25  | BA    | 1156    | A    |
| 25  | BA    | 1157    | G    |
| 25  | BA    | 1170    | G    |
| 25  | BA    | 1171    | G    |
| 25  | BA    | 1173    | G    |
| 25  | BA    | 1174    | A    |
| 25  | BA    | 1175    | U    |
| 25  | BA    | 1176    | G    |
| 25  | BA    | 1177    | A    |
| 25  | BA    | 1178    | C    |
| 25  | BA    | 1180    | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 25  | BA    | 1195 | G    |
| 25  | BA    | 1204 | A    |
| 25  | BA    | 1205 | U    |
| 25  | BA    | 1206 | G    |
| 25  | BA    | 1210 | A    |
| 25  | BA    | 1211 | U    |
| 25  | BA    | 1212 | G    |
| 25  | BA    | 1220 | A    |
| 25  | BA    | 1236 | G    |
| 25  | BA    | 1237 | A    |
| 25  | BA    | 1238 | G    |
| 25  | BA    | 1244 | G    |
| 25  | BA    | 1248 | G    |
| 25  | BA    | 1249 | U    |
| 25  | BA    | 1250 | G    |
| 25  | BA    | 1251 | C    |
| 25  | BA    | 1252 | G    |
| 25  | BA    | 1253 | A    |
| 25  | BA    | 1256 | G    |
| 25  | BA    | 1265 | A    |
| 25  | BA    | 1266 | G    |
| 25  | BA    | 1271 | G    |
| 25  | BA    | 1272 | A    |
| 25  | BA    | 1273 | U    |
| 25  | BA    | 1276 | A    |
| 25  | BA    | 1281 | G    |
| 25  | BA    | 1286 | A    |
| 25  | BA    | 1287 | A    |
| 25  | BA    | 1300 | U    |
| 25  | BA    | 1301 | A    |
| 25  | BA    | 1302 | A    |
| 25  | BA    | 1303 | G    |
| 25  | BA    | 1304 | C    |
| 25  | BA    | 1306 | C    |
| 25  | BA    | 1311 | G    |
| 25  | BA    | 1312 | U    |
| 25  | BA    | 1313 | U    |
| 25  | BA    | 1314 | C    |
| 25  | BA    | 1319 | G    |
| 25  | BA    | 1321 | A    |
| 25  | BA    | 1324 | G    |
| 25  | BA    | 1325 | G    |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 25  | BA    | 1329    | U    |
| 25  | BA    | 1330    | C    |
| 25  | BA    | 1332    | G    |
| 25  | BA    | 1333    | C    |
| 25  | BA    | 1341    | U    |
| 25  | BA    | 1342    | A    |
| 25  | BA    | 1345    | C    |
| 25  | BA    | 1349    | A    |
| 25  | BA    | 1352    | U    |
| 25  | BA    | 1359    | A    |
| 25  | BA    | 1360    | A    |
| 25  | BA    | 1365    | A    |
| 25  | BA    | 1368    | G    |
| 25  | BA    | 1378    | A    |
| 25  | BA    | 1379    | A    |
| 25  | BA    | 1380    | G    |
| 25  | BA    | 1384    | A    |
| 25  | BA    | 1385    | G    |
| 25  | BA    | 1386    | C    |
| 25  | BA    | 1391    | U    |
| 25  | BA    | 1392    | A    |
| 25  | BA    | 1395    | A    |
| 25  | BA    | 1396    | U    |
| 25  | BA    | 1397    | U    |
| 25  | BA    | 1406    | U    |
| 25  | BA    | 1407    | C    |
| 25  | BA    | 1416    | G    |
| 25  | BA    | 1419    | A    |
| 25  | BA    | 1420    | U    |
| 25  | BA    | 1421    | G    |
| 25  | BA    | 1427    | A    |
| 25  | BA    | 1428    | C    |
| 25  | BA    | 1429    | G    |
| 25  | BA    | 1437    | C    |
| 25  | BA    | 1445    | A    |
| 25  | BA    | 1445(A) | C    |
| 25  | BA    | 1447    | G    |
| 25  | BA    | 1449    | A    |
| 25  | BA    | 1450    | G    |
| 25  | BA    | 1451    | C    |
| 25  | BA    | 1452    | A    |
| 25  | BA    | 1453    | U    |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 25  | BA    | 1455    | G    |
| 25  | BA    | 1459    | G    |
| 25  | BA    | 1461    | G    |
| 25  | BA    | 1466    | G    |
| 25  | BA    | 1467    | C    |
| 25  | BA    | 1471    | A    |
| 25  | BA    | 1478    | G    |
| 25  | BA    | 1481    | U    |
| 25  | BA    | 1482    | G    |
| 25  | BA    | 1485    | G    |
| 25  | BA    | 1488    | G    |
| 25  | BA    | 1490    | A    |
| 25  | BA    | 1491    | G    |
| 25  | BA    | 1493    | C    |
| 25  | BA    | 1494    | A    |
| 25  | BA    | 1495    | A    |
| 25  | BA    | 1496    | A    |
| 25  | BA    | 1497    | U    |
| 25  | BA    | 1498    | C    |
| 25  | BA    | 1502    | C    |
| 25  | BA    | 1504    | C    |
| 25  | BA    | 1505    | C    |
| 25  | BA    | 1509    | C    |
| 25  | BA    | 1509(A) | A    |
| 25  | BA    | 1520    | G    |
| 25  | BA    | 1542    | A    |
| 25  | BA    | 1544    | A    |
| 25  | BA    | 1547    | C    |
| 25  | BA    | 1555    | G    |
| 25  | BA    | 1558    | A    |
| 25  | BA    | 1559    | G    |
| 25  | BA    | 1560    | G    |
| 25  | BA    | 1566    | A    |
| 25  | BA    | 1567    | A    |
| 25  | BA    | 1569    | A    |
| 25  | BA    | 1578    | U    |
| 25  | BA    | 1579    | A    |
| 25  | BA    | 1581    | G    |
| 25  | BA    | 1584    | C    |
| 25  | BA    | 1586    | A    |
| 25  | BA    | 1588    | C    |
| 25  | BA    | 1594    | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 25  | BA    | 1595 | G    |
| 25  | BA    | 1602 | U    |
| 25  | BA    | 1603 | A    |
| 25  | BA    | 1608 | A    |
| 25  | BA    | 1611 | C    |
| 25  | BA    | 1615 | C    |
| 25  | BA    | 1617 | C    |
| 25  | BA    | 1618 | A    |
| 25  | BA    | 1619 | G    |
| 25  | BA    | 1634 | A    |
| 25  | BA    | 1635 | G    |
| 25  | BA    | 1640 | C    |
| 25  | BA    | 1646 | C    |
| 25  | BA    | 1647 | G    |
| 25  | BA    | 1648 | C    |
| 25  | BA    | 1651 | G    |
| 25  | BA    | 1654 | A    |
| 25  | BA    | 1667 | G    |
| 25  | BA    | 1668 | A    |
| 25  | BA    | 1669 | A    |
| 25  | BA    | 1674 | G    |
| 25  | BA    | 1675 | C    |
| 25  | BA    | 1678 | G    |
| 25  | BA    | 1681 | G    |
| 25  | BA    | 1682 | G    |
| 25  | BA    | 1694 | C    |
| 25  | BA    | 1695 | G    |
| 25  | BA    | 1696 | G    |
| 25  | BA    | 1698 | A    |
| 25  | BA    | 1699 | G    |
| 25  | BA    | 1700 | A    |
| 25  | BA    | 1718 | G    |
| 25  | BA    | 1719 | G    |
| 25  | BA    | 1721 | G    |
| 25  | BA    | 1722 | A    |
| 25  | BA    | 1739 | U    |
| 25  | BA    | 1740 | G    |
| 25  | BA    | 1741 | A    |
| 25  | BA    | 1743 | C    |
| 25  | BA    | 1744 | C    |
| 25  | BA    | 1748 | G    |
| 25  | BA    | 1750 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 25  | BA    | 1755 | A    |
| 25  | BA    | 1756 | G    |
| 25  | BA    | 1758 | G    |
| 25  | BA    | 1759 | A    |
| 25  | BA    | 1763 | G    |
| 25  | BA    | 1764 | G    |
| 25  | BA    | 1773 | A    |
| 25  | BA    | 1776 | G    |
| 25  | BA    | 1780 | A    |
| 25  | BA    | 1781 | C    |
| 25  | BA    | 1783 | A    |
| 25  | BA    | 1784 | A    |
| 25  | BA    | 1785 | A    |
| 25  | BA    | 1787 | A    |
| 25  | BA    | 1791 | A    |
| 25  | BA    | 1799 | G    |
| 25  | BA    | 1800 | C    |
| 25  | BA    | 1801 | G    |
| 25  | BA    | 1815 | A    |
| 25  | BA    | 1816 | G    |
| 25  | BA    | 1820 | U    |
| 25  | BA    | 1821 | A    |
| 25  | BA    | 1828 | G    |
| 25  | BA    | 1829 | A    |
| 25  | BA    | 1835 | G    |
| 25  | BA    | 1838 | C    |
| 25  | BA    | 1839 | G    |
| 25  | BA    | 1847 | A    |
| 25  | BA    | 1848 | A    |
| 25  | BA    | 1858 | G    |
| 25  | BA    | 1865 | G    |
| 25  | BA    | 1866 | C    |
| 25  | BA    | 1877 | A    |
| 25  | BA    | 1878 | G    |
| 25  | BA    | 1881 | C    |
| 25  | BA    | 1882 | C    |
| 25  | BA    | 1884 | A    |
| 25  | BA    | 1888 | G    |
| 25  | BA    | 1889 | A    |
| 25  | BA    | 1896 | G    |
| 25  | BA    | 1901 | A    |
| 25  | BA    | 1906 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 25  | BA    | 1914 | C    |
| 25  | BA    | 1929 | G    |
| 25  | BA    | 1930 | G    |
| 25  | BA    | 1931 | U    |
| 25  | BA    | 1936 | A    |
| 25  | BA    | 1938 | A    |
| 25  | BA    | 1939 | U    |
| 25  | BA    | 1940 | U    |
| 25  | BA    | 1941 | C    |
| 25  | BA    | 1943 | U    |
| 25  | BA    | 1944 | U    |
| 25  | BA    | 1945 | G    |
| 25  | BA    | 1955 | U    |
| 25  | BA    | 1956 | U    |
| 25  | BA    | 1962 | C    |
| 25  | BA    | 1963 | U    |
| 25  | BA    | 1964 | G    |
| 25  | BA    | 1965 | C    |
| 25  | BA    | 1966 | A    |
| 25  | BA    | 1967 | C    |
| 25  | BA    | 1969 | A    |
| 25  | BA    | 1970 | A    |
| 25  | BA    | 1971 | A    |
| 25  | BA    | 1972 | A    |
| 25  | BA    | 1979 | C    |
| 25  | BA    | 1980 | G    |
| 25  | BA    | 1981 | A    |
| 25  | BA    | 1982 | C    |
| 25  | BA    | 1992 | G    |
| 25  | BA    | 1993 | U    |
| 25  | BA    | 1996 | C    |
| 25  | BA    | 1997 | G    |
| 25  | BA    | 2004 | G    |
| 25  | BA    | 2020 | A    |
| 25  | BA    | 2021 | C    |
| 25  | BA    | 2022 | U    |
| 25  | BA    | 2023 | G    |
| 25  | BA    | 2027 | G    |
| 25  | BA    | 2030 | A    |
| 25  | BA    | 2031 | A    |
| 25  | BA    | 2032 | G    |
| 25  | BA    | 2033 | A    |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 25         | BA           | 2034       | U           |
| 25         | BA           | 2036       | C           |
| 25         | BA           | 2043       | C           |
| 25         | BA           | 2049       | G           |
| 25         | BA           | 2051       | A           |
| 25         | BA           | 2052       | G           |
| 25         | BA           | 2055       | C           |
| 25         | BA           | 2056       | G           |
| 25         | BA           | 2059       | A           |
| 25         | BA           | 2060       | A           |
| 25         | BA           | 2061       | G           |
| 25         | BA           | 2062       | A           |
| 25         | BA           | 2063       | C           |
| 25         | BA           | 2068       | U           |
| 25         | BA           | 2069       | G           |
| 25         | BA           | 2089       | U           |
| 25         | BA           | 2092       | U           |
| 25         | BA           | 2093       | G           |
| 25         | BA           | 2099       | U           |
| 25         | BA           | 2103       | C           |
| 25         | BA           | 2104       | G           |
| 25         | BA           | 2111       | C           |
| 25         | BA           | 2112       | G           |
| 25         | BA           | 2116       | G           |
| 25         | BA           | 2117       | A           |
| 25         | BA           | 2121       | G           |
| 25         | BA           | 2126       | A           |
| 25         | BA           | 2127       | G           |
| 25         | BA           | 2131       | G           |
| 25         | BA           | 2133       | G           |
| 25         | BA           | 2146       | C           |
| 25         | BA           | 2147       | G           |
| 25         | BA           | 2148       | G           |
| 25         | BA           | 2154       | G           |
| 25         | BA           | 2157       | G           |
| 25         | BA           | 2159       | G           |
| 25         | BA           | 2172       | U           |
| 25         | BA           | 2173       | A           |
| 25         | BA           | 2185       | C           |
| 25         | BA           | 2186       | G           |
| 25         | BA           | 2187       | G           |
| 25         | BA           | 2190       | G           |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 25  | BA    | 2191 | G    |
| 25  | BA    | 2192 | G    |
| 25  | BA    | 2198 | A    |
| 25  | BA    | 2199 | A    |
| 25  | BA    | 2206 | G    |
| 25  | BA    | 2207 | G    |
| 25  | BA    | 2208 | A    |
| 25  | BA    | 2219 | G    |
| 25  | BA    | 2225 | A    |
| 25  | BA    | 2226 | C    |
| 25  | BA    | 2227 | A    |
| 25  | BA    | 2238 | G    |
| 25  | BA    | 2239 | G    |
| 25  | BA    | 2250 | G    |
| 25  | BA    | 2251 | G    |
| 25  | BA    | 2259 | G    |
| 25  | BA    | 2266 | A    |
| 25  | BA    | 2267 | A    |
| 25  | BA    | 2268 | A    |
| 25  | BA    | 2275 | C    |
| 25  | BA    | 2279 | G    |
| 25  | BA    | 2283 | C    |
| 25  | BA    | 2288 | A    |
| 25  | BA    | 2289 | G    |
| 25  | BA    | 2297 | C    |
| 25  | BA    | 2307 | G    |
| 25  | BA    | 2308 | G    |
| 25  | BA    | 2316 | C    |
| 25  | BA    | 2318 | G    |
| 25  | BA    | 2319 | G    |
| 25  | BA    | 2320 | A    |
| 25  | BA    | 2321 | G    |
| 25  | BA    | 2325 | G    |
| 25  | BA    | 2334 | G    |
| 25  | BA    | 2335 | A    |
| 25  | BA    | 2336 | A    |
| 25  | BA    | 2337 | G    |
| 25  | BA    | 2345 | G    |
| 25  | BA    | 2346 | A    |
| 25  | BA    | 2347 | C    |
| 25  | BA    | 2350 | C    |
| 25  | BA    | 2376 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 25  | BA    | 2383 | G    |
| 25  | BA    | 2385 | C    |
| 25  | BA    | 2388 | A    |
| 25  | BA    | 2392 | A    |
| 25  | BA    | 2394 | C    |
| 25  | BA    | 2398 | U    |
| 25  | BA    | 2399 | G    |
| 25  | BA    | 2400 | G    |
| 25  | BA    | 2402 | C    |
| 25  | BA    | 2403 | C    |
| 25  | BA    | 2406 | U    |
| 25  | BA    | 2407 | G    |
| 25  | BA    | 2420 | C    |
| 25  | BA    | 2422 | A    |
| 25  | BA    | 2423 | U    |
| 25  | BA    | 2424 | C    |
| 25  | BA    | 2425 | A    |
| 25  | BA    | 2426 | A    |
| 25  | BA    | 2427 | C    |
| 25  | BA    | 2429 | G    |
| 25  | BA    | 2430 | A    |
| 25  | BA    | 2435 | A    |
| 25  | BA    | 2439 | A    |
| 25  | BA    | 2440 | C    |
| 25  | BA    | 2441 | C    |
| 25  | BA    | 2447 | G    |
| 25  | BA    | 2448 | A    |
| 25  | BA    | 2449 | U    |
| 25  | BA    | 2450 | A    |
| 25  | BA    | 2468 | G    |
| 25  | BA    | 2469 | A    |
| 25  | BA    | 2470 | G    |
| 25  | BA    | 2474 | C    |
| 25  | BA    | 2475 | C    |
| 25  | BA    | 2476 | A    |
| 25  | BA    | 2477 | C    |
| 25  | BA    | 2478 | A    |
| 25  | BA    | 2482 | G    |
| 25  | BA    | 2483 | C    |
| 25  | BA    | 2484 | G    |
| 25  | BA    | 2491 | U    |
| 25  | BA    | 2497 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 25  | BA    | 2498 | C    |
| 25  | BA    | 2502 | G    |
| 25  | BA    | 2503 | A    |
| 25  | BA    | 2504 | U    |
| 25  | BA    | 2505 | G    |
| 25  | BA    | 2506 | U    |
| 25  | BA    | 2518 | A    |
| 25  | BA    | 2519 | U    |
| 25  | BA    | 2520 | C    |
| 25  | BA    | 2524 | G    |
| 25  | BA    | 2529 | G    |
| 25  | BA    | 2535 | G    |
| 25  | BA    | 2543 | G    |
| 25  | BA    | 2554 | U    |
| 25  | BA    | 2558 | C    |
| 25  | BA    | 2566 | A    |
| 25  | BA    | 2567 | G    |
| 25  | BA    | 2569 | G    |
| 25  | BA    | 2573 | C    |
| 25  | BA    | 2576 | G    |
| 25  | BA    | 2577 | A    |
| 25  | BA    | 2582 | G    |
| 25  | BA    | 2586 | C    |
| 25  | BA    | 2602 | A    |
| 25  | BA    | 2609 | U    |
| 25  | BA    | 2611 | U    |
| 25  | BA    | 2612 | C    |
| 25  | BA    | 2613 | U    |
| 25  | BA    | 2614 | A    |
| 25  | BA    | 2615 | U    |
| 25  | BA    | 2629 | A    |
| 25  | BA    | 2630 | G    |
| 25  | BA    | 2636 | U    |
| 25  | BA    | 2646 | C    |
| 25  | BA    | 2654 | A    |
| 25  | BA    | 2655 | G    |
| 25  | BA    | 2663 | G    |
| 25  | BA    | 2673 | G    |
| 25  | BA    | 2675 | A    |
| 25  | BA    | 2682 | U    |
| 25  | BA    | 2689 | U    |
| 25  | BA    | 2690 | C    |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 25  | BA    | 2691    | C    |
| 25  | BA    | 2702    | U    |
| 25  | BA    | 2703    | C    |
| 25  | BA    | 2707    | G    |
| 25  | BA    | 2712    | U    |
| 25  | BA    | 2712(A) | A    |
| 25  | BA    | 2713    | A    |
| 25  | BA    | 2726    | U    |
| 25  | BA    | 2732    | G    |
| 25  | BA    | 2733    | A    |
| 25  | BA    | 2734    | A    |
| 25  | BA    | 2750    | A    |
| 25  | BA    | 2751    | G    |
| 25  | BA    | 2752    | C    |
| 25  | BA    | 2753    | A    |
| 25  | BA    | 2756    | U    |
| 25  | BA    | 2757    | A    |
| 25  | BA    | 2759    | G    |
| 25  | BA    | 2762    | G    |
| 25  | BA    | 2764    | A    |
| 25  | BA    | 2765    | A    |
| 25  | BA    | 2766    | G    |
| 25  | BA    | 2777    | G    |
| 25  | BA    | 2778    | A    |
| 25  | BA    | 2779    | U    |
| 25  | BA    | 2780    | G    |
| 25  | BA    | 2781    | A    |
| 25  | BA    | 2789    | C    |
| 25  | BA    | 2790    | A    |
| 25  | BA    | 2791    | C    |
| 25  | BA    | 2792    | G    |
| 25  | BA    | 2796    | U    |
| 25  | BA    | 2799    | C    |
| 25  | BA    | 2801(A) | A    |
| 25  | BA    | 2802    | G    |
| 25  | BA    | 2803    | C    |
| 25  | BA    | 2804    | C    |
| 25  | BA    | 2807    | G    |
| 25  | BA    | 2808    | U    |
| 25  | BA    | 2818    | G    |
| 25  | BA    | 2820    | A    |
| 25  | BA    | 2827    | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 25  | BA    | 2828 | C    |
| 25  | BA    | 2830 | G    |
| 25  | BA    | 2833 | G    |
| 25  | BA    | 2834 | G    |
| 25  | BA    | 2835 | A    |
| 25  | BA    | 2836 | U    |
| 25  | BA    | 2849 | U    |
| 25  | BA    | 2850 | A    |
| 25  | BA    | 2866 | U    |
| 25  | BA    | 2867 | G    |
| 25  | BA    | 2872 | G    |
| 25  | BA    | 2874 | C    |
| 25  | BA    | 2876 | G    |
| 25  | BA    | 2879 | C    |
| 25  | BA    | 2892 | A    |
| 25  | BA    | 2893 | G    |
| 25  | BA    | 2894 | G    |
| 26  | BB    | 2    | C    |
| 26  | BB    | 3    | C    |
| 26  | BB    | 8    | U    |
| 26  | BB    | 12   | C    |
| 26  | BB    | 13   | A    |
| 26  | BB    | 14   | U    |
| 26  | BB    | 15   | A    |
| 26  | BB    | 16   | G    |
| 26  | BB    | 19   | G    |
| 26  | BB    | 21   | G    |
| 26  | BB    | 24   | G    |
| 26  | BB    | 25   | A    |
| 26  | BB    | 35   | U    |
| 26  | BB    | 42   | C    |
| 26  | BB    | 45   | A    |
| 26  | BB    | 52   | A    |
| 26  | BB    | 53   | A    |
| 26  | BB    | 57   | A    |
| 26  | BB    | 66   | A    |
| 26  | BB    | 67   | G    |
| 26  | BB    | 73   | A    |
| 26  | BB    | 92   | C    |
| 26  | BB    | 106  | G    |
| 26  | BB    | 109  | C    |
| 26  | BB    | 110  | G    |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 26  | BB    | 113    | G    |
| 1   | CA    | 6      | G    |
| 1   | CA    | 8      | A    |
| 1   | CA    | 9      | G    |
| 1   | CA    | 14     | U    |
| 1   | CA    | 31     | G    |
| 1   | CA    | 32     | A    |
| 1   | CA    | 39     | G    |
| 1   | CA    | 47     | C    |
| 1   | CA    | 48     | C    |
| 1   | CA    | 49     | U    |
| 1   | CA    | 50     | A    |
| 1   | CA    | 51     | A    |
| 1   | CA    | 54     | C    |
| 1   | CA    | 60     | A    |
| 1   | CA    | 61     | G    |
| 1   | CA    | 65     | U    |
| 1   | CA    | 66     | G    |
| 1   | CA    | 78     | G    |
| 1   | CA    | 79     | G    |
| 1   | CA    | 80     | G    |
| 1   | CA    | 81     | U    |
| 1   | CA    | 84     | U    |
| 1   | CA    | 89     | C    |
| 1   | CA    | 90     | U    |
| 1   | CA    | 101    | A    |
| 1   | CA    | 109    | A    |
| 1   | CA    | 110    | C    |
| 1   | CA    | 115    | G    |
| 1   | CA    | 116    | A    |
| 1   | CA    | 120    | A    |
| 1   | CA    | 121    | C    |
| 1   | CA    | 122    | G    |
| 1   | CA    | 129    | U    |
| 1   | CA    | 129(A) | G    |
| 1   | CA    | 130    | A    |
| 1   | CA    | 131    | C    |
| 1   | CA    | 137    | C    |
| 1   | CA    | 144    | G    |
| 1   | CA    | 151    | A    |
| 1   | CA    | 156    | G    |
| 1   | CA    | 163    | C    |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | CA    | 172    | A    |
| 1   | CA    | 173    | U    |
| 1   | CA    | 174    | C    |
| 1   | CA    | 180    | U    |
| 1   | CA    | 181    | G    |
| 1   | CA    | 182    | U    |
| 1   | CA    | 189(F) | U    |
| 1   | CA    | 189(G) | G    |
| 1   | CA    | 189(H) | G    |
| 1   | CA    | 195    | A    |
| 1   | CA    | 197    | A    |
| 1   | CA    | 198    | G    |
| 1   | CA    | 200    | G    |
| 1   | CA    | 201    | C    |
| 1   | CA    | 203    | U    |
| 1   | CA    | 204    | U    |
| 1   | CA    | 216    | G    |
| 1   | CA    | 220    | G    |
| 1   | CA    | 244    | U    |
| 1   | CA    | 245    | C    |
| 1   | CA    | 247    | G    |
| 1   | CA    | 251    | G    |
| 1   | CA    | 252    | U    |
| 1   | CA    | 267    | C    |
| 1   | CA    | 275    | G    |
| 1   | CA    | 279    | A    |
| 1   | CA    | 280    | C    |
| 1   | CA    | 281    | G    |
| 1   | CA    | 289    | G    |
| 1   | CA    | 301    | G    |
| 1   | CA    | 306    | G    |
| 1   | CA    | 314    | C    |
| 1   | CA    | 316    | G    |
| 1   | CA    | 321    | A    |
| 1   | CA    | 323    | U    |
| 1   | CA    | 328    | C    |
| 1   | CA    | 330    | C    |
| 1   | CA    | 332    | G    |
| 1   | CA    | 342    | C    |
| 1   | CA    | 343    | U    |
| 1   | CA    | 345    | C    |
| 1   | CA    | 346    | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | CA    | 347 | G    |
| 1   | CA    | 352 | C    |
| 1   | CA    | 353 | A    |
| 1   | CA    | 354 | G    |
| 1   | CA    | 367 | U    |
| 1   | CA    | 373 | A    |
| 1   | CA    | 384 | G    |
| 1   | CA    | 388 | G    |
| 1   | CA    | 389 | A    |
| 1   | CA    | 390 | C    |
| 1   | CA    | 397 | A    |
| 1   | CA    | 398 | C    |
| 1   | CA    | 406 | G    |
| 1   | CA    | 412 | A    |
| 1   | CA    | 413 | G    |
| 1   | CA    | 421 | U    |
| 1   | CA    | 422 | C    |
| 1   | CA    | 423 | G    |
| 1   | CA    | 424 | G    |
| 1   | CA    | 428 | G    |
| 1   | CA    | 429 | U    |
| 1   | CA    | 430 | A    |
| 1   | CA    | 435 | C    |
| 1   | CA    | 439 | A    |
| 1   | CA    | 442 | C    |
| 1   | CA    | 451 | A    |
| 1   | CA    | 461 | A    |
| 1   | CA    | 470 | C    |
| 1   | CA    | 471 | G    |
| 1   | CA    | 482 | A    |
| 1   | CA    | 484 | G    |
| 1   | CA    | 485 | G    |
| 1   | CA    | 486 | U    |
| 1   | CA    | 495 | A    |
| 1   | CA    | 496 | A    |
| 1   | CA    | 498 | U    |
| 1   | CA    | 500 | G    |
| 1   | CA    | 508 | C    |
| 1   | CA    | 509 | A    |
| 1   | CA    | 510 | A    |
| 1   | CA    | 511 | C    |
| 1   | CA    | 512 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | CA    | 517 | G    |
| 1   | CA    | 518 | C    |
| 1   | CA    | 519 | C    |
| 1   | CA    | 527 | G    |
| 1   | CA    | 532 | A    |
| 1   | CA    | 533 | A    |
| 1   | CA    | 534 | U    |
| 1   | CA    | 536 | C    |
| 1   | CA    | 548 | G    |
| 1   | CA    | 559 | A    |
| 1   | CA    | 560 | U    |
| 1   | CA    | 561 | U    |
| 1   | CA    | 562 | C    |
| 1   | CA    | 563 | A    |
| 1   | CA    | 564 | C    |
| 1   | CA    | 566 | G    |
| 1   | CA    | 572 | A    |
| 1   | CA    | 573 | A    |
| 1   | CA    | 575 | G    |
| 1   | CA    | 576 | G    |
| 1   | CA    | 577 | G    |
| 1   | CA    | 579 | G    |
| 1   | CA    | 595 | G    |
| 1   | CA    | 596 | C    |
| 1   | CA    | 630 | G    |
| 1   | CA    | 632 | A    |
| 1   | CA    | 633 | G    |
| 1   | CA    | 642 | A    |
| 1   | CA    | 652 | U    |
| 1   | CA    | 653 | A    |
| 1   | CA    | 665 | A    |
| 1   | CA    | 671 | G    |
| 1   | CA    | 687 | A    |
| 1   | CA    | 688 | G    |
| 1   | CA    | 701 | C    |
| 1   | CA    | 702 | A    |
| 1   | CA    | 703 | G    |
| 1   | CA    | 704 | A    |
| 1   | CA    | 721 | G    |
| 1   | CA    | 722 | A    |
| 1   | CA    | 723 | U    |
| 1   | CA    | 724 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | CA    | 731 | G    |
| 1   | CA    | 748 | C    |
| 1   | CA    | 749 | C    |
| 1   | CA    | 754 | C    |
| 1   | CA    | 755 | G    |
| 1   | CA    | 777 | A    |
| 1   | CA    | 786 | G    |
| 1   | CA    | 792 | A    |
| 1   | CA    | 793 | U    |
| 1   | CA    | 794 | A    |
| 1   | CA    | 812 | C    |
| 1   | CA    | 813 | U    |
| 1   | CA    | 815 | A    |
| 1   | CA    | 816 | A    |
| 1   | CA    | 817 | C    |
| 1   | CA    | 818 | G    |
| 1   | CA    | 819 | A    |
| 1   | CA    | 820 | U    |
| 1   | CA    | 821 | G    |
| 1   | CA    | 828 | A    |
| 1   | CA    | 839 | U    |
| 1   | CA    | 840 | C    |
| 1   | CA    | 841 | U    |
| 1   | CA    | 848 | C    |
| 1   | CA    | 855 | G    |
| 1   | CA    | 859 | A    |
| 1   | CA    | 871 | U    |
| 1   | CA    | 872 | A    |
| 1   | CA    | 873 | A    |
| 1   | CA    | 874 | G    |
| 1   | CA    | 885 | G    |
| 1   | CA    | 887 | G    |
| 1   | CA    | 889 | A    |
| 1   | CA    | 890 | G    |
| 1   | CA    | 902 | G    |
| 1   | CA    | 913 | A    |
| 1   | CA    | 914 | A    |
| 1   | CA    | 926 | G    |
| 1   | CA    | 927 | G    |
| 1   | CA    | 934 | C    |
| 1   | CA    | 935 | A    |
| 1   | CA    | 960 | U    |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 1   | CA    | 961     | U    |
| 1   | CA    | 965     | A    |
| 1   | CA    | 966     | G    |
| 1   | CA    | 968     | A    |
| 1   | CA    | 969     | A    |
| 1   | CA    | 971     | G    |
| 1   | CA    | 972     | C    |
| 1   | CA    | 974     | A    |
| 1   | CA    | 975     | A    |
| 1   | CA    | 976     | G    |
| 1   | CA    | 977     | A    |
| 1   | CA    | 980     | C    |
| 1   | CA    | 982     | U    |
| 1   | CA    | 983     | A    |
| 1   | CA    | 991     | U    |
| 1   | CA    | 992     | U    |
| 1   | CA    | 993     | G    |
| 1   | CA    | 1001(A) | G    |
| 1   | CA    | 1002    | G    |
| 1   | CA    | 1005    | A    |
| 1   | CA    | 1027    | C    |
| 1   | CA    | 1030    | C    |
| 1   | CA    | 1030(A) | G    |
| 1   | CA    | 1030(C) | G    |
| 1   | CA    | 1031    | G    |
| 1   | CA    | 1044    | A    |
| 1   | CA    | 1046    | A    |
| 1   | CA    | 1049    | U    |
| 1   | CA    | 1053    | G    |
| 1   | CA    | 1054    | C    |
| 1   | CA    | 1064    | G    |
| 1   | CA    | 1065    | U    |
| 1   | CA    | 1066    | C    |
| 1   | CA    | 1067    | A    |
| 1   | CA    | 1068    | G    |
| 1   | CA    | 1081    | G    |
| 1   | CA    | 1085    | U    |
| 1   | CA    | 1086    | U    |
| 1   | CA    | 1094    | G    |
| 1   | CA    | 1101    | A    |
| 1   | CA    | 1102    | A    |
| 1   | CA    | 1118    | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | CA    | 1124 | G    |
| 1   | CA    | 1125 | U    |
| 1   | CA    | 1126 | U    |
| 1   | CA    | 1128 | C    |
| 1   | CA    | 1129 | C    |
| 1   | CA    | 1130 | A    |
| 1   | CA    | 1131 | G    |
| 1   | CA    | 1136 | U    |
| 1   | CA    | 1137 | C    |
| 1   | CA    | 1139 | G    |
| 1   | CA    | 1140 | C    |
| 1   | CA    | 1142 | G    |
| 1   | CA    | 1145 | C    |
| 1   | CA    | 1146 | A    |
| 1   | CA    | 1157 | A    |
| 1   | CA    | 1158 | C    |
| 1   | CA    | 1159 | U    |
| 1   | CA    | 1160 | G    |
| 1   | CA    | 1162 | C    |
| 1   | CA    | 1181 | G    |
| 1   | CA    | 1182 | G    |
| 1   | CA    | 1183 | A    |
| 1   | CA    | 1184 | G    |
| 1   | CA    | 1190 | G    |
| 1   | CA    | 1191 | A    |
| 1   | CA    | 1196 | U    |
| 1   | CA    | 1197 | G    |
| 1   | CA    | 1200 | C    |
| 1   | CA    | 1201 | A    |
| 1   | CA    | 1202 | G    |
| 1   | CA    | 1212 | U    |
| 1   | CA    | 1213 | A    |
| 1   | CA    | 1215 | G    |
| 1   | CA    | 1224 | G    |
| 1   | CA    | 1225 | A    |
| 1   | CA    | 1226 | C    |
| 1   | CA    | 1227 | A    |
| 1   | CA    | 1236 | A    |
| 1   | CA    | 1238 | A    |
| 1   | CA    | 1239 | A    |
| 1   | CA    | 1240 | U    |
| 1   | CA    | 1241 | G    |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 1   | CA    | 1255    | G    |
| 1   | CA    | 1256    | A    |
| 1   | CA    | 1257    | U    |
| 1   | CA    | 1258    | G    |
| 1   | CA    | 1278    | U    |
| 1   | CA    | 1280    | A    |
| 1   | CA    | 1281    | U    |
| 1   | CA    | 1282    | C    |
| 1   | CA    | 1285    | A    |
| 1   | CA    | 1286    | A    |
| 1   | CA    | 1287    | A    |
| 1   | CA    | 1288    | A    |
| 1   | CA    | 1297    | C    |
| 1   | CA    | 1298    | C    |
| 1   | CA    | 1300    | G    |
| 1   | CA    | 1301    | U    |
| 1   | CA    | 1302    | U    |
| 1   | CA    | 1303    | C    |
| 1   | CA    | 1305    | G    |
| 1   | CA    | 1319    | A    |
| 1   | CA    | 1320    | C    |
| 1   | CA    | 1322    | C    |
| 1   | CA    | 1323    | G    |
| 1   | CA    | 1331    | G    |
| 1   | CA    | 1334    | G    |
| 1   | CA    | 1336    | C    |
| 1   | CA    | 1338    | G    |
| 1   | CA    | 1340    | A    |
| 1   | CA    | 1347    | G    |
| 1   | CA    | 1353    | G    |
| 1   | CA    | 1360    | A    |
| 1   | CA    | 1363    | C    |
| 1   | CA    | 1363(A) | A    |
| 1   | CA    | 1364    | U    |
| 1   | CA    | 1365    | G    |
| 1   | CA    | 1370    | G    |
| 1   | CA    | 1381    | U    |
| 1   | CA    | 1390    | U    |
| 1   | CA    | 1394    | A    |
| 1   | CA    | 1395    | C    |
| 1   | CA    | 1397    | C    |
| 1   | CA    | 1398    | A    |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 1   | CA    | 1400    | C    |
| 1   | CA    | 1401    | G    |
| 1   | CA    | 1419    | G    |
| 1   | CA    | 1442    | G    |
| 1   | CA    | 1442(A) | G    |
| 1   | CA    | 1442(B) | A    |
| 1   | CA    | 1443    | G    |
| 1   | CA    | 1446    | U    |
| 1   | CA    | 1447    | A    |
| 1   | CA    | 1452    | C    |
| 1   | CA    | 1456    | G    |
| 1   | CA    | 1457    | G    |
| 1   | CA    | 1487    | G    |
| 1   | CA    | 1492    | A    |
| 1   | CA    | 1497    | G    |
| 1   | CA    | 1498    | U    |
| 1   | CA    | 1499    | A    |
| 1   | CA    | 1502    | A    |
| 1   | CA    | 1503    | A    |
| 1   | CA    | 1504    | G    |
| 1   | CA    | 1505    | G    |
| 1   | CA    | 1506    | U    |
| 1   | CA    | 1507    | A    |
| 1   | CA    | 1517    | G    |
| 1   | CA    | 1519    | A    |
| 1   | CA    | 1520    | G    |
| 1   | CA    | 1529    | G    |
| 1   | CA    | 1530    | G    |
| 22  | CV    | 4       | G    |
| 22  | CV    | 5       | G    |
| 22  | CV    | 9       | G    |
| 22  | CV    | 15      | G    |
| 22  | CV    | 18      | U    |
| 22  | CV    | 19      | G    |
| 22  | CV    | 20      | G    |
| 22  | CV    | 21      | U    |
| 22  | CV    | 22      | A    |
| 22  | CV    | 25      | U    |
| 22  | CV    | 26      | C    |
| 22  | CV    | 30      | G    |
| 22  | CV    | 32      | G    |
| 22  | CV    | 33      | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 22  | CV    | 35  | C    |
| 22  | CV    | 36  | A    |
| 22  | CV    | 44  | A    |
| 22  | CV    | 45  | A    |
| 22  | CV    | 48  | U    |
| 22  | CV    | 49  | C    |
| 22  | CV    | 50  | G    |
| 22  | CV    | 52  | C    |
| 22  | CV    | 54  | G    |
| 22  | CV    | 55  | U    |
| 22  | CV    | 57  | C    |
| 22  | CV    | 65  | G    |
| 22  | CV    | 70  | C    |
| 22  | CV    | 71  | G    |
| 22  | CV    | 76  | C    |
| 22  | CV    | 77  | A    |
| 23  | CW    | 6   | G    |
| 23  | CW    | 9   | A    |
| 23  | CW    | 11  | C    |
| 23  | CW    | 14  | A    |
| 23  | CW    | 15  | G    |
| 23  | CW    | 16  | U    |
| 23  | CW    | 17  | C    |
| 23  | CW    | 18  | G    |
| 23  | CW    | 19  | G    |
| 23  | CW    | 21  | A    |
| 23  | CW    | 30  | G    |
| 23  | CW    | 34  | G    |
| 23  | CW    | 37  | A    |
| 23  | CW    | 39  | U    |
| 23  | CW    | 42  | C    |
| 23  | CW    | 43  | C    |
| 23  | CW    | 46  | G    |
| 23  | CW    | 47  | U    |
| 23  | CW    | 48  | C    |
| 23  | CW    | 49  | C    |
| 23  | CW    | 52  | G    |
| 23  | CW    | 57  | G    |
| 23  | CW    | 58  | A    |
| 23  | CW    | 61  | C    |
| 23  | CW    | 68  | C    |
| 23  | CW    | 70  | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 24  | CX    | 14  | A    |
| 24  | CX    | 15  | A    |
| 24  | CX    | 18  | G    |
| 24  | CX    | 19  | U    |
| 23  | CY    | 29  | G    |
| 23  | CY    | 30  | G    |
| 23  | CY    | 33  | U    |
| 23  | CY    | 34  | G    |
| 23  | CY    | 36  | A    |
| 23  | CY    | 37  | A    |
| 23  | CY    | 42  | C    |
| 23  | CY    | 43  | C    |
| 25  | DA    | 34  | C    |
| 25  | DA    | 35  | G    |
| 25  | DA    | 45  | C    |
| 25  | DA    | 50  | U    |
| 25  | DA    | 51  | G    |
| 25  | DA    | 52  | A    |
| 25  | DA    | 55  | G    |
| 25  | DA    | 59  | U    |
| 25  | DA    | 60  | G    |
| 25  | DA    | 61  | G    |
| 25  | DA    | 69  | C    |
| 25  | DA    | 70  | G    |
| 25  | DA    | 71  | A    |
| 25  | DA    | 72  | U    |
| 25  | DA    | 73  | A    |
| 25  | DA    | 75  | G    |
| 25  | DA    | 83  | G    |
| 25  | DA    | 84  | A    |
| 25  | DA    | 90  | U    |
| 25  | DA    | 92  | A    |
| 25  | DA    | 94  | C    |
| 25  | DA    | 95  | G    |
| 25  | DA    | 99  | U    |
| 25  | DA    | 100 | G    |
| 25  | DA    | 102 | G    |
| 25  | DA    | 118 | A    |
| 25  | DA    | 119 | A    |
| 25  | DA    | 120 | U    |
| 25  | DA    | 121 | G    |
| 25  | DA    | 126 | A    |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 25  | DA    | 129    | C    |
| 25  | DA    | 137    | C    |
| 25  | DA    | 139(A) | G    |
| 25  | DA    | 141    | A    |
| 25  | DA    | 142    | A    |
| 25  | DA    | 146    | G    |
| 25  | DA    | 148    | C    |
| 25  | DA    | 154    | G    |
| 25  | DA    | 154(A) | C    |
| 25  | DA    | 174    | C    |
| 25  | DA    | 175    | G    |
| 25  | DA    | 178    | G    |
| 25  | DA    | 182    | A    |
| 25  | DA    | 196    | A    |
| 25  | DA    | 197    | A    |
| 25  | DA    | 199    | A    |
| 25  | DA    | 204    | A    |
| 25  | DA    | 205    | G    |
| 25  | DA    | 215    | G    |
| 25  | DA    | 216    | A    |
| 25  | DA    | 221    | A    |
| 25  | DA    | 222    | A    |
| 25  | DA    | 223    | A    |
| 25  | DA    | 227    | A    |
| 25  | DA    | 228    | A    |
| 25  | DA    | 229    | A    |
| 25  | DA    | 232    | G    |
| 25  | DA    | 233    | A    |
| 25  | DA    | 241    | A    |
| 25  | DA    | 242    | G    |
| 25  | DA    | 248    | G    |
| 25  | DA    | 252    | G    |
| 25  | DA    | 261    | G    |
| 25  | DA    | 265    | A    |
| 25  | DA    | 266    | G    |
| 25  | DA    | 271(J) | C    |
| 25  | DA    | 271(K) | U    |
| 25  | DA    | 271(L) | U    |
| 25  | DA    | 271(M) | G    |
| 25  | DA    | 271(N) | U    |
| 25  | DA    | 271(O) | C    |
| 25  | DA    | 271(T) | C    |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 25  | DA    | 9274   | U    |
| 25  | DA    | 272    | G    |
| 25  | DA    | 272(A) | U    |
| 25  | DA    | 272(B) | G    |
| 25  | DA    | 272(H) | C    |
| 25  | DA    | 272(I) | U    |
| 25  | DA    | 272(J) | C    |
| 25  | DA    | 274    | G    |
| 25  | DA    | 284    | U    |
| 25  | DA    | 286    | C    |
| 25  | DA    | 287    | C    |
| 25  | DA    | 289    | A    |
| 25  | DA    | 298    | G    |
| 25  | DA    | 301    | G    |
| 25  | DA    | 310    | A    |
| 25  | DA    | 311    | A    |
| 25  | DA    | 316    | C    |
| 25  | DA    | 321    | G    |
| 25  | DA    | 322    | A    |
| 25  | DA    | 323    | G    |
| 25  | DA    | 324    | A    |
| 25  | DA    | 329    | G    |
| 25  | DA    | 330    | A    |
| 25  | DA    | 332    | A    |
| 25  | DA    | 333    | G    |
| 25  | DA    | 340    | A    |
| 25  | DA    | 343    | C    |
| 25  | DA    | 346    | A    |
| 25  | DA    | 352    | G    |
| 25  | DA    | 353    | G    |
| 25  | DA    | 358    | U    |
| 25  | DA    | 362    | U    |
| 25  | DA    | 363(B) | G    |
| 25  | DA    | 363(E) | U    |
| 25  | DA    | 362(F) | A    |
| 25  | DA    | 364    | C    |
| 25  | DA    | 365    | C    |
| 25  | DA    | 370    | G    |
| 25  | DA    | 371    | A    |
| 25  | DA    | 372    | G    |
| 25  | DA    | 380    | U    |
| 25  | DA    | 386    | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 25  | DA    | 387 | U    |
| 25  | DA    | 388 | G    |
| 25  | DA    | 390 | A    |
| 25  | DA    | 391 | G    |
| 25  | DA    | 395 | U    |
| 25  | DA    | 396 | G    |
| 25  | DA    | 403 | U    |
| 25  | DA    | 404 | C    |
| 25  | DA    | 405 | U    |
| 25  | DA    | 411 | G    |
| 25  | DA    | 412 | A    |
| 25  | DA    | 414 | C    |
| 25  | DA    | 428 | A    |
| 25  | DA    | 434 | U    |
| 25  | DA    | 435 | C    |
| 25  | DA    | 443 | A    |
| 25  | DA    | 444 | C    |
| 25  | DA    | 446 | G    |
| 25  | DA    | 447 | A    |
| 25  | DA    | 448 | U    |
| 25  | DA    | 454 | A    |
| 25  | DA    | 455 | C    |
| 25  | DA    | 457 | A    |
| 25  | DA    | 458 | G    |
| 25  | DA    | 470 | A    |
| 25  | DA    | 475 | U    |
| 25  | DA    | 480 | A    |
| 25  | DA    | 481 | G    |
| 25  | DA    | 482 | A    |
| 25  | DA    | 483 | A    |
| 25  | DA    | 503 | A    |
| 25  | DA    | 504 | U    |
| 25  | DA    | 505 | A    |
| 25  | DA    | 506 | G    |
| 25  | DA    | 507 | A    |
| 25  | DA    | 508 | G    |
| 25  | DA    | 509 | C    |
| 25  | DA    | 512 | G    |
| 25  | DA    | 527 | C    |
| 25  | DA    | 528 | A    |
| 25  | DA    | 529 | A    |
| 25  | DA    | 530 | G    |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 25  | DA    | 531    | C    |
| 25  | DA    | 532    | A    |
| 25  | DA    | 533    | G    |
| 25  | DA    | 545    | C    |
| 25  | DA    | 555    | U    |
| 25  | DA    | 556    | G    |
| 25  | DA    | 561    | G    |
| 25  | DA    | 562    | U    |
| 25  | DA    | 563    | G    |
| 25  | DA    | 571    | A    |
| 25  | DA    | 572    | A    |
| 25  | DA    | 573    | G    |
| 25  | DA    | 574    | C    |
| 25  | DA    | 575    | A    |
| 25  | DA    | 586    | A    |
| 25  | DA    | 588    | U    |
| 25  | DA    | 603    | A    |
| 25  | DA    | 604    | G    |
| 25  | DA    | 607    | U    |
| 25  | DA    | 608    | A    |
| 25  | DA    | 613    | G    |
| 25  | DA    | 614(A) | U    |
| 25  | DA    | 614(B) | G    |
| 25  | DA    | 614(C) | A    |
| 25  | DA    | 615    | G    |
| 25  | DA    | 620    | G    |
| 25  | DA    | 621    | A    |
| 25  | DA    | 626    | U    |
| 25  | DA    | 627    | A    |
| 25  | DA    | 628    | G    |
| 25  | DA    | 634    | C    |
| 25  | DA    | 638    | G    |
| 25  | DA    | 645    | C    |
| 25  | DA    | 646    | A    |
| 25  | DA    | 651    | G    |
| 25  | DA    | 652    | C    |
| 25  | DA    | 668    | G    |
| 25  | DA    | 670    | A    |
| 25  | DA    | 671    | C    |
| 25  | DA    | 686    | G    |
| 25  | DA    | 687    | C    |
| 25  | DA    | 708    | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 25  | DA    | 717 | G    |
| 25  | DA    | 722 | A    |
| 25  | DA    | 726 | G    |
| 25  | DA    | 727 | A    |
| 25  | DA    | 728 | G    |
| 25  | DA    | 729 | G    |
| 25  | DA    | 730 | C    |
| 25  | DA    | 747 | U    |
| 25  | DA    | 752 | A    |
| 25  | DA    | 753 | C    |
| 25  | DA    | 763 | G    |
| 25  | DA    | 765 | G    |
| 25  | DA    | 775 | G    |
| 25  | DA    | 776 | G    |
| 25  | DA    | 777 | A    |
| 25  | DA    | 782 | A    |
| 25  | DA    | 784 | A    |
| 25  | DA    | 785 | G    |
| 25  | DA    | 788 | A    |
| 25  | DA    | 789 | A    |
| 25  | DA    | 790 | C    |
| 25  | DA    | 791 | C    |
| 25  | DA    | 792 | G    |
| 25  | DA    | 793 | A    |
| 25  | DA    | 794 | G    |
| 25  | DA    | 800 | A    |
| 25  | DA    | 801 | G    |
| 25  | DA    | 802 | A    |
| 25  | DA    | 805 | G    |
| 25  | DA    | 806 | C    |
| 25  | DA    | 811 | U    |
| 25  | DA    | 812 | C    |
| 25  | DA    | 819 | A    |
| 25  | DA    | 827 | U    |
| 25  | DA    | 828 | U    |
| 25  | DA    | 829 | A    |
| 25  | DA    | 830 | G    |
| 25  | DA    | 831 | G    |
| 25  | DA    | 845 | G    |
| 25  | DA    | 846 | C    |
| 25  | DA    | 847 | U    |
| 25  | DA    | 848 | G    |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 25  | DA    | 856    | C    |
| 25  | DA    | 857    | C    |
| 25  | DA    | 858    | U    |
| 25  | DA    | 859    | G    |
| 25  | DA    | 866    | A    |
| 25  | DA    | 886    | C    |
| 25  | DA    | 887    | A    |
| 25  | DA    | 888    | C    |
| 25  | DA    | 889    | C    |
| 25  | DA    | 890    | A    |
| 25  | DA    | 896    | A    |
| 25  | DA    | 897    | C    |
| 25  | DA    | 904    | C    |
| 25  | DA    | 910    | A    |
| 25  | DA    | 913    | U    |
| 25  | DA    | 914    | C    |
| 25  | DA    | 915    | C    |
| 25  | DA    | 917    | A    |
| 25  | DA    | 919    | G    |
| 25  | DA    | 926    | A    |
| 25  | DA    | 931    | G    |
| 25  | DA    | 932    | G    |
| 25  | DA    | 933    | A    |
| 25  | DA    | 941    | A    |
| 25  | DA    | 943    | U    |
| 25  | DA    | 945    | A    |
| 25  | DA    | 946    | G    |
| 25  | DA    | 953    | A    |
| 25  | DA    | 957    | A    |
| 25  | DA    | 958    | U    |
| 25  | DA    | 959    | A    |
| 25  | DA    | 961    | C    |
| 25  | DA    | 962    | G    |
| 25  | DA    | 965    | C    |
| 25  | DA    | 973    | A    |
| 25  | DA    | 974    | G    |
| 25  | DA    | 975(A) | G    |
| 25  | DA    | 983    | A    |
| 25  | DA    | 990    | A    |
| 25  | DA    | 991    | C    |
| 25  | DA    | 996    | A    |
| 25  | DA    | 1005   | C    |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 25  | DA    | 1008    | C    |
| 25  | DA    | 1009    | A    |
| 25  | DA    | 1011    | G    |
| 25  | DA    | 1012    | U    |
| 25  | DA    | 1013    | C    |
| 25  | DA    | 1015    | G    |
| 25  | DA    | 1017    | G    |
| 25  | DA    | 1020    | A    |
| 25  | DA    | 1021    | A    |
| 25  | DA    | 1022    | G    |
| 25  | DA    | 1023    | U    |
| 25  | DA    | 1025    | G    |
| 25  | DA    | 1026    | U    |
| 25  | DA    | 1044    | G    |
| 25  | DA    | 1045    | A    |
| 25  | DA    | 1046    | A    |
| 25  | DA    | 1047    | G    |
| 25  | DA    | 1048    | A    |
| 25  | DA    | 1049    | C    |
| 25  | DA    | 1050    | A    |
| 25  | DA    | 1054    | A    |
| 25  | DA    | 1055    | G    |
| 25  | DA    | 1097    | U    |
| 25  | DA    | 1099    | G    |
| 25  | DA    | 1103    | A    |
| 25  | DA    | 1104    | C    |
| 25  | DA    | 1105    | U    |
| 25  | DA    | 1110    | G    |
| 25  | DA    | 1111    | A    |
| 25  | DA    | 1112    | G    |
| 25  | DA    | 1122    | G    |
| 25  | DA    | 1126    | A    |
| 25  | DA    | 1127    | A    |
| 25  | DA    | 1128    | A    |
| 25  | DA    | 1130    | U    |
| 25  | DA    | 1131    | G    |
| 25  | DA    | 1132    | A    |
| 25  | DA    | 1135    | C    |
| 25  | DA    | 1136    | G    |
| 25  | DA    | 1142(A) | A    |
| 25  | DA    | 1143    | A    |
| 25  | DA    | 1144    | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 25  | DA    | 1155 | A    |
| 25  | DA    | 1157 | G    |
| 25  | DA    | 1171 | G    |
| 25  | DA    | 1173 | G    |
| 25  | DA    | 1174 | A    |
| 25  | DA    | 1175 | U    |
| 25  | DA    | 1176 | G    |
| 25  | DA    | 1177 | A    |
| 25  | DA    | 1178 | C    |
| 25  | DA    | 1195 | G    |
| 25  | DA    | 1204 | A    |
| 25  | DA    | 1205 | U    |
| 25  | DA    | 1206 | G    |
| 25  | DA    | 1208 | C    |
| 25  | DA    | 1210 | A    |
| 25  | DA    | 1211 | U    |
| 25  | DA    | 1212 | G    |
| 25  | DA    | 1220 | A    |
| 25  | DA    | 1221 | C    |
| 25  | DA    | 1236 | G    |
| 25  | DA    | 1237 | A    |
| 25  | DA    | 1238 | G    |
| 25  | DA    | 1247 | A    |
| 25  | DA    | 1248 | G    |
| 25  | DA    | 1249 | U    |
| 25  | DA    | 1250 | G    |
| 25  | DA    | 1251 | C    |
| 25  | DA    | 1252 | G    |
| 25  | DA    | 1253 | A    |
| 25  | DA    | 1254 | A    |
| 25  | DA    | 1256 | G    |
| 25  | DA    | 1265 | A    |
| 25  | DA    | 1266 | G    |
| 25  | DA    | 1271 | G    |
| 25  | DA    | 1272 | A    |
| 25  | DA    | 1273 | U    |
| 25  | DA    | 1276 | A    |
| 25  | DA    | 1281 | G    |
| 25  | DA    | 1288 | U    |
| 25  | DA    | 1289 | C    |
| 25  | DA    | 1300 | U    |
| 25  | DA    | 1301 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 25  | DA    | 1302 | A    |
| 25  | DA    | 1303 | G    |
| 25  | DA    | 1311 | G    |
| 25  | DA    | 1312 | U    |
| 25  | DA    | 1313 | U    |
| 25  | DA    | 1314 | C    |
| 25  | DA    | 1319 | G    |
| 25  | DA    | 1321 | A    |
| 25  | DA    | 1324 | G    |
| 25  | DA    | 1325 | G    |
| 25  | DA    | 1329 | U    |
| 25  | DA    | 1330 | C    |
| 25  | DA    | 1332 | G    |
| 25  | DA    | 1333 | C    |
| 25  | DA    | 1341 | U    |
| 25  | DA    | 1344 | G    |
| 25  | DA    | 1345 | C    |
| 25  | DA    | 1349 | A    |
| 25  | DA    | 1352 | U    |
| 25  | DA    | 1359 | A    |
| 25  | DA    | 1360 | A    |
| 25  | DA    | 1365 | A    |
| 25  | DA    | 1368 | G    |
| 25  | DA    | 1379 | A    |
| 25  | DA    | 1380 | G    |
| 25  | DA    | 1384 | A    |
| 25  | DA    | 1386 | C    |
| 25  | DA    | 1391 | U    |
| 25  | DA    | 1395 | A    |
| 25  | DA    | 1397 | U    |
| 25  | DA    | 1407 | C    |
| 25  | DA    | 1408 | C    |
| 25  | DA    | 1416 | G    |
| 25  | DA    | 1417 | C    |
| 25  | DA    | 1419 | A    |
| 25  | DA    | 1420 | U    |
| 25  | DA    | 1421 | G    |
| 25  | DA    | 1427 | A    |
| 25  | DA    | 1428 | C    |
| 25  | DA    | 1429 | G    |
| 25  | DA    | 1437 | C    |
| 25  | DA    | 1445 | A    |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 25  | DA    | 1445(A) | C    |
| 25  | DA    | 1449    | A    |
| 25  | DA    | 1450    | G    |
| 25  | DA    | 1451    | C    |
| 25  | DA    | 1452    | A    |
| 25  | DA    | 1453    | U    |
| 25  | DA    | 1455    | G    |
| 25  | DA    | 1458    | C    |
| 25  | DA    | 1459    | G    |
| 25  | DA    | 1461    | G    |
| 25  | DA    | 1467    | C    |
| 25  | DA    | 1471    | A    |
| 25  | DA    | 1475    | G    |
| 25  | DA    | 1481    | U    |
| 25  | DA    | 1482    | G    |
| 25  | DA    | 1488    | G    |
| 25  | DA    | 1490    | A    |
| 25  | DA    | 1493    | C    |
| 25  | DA    | 1494    | A    |
| 25  | DA    | 1496    | A    |
| 25  | DA    | 1497    | U    |
| 25  | DA    | 1498    | C    |
| 25  | DA    | 1502    | C    |
| 25  | DA    | 1504    | C    |
| 25  | DA    | 1508    | A    |
| 25  | DA    | 1509    | C    |
| 25  | DA    | 1509(A) | A    |
| 25  | DA    | 1513    | C    |
| 25  | DA    | 1520    | G    |
| 25  | DA    | 1529    | G    |
| 25  | DA    | 1542    | A    |
| 25  | DA    | 1543    | C    |
| 25  | DA    | 1544    | A    |
| 25  | DA    | 1547    | C    |
| 25  | DA    | 1549    | C    |
| 25  | DA    | 1554    | A    |
| 25  | DA    | 1558    | A    |
| 25  | DA    | 1559    | G    |
| 25  | DA    | 1560    | G    |
| 25  | DA    | 1566    | A    |
| 25  | DA    | 1567    | A    |
| 25  | DA    | 1568    | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 25  | DA    | 1569 | A    |
| 25  | DA    | 1578 | U    |
| 25  | DA    | 1579 | A    |
| 25  | DA    | 1583 | A    |
| 25  | DA    | 1584 | C    |
| 25  | DA    | 1586 | A    |
| 25  | DA    | 1588 | C    |
| 25  | DA    | 1589 | C    |
| 25  | DA    | 1594 | G    |
| 25  | DA    | 1595 | G    |
| 25  | DA    | 1598 | C    |
| 25  | DA    | 1602 | U    |
| 25  | DA    | 1603 | A    |
| 25  | DA    | 1608 | A    |
| 25  | DA    | 1611 | C    |
| 25  | DA    | 1616 | A    |
| 25  | DA    | 1617 | C    |
| 25  | DA    | 1618 | A    |
| 25  | DA    | 1634 | A    |
| 25  | DA    | 1635 | G    |
| 25  | DA    | 1640 | C    |
| 25  | DA    | 1648 | C    |
| 25  | DA    | 1651 | G    |
| 25  | DA    | 1653 | G    |
| 25  | DA    | 1654 | A    |
| 25  | DA    | 1668 | A    |
| 25  | DA    | 1669 | A    |
| 25  | DA    | 1674 | G    |
| 25  | DA    | 1675 | C    |
| 25  | DA    | 1678 | G    |
| 25  | DA    | 1681 | G    |
| 25  | DA    | 1682 | G    |
| 25  | DA    | 1693 | U    |
| 25  | DA    | 1694 | C    |
| 25  | DA    | 1696 | G    |
| 25  | DA    | 1699 | G    |
| 25  | DA    | 1700 | A    |
| 25  | DA    | 1701 | A    |
| 25  | DA    | 1706 | U    |
| 25  | DA    | 1707 | G    |
| 25  | DA    | 1718 | G    |
| 25  | DA    | 1722 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 25  | DA    | 1739 | U    |
| 25  | DA    | 1740 | G    |
| 25  | DA    | 1741 | A    |
| 25  | DA    | 1744 | C    |
| 25  | DA    | 1746 | G    |
| 25  | DA    | 1748 | G    |
| 25  | DA    | 1752 | C    |
| 25  | DA    | 1754 | C    |
| 25  | DA    | 1756 | G    |
| 25  | DA    | 1758 | G    |
| 25  | DA    | 1759 | A    |
| 25  | DA    | 1762 | A    |
| 25  | DA    | 1763 | G    |
| 25  | DA    | 1764 | G    |
| 25  | DA    | 1773 | A    |
| 25  | DA    | 1780 | A    |
| 25  | DA    | 1782 | C    |
| 25  | DA    | 1784 | A    |
| 25  | DA    | 1785 | A    |
| 25  | DA    | 1787 | A    |
| 25  | DA    | 1791 | A    |
| 25  | DA    | 1799 | G    |
| 25  | DA    | 1800 | C    |
| 25  | DA    | 1801 | G    |
| 25  | DA    | 1802 | A    |
| 25  | DA    | 1815 | A    |
| 25  | DA    | 1816 | G    |
| 25  | DA    | 1820 | U    |
| 25  | DA    | 1821 | A    |
| 25  | DA    | 1828 | G    |
| 25  | DA    | 1829 | A    |
| 25  | DA    | 1835 | G    |
| 25  | DA    | 1836 | C    |
| 25  | DA    | 1838 | C    |
| 25  | DA    | 1839 | G    |
| 25  | DA    | 1847 | A    |
| 25  | DA    | 1848 | A    |
| 25  | DA    | 1853 | A    |
| 25  | DA    | 1858 | G    |
| 25  | DA    | 1865 | G    |
| 25  | DA    | 1866 | C    |
| 25  | DA    | 1877 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 25  | DA    | 1878 | G    |
| 25  | DA    | 1880 | C    |
| 25  | DA    | 1882 | C    |
| 25  | DA    | 1885 | A    |
| 25  | DA    | 1888 | G    |
| 25  | DA    | 1889 | A    |
| 25  | DA    | 1900 | A    |
| 25  | DA    | 1906 | G    |
| 25  | DA    | 1912 | A    |
| 25  | DA    | 1914 | C    |
| 25  | DA    | 1918 | A    |
| 25  | DA    | 1919 | A    |
| 25  | DA    | 1929 | G    |
| 25  | DA    | 1930 | G    |
| 25  | DA    | 1936 | A    |
| 25  | DA    | 1937 | A    |
| 25  | DA    | 1938 | A    |
| 25  | DA    | 1939 | U    |
| 25  | DA    | 1940 | U    |
| 25  | DA    | 1941 | C    |
| 25  | DA    | 1943 | U    |
| 25  | DA    | 1944 | U    |
| 25  | DA    | 1945 | G    |
| 25  | DA    | 1954 | G    |
| 25  | DA    | 1955 | U    |
| 25  | DA    | 1956 | U    |
| 25  | DA    | 1962 | C    |
| 25  | DA    | 1963 | U    |
| 25  | DA    | 1964 | G    |
| 25  | DA    | 1965 | C    |
| 25  | DA    | 1967 | C    |
| 25  | DA    | 1969 | A    |
| 25  | DA    | 1970 | A    |
| 25  | DA    | 1971 | A    |
| 25  | DA    | 1972 | A    |
| 25  | DA    | 1980 | G    |
| 25  | DA    | 1981 | A    |
| 25  | DA    | 1982 | C    |
| 25  | DA    | 1987 | G    |
| 25  | DA    | 1991 | U    |
| 25  | DA    | 1992 | G    |
| 25  | DA    | 1993 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 25  | DA    | 1996 | C    |
| 25  | DA    | 1997 | G    |
| 25  | DA    | 2020 | A    |
| 25  | DA    | 2021 | C    |
| 25  | DA    | 2022 | U    |
| 25  | DA    | 2023 | G    |
| 25  | DA    | 2031 | A    |
| 25  | DA    | 2032 | G    |
| 25  | DA    | 2033 | A    |
| 25  | DA    | 2034 | U    |
| 25  | DA    | 2036 | C    |
| 25  | DA    | 2043 | C    |
| 25  | DA    | 2051 | A    |
| 25  | DA    | 2052 | G    |
| 25  | DA    | 2055 | C    |
| 25  | DA    | 2056 | G    |
| 25  | DA    | 2059 | A    |
| 25  | DA    | 2060 | A    |
| 25  | DA    | 2061 | G    |
| 25  | DA    | 2062 | A    |
| 25  | DA    | 2067 | G    |
| 25  | DA    | 2068 | U    |
| 25  | DA    | 2069 | G    |
| 25  | DA    | 2092 | U    |
| 25  | DA    | 2093 | G    |
| 25  | DA    | 2099 | U    |
| 25  | DA    | 2103 | C    |
| 25  | DA    | 2104 | G    |
| 25  | DA    | 2105 | C    |
| 25  | DA    | 2110 | G    |
| 25  | DA    | 2111 | C    |
| 25  | DA    | 2112 | G    |
| 25  | DA    | 2116 | G    |
| 25  | DA    | 2117 | A    |
| 25  | DA    | 2126 | A    |
| 25  | DA    | 2127 | G    |
| 25  | DA    | 2131 | G    |
| 25  | DA    | 2133 | G    |
| 25  | DA    | 2146 | C    |
| 25  | DA    | 2147 | G    |
| 25  | DA    | 2148 | G    |
| 25  | DA    | 2157 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 25  | DA    | 2159 | G    |
| 25  | DA    | 2172 | U    |
| 25  | DA    | 2173 | A    |
| 25  | DA    | 2174 | C    |
| 25  | DA    | 2176 | A    |
| 25  | DA    | 2179 | C    |
| 25  | DA    | 2187 | G    |
| 25  | DA    | 2190 | G    |
| 25  | DA    | 2192 | G    |
| 25  | DA    | 2193 | G    |
| 25  | DA    | 2199 | A    |
| 25  | DA    | 2206 | G    |
| 25  | DA    | 2207 | G    |
| 25  | DA    | 2208 | A    |
| 25  | DA    | 2218 | U    |
| 25  | DA    | 2219 | G    |
| 25  | DA    | 2225 | A    |
| 25  | DA    | 2226 | C    |
| 25  | DA    | 2238 | G    |
| 25  | DA    | 2239 | G    |
| 25  | DA    | 2246 | G    |
| 25  | DA    | 2249 | U    |
| 25  | DA    | 2250 | G    |
| 25  | DA    | 2251 | G    |
| 25  | DA    | 2259 | G    |
| 25  | DA    | 2266 | A    |
| 25  | DA    | 2267 | A    |
| 25  | DA    | 2275 | C    |
| 25  | DA    | 2276 | G    |
| 25  | DA    | 2283 | C    |
| 25  | DA    | 2286 | A    |
| 25  | DA    | 2287 | A    |
| 25  | DA    | 2288 | A    |
| 25  | DA    | 2289 | G    |
| 25  | DA    | 2290 | G    |
| 25  | DA    | 2296 | U    |
| 25  | DA    | 2297 | C    |
| 25  | DA    | 2305 | A    |
| 25  | DA    | 2307 | G    |
| 25  | DA    | 2308 | G    |
| 25  | DA    | 2309 | A    |
| 25  | DA    | 2319 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 25  | DA    | 2320 | A    |
| 25  | DA    | 2325 | G    |
| 25  | DA    | 2334 | G    |
| 25  | DA    | 2335 | A    |
| 25  | DA    | 2336 | A    |
| 25  | DA    | 2337 | G    |
| 25  | DA    | 2345 | G    |
| 25  | DA    | 2346 | A    |
| 25  | DA    | 2347 | C    |
| 25  | DA    | 2349 | G    |
| 25  | DA    | 2350 | C    |
| 25  | DA    | 2379 | G    |
| 25  | DA    | 2382 | G    |
| 25  | DA    | 2383 | G    |
| 25  | DA    | 2384 | G    |
| 25  | DA    | 2385 | C    |
| 25  | DA    | 2388 | A    |
| 25  | DA    | 2392 | A    |
| 25  | DA    | 2394 | C    |
| 25  | DA    | 2399 | G    |
| 25  | DA    | 2400 | G    |
| 25  | DA    | 2402 | C    |
| 25  | DA    | 2406 | U    |
| 25  | DA    | 2407 | G    |
| 25  | DA    | 2423 | U    |
| 25  | DA    | 2424 | C    |
| 25  | DA    | 2425 | A    |
| 25  | DA    | 2426 | A    |
| 25  | DA    | 2429 | G    |
| 25  | DA    | 2430 | A    |
| 25  | DA    | 2435 | A    |
| 25  | DA    | 2439 | A    |
| 25  | DA    | 2441 | C    |
| 25  | DA    | 2447 | G    |
| 25  | DA    | 2448 | A    |
| 25  | DA    | 2449 | U    |
| 25  | DA    | 2450 | A    |
| 25  | DA    | 2458 | G    |
| 25  | DA    | 2468 | G    |
| 25  | DA    | 2469 | A    |
| 25  | DA    | 2470 | G    |
| 25  | DA    | 2476 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 25  | DA    | 2477 | C    |
| 25  | DA    | 2478 | A    |
| 25  | DA    | 2482 | G    |
| 25  | DA    | 2483 | C    |
| 25  | DA    | 2484 | G    |
| 25  | DA    | 2491 | U    |
| 25  | DA    | 2497 | A    |
| 25  | DA    | 2498 | C    |
| 25  | DA    | 2502 | G    |
| 25  | DA    | 2505 | G    |
| 25  | DA    | 2506 | U    |
| 25  | DA    | 2507 | C    |
| 25  | DA    | 2518 | A    |
| 25  | DA    | 2519 | U    |
| 25  | DA    | 2520 | C    |
| 25  | DA    | 2529 | G    |
| 25  | DA    | 2534 | A    |
| 25  | DA    | 2542 | A    |
| 25  | DA    | 2543 | G    |
| 25  | DA    | 2554 | U    |
| 25  | DA    | 2566 | A    |
| 25  | DA    | 2567 | G    |
| 25  | DA    | 2569 | G    |
| 25  | DA    | 2571 | C    |
| 25  | DA    | 2573 | C    |
| 25  | DA    | 2576 | G    |
| 25  | DA    | 2577 | A    |
| 25  | DA    | 2582 | G    |
| 25  | DA    | 2585 | U    |
| 25  | DA    | 2602 | A    |
| 25  | DA    | 2609 | U    |
| 25  | DA    | 2610 | C    |
| 25  | DA    | 2611 | U    |
| 25  | DA    | 2612 | C    |
| 25  | DA    | 2621 | A    |
| 25  | DA    | 2629 | A    |
| 25  | DA    | 2630 | G    |
| 25  | DA    | 2636 | U    |
| 25  | DA    | 2638 | G    |
| 25  | DA    | 2639 | A    |
| 25  | DA    | 2641 | G    |
| 25  | DA    | 2645 | G    |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 25  | DA    | 2646    | C    |
| 25  | DA    | 2654    | A    |
| 25  | DA    | 2655    | G    |
| 25  | DA    | 2669    | G    |
| 25  | DA    | 2673    | G    |
| 25  | DA    | 2681    | C    |
| 25  | DA    | 2682    | U    |
| 25  | DA    | 2690    | C    |
| 25  | DA    | 2691    | C    |
| 25  | DA    | 2701    | C    |
| 25  | DA    | 2702    | U    |
| 25  | DA    | 2703    | C    |
| 25  | DA    | 2707    | G    |
| 25  | DA    | 2712    | U    |
| 25  | DA    | 2712(A) | A    |
| 25  | DA    | 2713    | A    |
| 25  | DA    | 2714    | G    |
| 25  | DA    | 2720    | U    |
| 25  | DA    | 2721    | A    |
| 25  | DA    | 2726    | U    |
| 25  | DA    | 2732    | G    |
| 25  | DA    | 2733    | A    |
| 25  | DA    | 2744    | G    |
| 25  | DA    | 2748    | A    |
| 25  | DA    | 2750    | A    |
| 25  | DA    | 2751    | G    |
| 25  | DA    | 2752    | C    |
| 25  | DA    | 2754    | U    |
| 25  | DA    | 2756    | U    |
| 25  | DA    | 2757    | A    |
| 25  | DA    | 2758    | A    |
| 25  | DA    | 2762    | G    |
| 25  | DA    | 2764    | A    |
| 25  | DA    | 2765    | A    |
| 25  | DA    | 2776    | A    |
| 25  | DA    | 2777    | G    |
| 25  | DA    | 2778    | A    |
| 25  | DA    | 2779    | U    |
| 25  | DA    | 2780    | G    |
| 25  | DA    | 2781    | A    |
| 25  | DA    | 2789    | C    |
| 25  | DA    | 2790    | A    |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 25  | DA    | 2791    | C    |
| 25  | DA    | 2792    | G    |
| 25  | DA    | 2799    | C    |
| 25  | DA    | 2801    | A    |
| 25  | DA    | 2801(A) | A    |
| 25  | DA    | 2802    | G    |
| 25  | DA    | 2803    | C    |
| 25  | DA    | 2804    | C    |
| 25  | DA    | 2807    | G    |
| 25  | DA    | 2808    | U    |
| 25  | DA    | 2820    | A    |
| 25  | DA    | 2823    | A    |
| 25  | DA    | 2827    | C    |
| 25  | DA    | 2830    | G    |
| 25  | DA    | 2833    | G    |
| 25  | DA    | 2834    | G    |
| 25  | DA    | 2835    | A    |
| 25  | DA    | 2836    | U    |
| 25  | DA    | 2848    | G    |
| 25  | DA    | 2849    | U    |
| 25  | DA    | 2864    | G    |
| 25  | DA    | 2867    | G    |
| 25  | DA    | 2872    | G    |
| 25  | DA    | 2874    | C    |
| 25  | DA    | 2876    | G    |
| 25  | DA    | 2879    | C    |
| 25  | DA    | 2880    | C    |
| 25  | DA    | 2893    | G    |
| 26  | DB    | 2       | C    |
| 26  | DB    | 3       | C    |
| 26  | DB    | 8       | U    |
| 26  | DB    | 9       | G    |
| 26  | DB    | 12      | C    |
| 26  | DB    | 13      | A    |
| 26  | DB    | 14      | U    |
| 26  | DB    | 15      | A    |
| 26  | DB    | 25      | A    |
| 26  | DB    | 27      | C    |
| 26  | DB    | 31      | C    |
| 26  | DB    | 35      | U    |
| 26  | DB    | 40      | U    |
| 26  | DB    | 42      | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 26  | DB    | 45  | A    |
| 26  | DB    | 52  | A    |
| 26  | DB    | 53  | A    |
| 26  | DB    | 57  | A    |
| 26  | DB    | 67  | G    |
| 26  | DB    | 73  | A    |
| 26  | DB    | 89  | G    |
| 26  | DB    | 91  | C    |
| 26  | DB    | 109 | C    |
| 26  | DB    | 110 | G    |
| 26  | DB    | 116 | G    |

All (768) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AA    | 7   | G    |
| 1   | AA    | 30  | U    |
| 1   | AA    | 47  | C    |
| 1   | AA    | 48  | C    |
| 1   | AA    | 50  | A    |
| 1   | AA    | 51  | A    |
| 1   | AA    | 60  | A    |
| 1   | AA    | 79  | G    |
| 1   | AA    | 109 | A    |
| 1   | AA    | 115 | G    |
| 1   | AA    | 119 | A    |
| 1   | AA    | 121 | C    |
| 1   | AA    | 154 | C    |
| 1   | AA    | 173 | U    |
| 1   | AA    | 197 | A    |
| 1   | AA    | 204 | U    |
| 1   | AA    | 243 | A    |
| 1   | AA    | 244 | U    |
| 1   | AA    | 250 | A    |
| 1   | AA    | 251 | G    |
| 1   | AA    | 266 | G    |
| 1   | AA    | 274 | A    |
| 1   | AA    | 344 | A    |
| 1   | AA    | 345 | C    |
| 1   | AA    | 351 | G    |
| 1   | AA    | 366 | C    |
| 1   | AA    | 367 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AA    | 388 | G    |
| 1   | AA    | 412 | A    |
| 1   | AA    | 428 | G    |
| 1   | AA    | 429 | U    |
| 1   | AA    | 438 | G    |
| 1   | AA    | 451 | A    |
| 1   | AA    | 484 | G    |
| 1   | AA    | 485 | G    |
| 1   | AA    | 495 | A    |
| 1   | AA    | 496 | A    |
| 1   | AA    | 499 | A    |
| 1   | AA    | 508 | C    |
| 1   | AA    | 509 | A    |
| 1   | AA    | 517 | G    |
| 1   | AA    | 518 | C    |
| 1   | AA    | 530 | G    |
| 1   | AA    | 531 | U    |
| 1   | AA    | 533 | A    |
| 1   | AA    | 535 | A    |
| 1   | AA    | 547 | A    |
| 1   | AA    | 559 | A    |
| 1   | AA    | 562 | C    |
| 1   | AA    | 566 | G    |
| 1   | AA    | 575 | G    |
| 1   | AA    | 576 | G    |
| 1   | AA    | 595 | G    |
| 1   | AA    | 687 | A    |
| 1   | AA    | 702 | A    |
| 1   | AA    | 703 | G    |
| 1   | AA    | 721 | G    |
| 1   | AA    | 733 | A    |
| 1   | AA    | 748 | C    |
| 1   | AA    | 817 | C    |
| 1   | AA    | 819 | A    |
| 1   | AA    | 820 | U    |
| 1   | AA    | 840 | C    |
| 1   | AA    | 871 | U    |
| 1   | AA    | 873 | A    |
| 1   | AA    | 889 | A    |
| 1   | AA    | 913 | A    |
| 1   | AA    | 934 | C    |
| 1   | AA    | 960 | U    |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 1   | AA    | 965     | A    |
| 1   | AA    | 968     | A    |
| 1   | AA    | 974     | A    |
| 1   | AA    | 991     | U    |
| 1   | AA    | 992     | U    |
| 1   | AA    | 1049    | U    |
| 1   | AA    | 1064    | G    |
| 1   | AA    | 1065    | U    |
| 1   | AA    | 1067    | A    |
| 1   | AA    | 1085    | U    |
| 1   | AA    | 1101    | A    |
| 1   | AA    | 1139    | G    |
| 1   | AA    | 1157    | A    |
| 1   | AA    | 1159    | U    |
| 1   | AA    | 1182    | G    |
| 1   | AA    | 1201    | A    |
| 1   | AA    | 1211    | U    |
| 1   | AA    | 1214    | C    |
| 1   | AA    | 1226    | C    |
| 1   | AA    | 1239    | A    |
| 1   | AA    | 1240    | U    |
| 1   | AA    | 1281    | U    |
| 1   | AA    | 1285    | A    |
| 1   | AA    | 1297    | C    |
| 1   | AA    | 1298    | C    |
| 1   | AA    | 1300    | G    |
| 1   | AA    | 1302    | U    |
| 1   | AA    | 1319    | A    |
| 1   | AA    | 1363(A) | A    |
| 1   | AA    | 1364    | U    |
| 1   | AA    | 1380    | U    |
| 1   | AA    | 1394    | A    |
| 1   | AA    | 1399    | C    |
| 1   | AA    | 1400    | C    |
| 1   | AA    | 1442(A) | G    |
| 1   | AA    | 1498    | U    |
| 1   | AA    | 1503    | A    |
| 1   | AA    | 1505    | G    |
| 1   | AA    | 1506    | U    |
| 1   | AA    | 1528    | U    |
| 22  | AV    | 18      | U    |
| 22  | AV    | 35      | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 22  | AV    | 53  | G    |
| 25  | BA    | 13  | A    |
| 25  | BA    | 27  | G    |
| 25  | BA    | 34  | C    |
| 25  | BA    | 49  | A    |
| 25  | BA    | 50  | U    |
| 25  | BA    | 51  | G    |
| 25  | BA    | 60  | G    |
| 25  | BA    | 63  | U    |
| 25  | BA    | 70  | G    |
| 25  | BA    | 71  | A    |
| 25  | BA    | 72  | U    |
| 25  | BA    | 74  | A    |
| 25  | BA    | 83  | G    |
| 25  | BA    | 84  | A    |
| 25  | BA    | 99  | U    |
| 25  | BA    | 119 | A    |
| 25  | BA    | 120 | U    |
| 25  | BA    | 125 | G    |
| 25  | BA    | 177 | G    |
| 25  | BA    | 215 | G    |
| 25  | BA    | 221 | A    |
| 25  | BA    | 222 | A    |
| 25  | BA    | 226 | G    |
| 25  | BA    | 227 | A    |
| 25  | BA    | 232 | G    |
| 25  | BA    | 241 | A    |
| 25  | BA    | 249 | C    |
| 25  | BA    | 265 | A    |
| 25  | BA    | 272 | G    |
| 25  | BA    | 283 | A    |
| 25  | BA    | 311 | A    |
| 25  | BA    | 322 | A    |
| 25  | BA    | 323 | G    |
| 25  | BA    | 329 | G    |
| 25  | BA    | 331 | A    |
| 25  | BA    | 332 | A    |
| 25  | BA    | 345 | A    |
| 25  | BA    | 370 | G    |
| 25  | BA    | 386 | G    |
| 25  | BA    | 387 | U    |
| 25  | BA    | 390 | A    |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 25  | BA    | 403    | U    |
| 25  | BA    | 404    | C    |
| 25  | BA    | 411    | G    |
| 25  | BA    | 434    | U    |
| 25  | BA    | 442    | G    |
| 25  | BA    | 446    | G    |
| 25  | BA    | 454    | A    |
| 25  | BA    | 455    | C    |
| 25  | BA    | 457    | A    |
| 25  | BA    | 474    | G    |
| 25  | BA    | 479    | A    |
| 25  | BA    | 481    | G    |
| 25  | BA    | 503    | A    |
| 25  | BA    | 506    | G    |
| 25  | BA    | 527    | C    |
| 25  | BA    | 531    | C    |
| 25  | BA    | 571    | A    |
| 25  | BA    | 573    | G    |
| 25  | BA    | 574    | C    |
| 25  | BA    | 587    | C    |
| 25  | BA    | 603    | A    |
| 25  | BA    | 614(C) | A    |
| 25  | BA    | 620    | G    |
| 25  | BA    | 627    | A    |
| 25  | BA    | 637    | A    |
| 25  | BA    | 685    | A    |
| 25  | BA    | 686    | G    |
| 25  | BA    | 728    | G    |
| 25  | BA    | 739    | G    |
| 25  | BA    | 752    | A    |
| 25  | BA    | 762    | U    |
| 25  | BA    | 764    | A    |
| 25  | BA    | 775    | G    |
| 25  | BA    | 776    | G    |
| 25  | BA    | 788    | A    |
| 25  | BA    | 789    | A    |
| 25  | BA    | 790    | C    |
| 25  | BA    | 791    | C    |
| 25  | BA    | 792    | G    |
| 25  | BA    | 793    | A    |
| 25  | BA    | 800    | A    |
| 25  | BA    | 801    | G    |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 25  | BA    | 830     | G    |
| 25  | BA    | 846     | C    |
| 25  | BA    | 856     | C    |
| 25  | BA    | 858     | U    |
| 25  | BA    | 859     | G    |
| 25  | BA    | 865     | C    |
| 25  | BA    | 913     | U    |
| 25  | BA    | 930     | U    |
| 25  | BA    | 932     | G    |
| 25  | BA    | 945     | A    |
| 25  | BA    | 961     | C    |
| 25  | BA    | 973     | A    |
| 25  | BA    | 975     | C    |
| 25  | BA    | 1008    | C    |
| 25  | BA    | 1020    | A    |
| 25  | BA    | 1022    | G    |
| 25  | BA    | 1025    | G    |
| 25  | BA    | 1051    | G    |
| 25  | BA    | 1126    | A    |
| 25  | BA    | 1128    | A    |
| 25  | BA    | 1130    | U    |
| 25  | BA    | 1142(A) | A    |
| 25  | BA    | 1143    | A    |
| 25  | BA    | 1156    | A    |
| 25  | BA    | 1175    | U    |
| 25  | BA    | 1204    | A    |
| 25  | BA    | 1205    | U    |
| 25  | BA    | 1210    | A    |
| 25  | BA    | 1211    | U    |
| 25  | BA    | 1220    | A    |
| 25  | BA    | 1236    | G    |
| 25  | BA    | 1237    | A    |
| 25  | BA    | 1247    | A    |
| 25  | BA    | 1248    | G    |
| 25  | BA    | 1253    | A    |
| 25  | BA    | 1265    | A    |
| 25  | BA    | 1275    | A    |
| 25  | BA    | 1300    | U    |
| 25  | BA    | 1301    | A    |
| 25  | BA    | 1302    | A    |
| 25  | BA    | 1311    | G    |
| 25  | BA    | 1312    | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 25  | BA    | 1320 | C    |
| 25  | BA    | 1324 | G    |
| 25  | BA    | 1329 | U    |
| 25  | BA    | 1332 | G    |
| 25  | BA    | 1340 | U    |
| 25  | BA    | 1344 | G    |
| 25  | BA    | 1359 | A    |
| 25  | BA    | 1379 | A    |
| 25  | BA    | 1385 | G    |
| 25  | BA    | 1396 | U    |
| 25  | BA    | 1427 | A    |
| 25  | BA    | 1428 | C    |
| 25  | BA    | 1445 | A    |
| 25  | BA    | 1451 | C    |
| 25  | BA    | 1452 | A    |
| 25  | BA    | 1453 | U    |
| 25  | BA    | 1458 | C    |
| 25  | BA    | 1504 | C    |
| 25  | BA    | 1554 | A    |
| 25  | BA    | 1558 | A    |
| 25  | BA    | 1566 | A    |
| 25  | BA    | 1607 | C    |
| 25  | BA    | 1608 | A    |
| 25  | BA    | 1610 | A    |
| 25  | BA    | 1616 | A    |
| 25  | BA    | 1617 | C    |
| 25  | BA    | 1618 | A    |
| 25  | BA    | 1634 | A    |
| 25  | BA    | 1646 | C    |
| 25  | BA    | 1647 | G    |
| 25  | BA    | 1653 | G    |
| 25  | BA    | 1668 | A    |
| 25  | BA    | 1681 | G    |
| 25  | BA    | 1694 | C    |
| 25  | BA    | 1706 | U    |
| 25  | BA    | 1740 | G    |
| 25  | BA    | 1758 | G    |
| 25  | BA    | 1762 | A    |
| 25  | BA    | 1784 | A    |
| 25  | BA    | 1786 | A    |
| 25  | BA    | 1799 | G    |
| 25  | BA    | 1800 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 25  | BA    | 1801 | G    |
| 25  | BA    | 1815 | A    |
| 25  | BA    | 1819 | A    |
| 25  | BA    | 1820 | U    |
| 25  | BA    | 1847 | A    |
| 25  | BA    | 1913 | A    |
| 25  | BA    | 1929 | G    |
| 25  | BA    | 1930 | G    |
| 25  | BA    | 1936 | A    |
| 25  | BA    | 1939 | U    |
| 25  | BA    | 1940 | U    |
| 25  | BA    | 1943 | U    |
| 25  | BA    | 1944 | U    |
| 25  | BA    | 1955 | U    |
| 25  | BA    | 1962 | C    |
| 25  | BA    | 1963 | U    |
| 25  | BA    | 1964 | G    |
| 25  | BA    | 1966 | A    |
| 25  | BA    | 1970 | A    |
| 25  | BA    | 1980 | G    |
| 25  | BA    | 1992 | G    |
| 25  | BA    | 1996 | C    |
| 25  | BA    | 2021 | C    |
| 25  | BA    | 2031 | A    |
| 25  | BA    | 2032 | G    |
| 25  | BA    | 2033 | A    |
| 25  | BA    | 2035 | G    |
| 25  | BA    | 2051 | A    |
| 25  | BA    | 2067 | G    |
| 25  | BA    | 2092 | U    |
| 25  | BA    | 2110 | G    |
| 25  | BA    | 2111 | C    |
| 25  | BA    | 2116 | G    |
| 25  | BA    | 2126 | A    |
| 25  | BA    | 2145 | C    |
| 25  | BA    | 2146 | C    |
| 25  | BA    | 2158 | A    |
| 25  | BA    | 2171 | A    |
| 25  | BA    | 2172 | U    |
| 25  | BA    | 2198 | A    |
| 25  | BA    | 2225 | A    |
| 25  | BA    | 2238 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 25  | BA    | 2249 | U    |
| 25  | BA    | 2258 | C    |
| 25  | BA    | 2266 | A    |
| 25  | BA    | 2282 | G    |
| 25  | BA    | 2296 | U    |
| 25  | BA    | 2311 | A    |
| 25  | BA    | 2318 | G    |
| 25  | BA    | 2334 | G    |
| 25  | BA    | 2336 | A    |
| 25  | BA    | 2344 | U    |
| 25  | BA    | 2405 | G    |
| 25  | BA    | 2406 | U    |
| 25  | BA    | 2422 | A    |
| 25  | BA    | 2423 | U    |
| 25  | BA    | 2425 | A    |
| 25  | BA    | 2426 | A    |
| 25  | BA    | 2447 | G    |
| 25  | BA    | 2448 | A    |
| 25  | BA    | 2449 | U    |
| 25  | BA    | 2481 | G    |
| 25  | BA    | 2490 | G    |
| 25  | BA    | 2497 | A    |
| 25  | BA    | 2503 | A    |
| 25  | BA    | 2519 | U    |
| 25  | BA    | 2581 | G    |
| 25  | BA    | 2585 | U    |
| 25  | BA    | 2602 | A    |
| 25  | BA    | 2609 | U    |
| 25  | BA    | 2610 | C    |
| 25  | BA    | 2613 | U    |
| 25  | BA    | 2614 | A    |
| 25  | BA    | 2654 | A    |
| 25  | BA    | 2689 | U    |
| 25  | BA    | 2702 | U    |
| 25  | BA    | 2712 | U    |
| 25  | BA    | 2732 | G    |
| 25  | BA    | 2750 | A    |
| 25  | BA    | 2751 | G    |
| 25  | BA    | 2756 | U    |
| 25  | BA    | 2776 | A    |
| 25  | BA    | 2778 | A    |
| 25  | BA    | 2779 | U    |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 25  | BA    | 2780    | G    |
| 25  | BA    | 2791    | C    |
| 25  | BA    | 2801    | A    |
| 25  | BA    | 2801(A) | A    |
| 25  | BA    | 2835    | A    |
| 25  | BA    | 2848    | G    |
| 25  | BA    | 2849    | U    |
| 25  | BA    | 2866    | U    |
| 25  | BA    | 2873    | A    |
| 26  | BB    | 14      | U    |
| 26  | BB    | 15      | A    |
| 26  | BB    | 34      | U    |
| 26  | BB    | 56      | G    |
| 26  | BB    | 66      | A    |
| 1   | CA    | 8       | A    |
| 1   | CA    | 13      | U    |
| 1   | CA    | 30      | U    |
| 1   | CA    | 47      | C    |
| 1   | CA    | 48      | C    |
| 1   | CA    | 50      | A    |
| 1   | CA    | 51      | A    |
| 1   | CA    | 60      | A    |
| 1   | CA    | 79      | G    |
| 1   | CA    | 109     | A    |
| 1   | CA    | 115     | G    |
| 1   | CA    | 119     | A    |
| 1   | CA    | 121     | C    |
| 1   | CA    | 129(A)  | G    |
| 1   | CA    | 173     | U    |
| 1   | CA    | 181     | G    |
| 1   | CA    | 197     | A    |
| 1   | CA    | 204     | U    |
| 1   | CA    | 243     | A    |
| 1   | CA    | 244     | U    |
| 1   | CA    | 246     | A    |
| 1   | CA    | 250     | A    |
| 1   | CA    | 251     | G    |
| 1   | CA    | 266     | G    |
| 1   | CA    | 274     | A    |
| 1   | CA    | 279     | A    |
| 1   | CA    | 327     | A    |
| 1   | CA    | 328     | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | CA    | 329 | A    |
| 1   | CA    | 344 | A    |
| 1   | CA    | 345 | C    |
| 1   | CA    | 351 | G    |
| 1   | CA    | 372 | C    |
| 1   | CA    | 388 | G    |
| 1   | CA    | 412 | A    |
| 1   | CA    | 428 | G    |
| 1   | CA    | 429 | U    |
| 1   | CA    | 451 | A    |
| 1   | CA    | 481 | G    |
| 1   | CA    | 484 | G    |
| 1   | CA    | 495 | A    |
| 1   | CA    | 496 | A    |
| 1   | CA    | 499 | A    |
| 1   | CA    | 508 | C    |
| 1   | CA    | 509 | A    |
| 1   | CA    | 517 | G    |
| 1   | CA    | 518 | C    |
| 1   | CA    | 533 | A    |
| 1   | CA    | 535 | A    |
| 1   | CA    | 547 | A    |
| 1   | CA    | 559 | A    |
| 1   | CA    | 562 | C    |
| 1   | CA    | 575 | G    |
| 1   | CA    | 576 | G    |
| 1   | CA    | 595 | G    |
| 1   | CA    | 641 | U    |
| 1   | CA    | 687 | A    |
| 1   | CA    | 702 | A    |
| 1   | CA    | 721 | G    |
| 1   | CA    | 733 | A    |
| 1   | CA    | 748 | C    |
| 1   | CA    | 753 | A    |
| 1   | CA    | 792 | A    |
| 1   | CA    | 812 | C    |
| 1   | CA    | 815 | A    |
| 1   | CA    | 817 | C    |
| 1   | CA    | 819 | A    |
| 1   | CA    | 820 | U    |
| 1   | CA    | 840 | C    |
| 1   | CA    | 871 | U    |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 1   | CA    | 873     | A    |
| 1   | CA    | 889     | A    |
| 1   | CA    | 913     | A    |
| 1   | CA    | 934     | C    |
| 1   | CA    | 960     | U    |
| 1   | CA    | 965     | A    |
| 1   | CA    | 968     | A    |
| 1   | CA    | 974     | A    |
| 1   | CA    | 976     | G    |
| 1   | CA    | 982     | U    |
| 1   | CA    | 992     | U    |
| 1   | CA    | 1049    | U    |
| 1   | CA    | 1064    | G    |
| 1   | CA    | 1065    | U    |
| 1   | CA    | 1067    | A    |
| 1   | CA    | 1085    | U    |
| 1   | CA    | 1101    | A    |
| 1   | CA    | 1139    | G    |
| 1   | CA    | 1157    | A    |
| 1   | CA    | 1182    | G    |
| 1   | CA    | 1201    | A    |
| 1   | CA    | 1211    | U    |
| 1   | CA    | 1214    | C    |
| 1   | CA    | 1224    | G    |
| 1   | CA    | 1226    | C    |
| 1   | CA    | 1239    | A    |
| 1   | CA    | 1240    | U    |
| 1   | CA    | 1285    | A    |
| 1   | CA    | 1298    | C    |
| 1   | CA    | 1302    | U    |
| 1   | CA    | 1319    | A    |
| 1   | CA    | 1363(A) | A    |
| 1   | CA    | 1380    | U    |
| 1   | CA    | 1394    | A    |
| 1   | CA    | 1396    | A    |
| 1   | CA    | 1397    | C    |
| 1   | CA    | 1399    | C    |
| 1   | CA    | 1400    | C    |
| 1   | CA    | 1442(B) | A    |
| 1   | CA    | 1498    | U    |
| 1   | CA    | 1502    | A    |
| 1   | CA    | 1504    | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | CA    | 1506 | U    |
| 1   | CA    | 1528 | U    |
| 1   | CA    | 1529 | G    |
| 22  | CV    | 18   | U    |
| 22  | CV    | 21   | U    |
| 22  | CV    | 35   | C    |
| 22  | CV    | 53   | G    |
| 24  | CX    | 14   | A    |
| 25  | DA    | 33   | U    |
| 25  | DA    | 49   | A    |
| 25  | DA    | 50   | U    |
| 25  | DA    | 51   | G    |
| 25  | DA    | 60   | G    |
| 25  | DA    | 70   | G    |
| 25  | DA    | 71   | A    |
| 25  | DA    | 72   | U    |
| 25  | DA    | 74   | A    |
| 25  | DA    | 90   | U    |
| 25  | DA    | 119  | A    |
| 25  | DA    | 120  | U    |
| 25  | DA    | 125  | G    |
| 25  | DA    | 177  | G    |
| 25  | DA    | 196  | A    |
| 25  | DA    | 199  | A    |
| 25  | DA    | 204  | A    |
| 25  | DA    | 215  | G    |
| 25  | DA    | 221  | A    |
| 25  | DA    | 222  | A    |
| 25  | DA    | 226  | G    |
| 25  | DA    | 227  | A    |
| 25  | DA    | 232  | G    |
| 25  | DA    | 241  | A    |
| 25  | DA    | 283  | A    |
| 25  | DA    | 297  | C    |
| 25  | DA    | 311  | A    |
| 25  | DA    | 321  | G    |
| 25  | DA    | 322  | A    |
| 25  | DA    | 323  | G    |
| 25  | DA    | 329  | G    |
| 25  | DA    | 331  | A    |
| 25  | DA    | 332  | A    |
| 25  | DA    | 345  | A    |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 25  | DA    | 370    | G    |
| 25  | DA    | 386    | G    |
| 25  | DA    | 387    | U    |
| 25  | DA    | 390    | A    |
| 25  | DA    | 395    | U    |
| 25  | DA    | 403    | U    |
| 25  | DA    | 404    | C    |
| 25  | DA    | 411    | G    |
| 25  | DA    | 434    | U    |
| 25  | DA    | 442    | G    |
| 25  | DA    | 446    | G    |
| 25  | DA    | 454    | A    |
| 25  | DA    | 455    | C    |
| 25  | DA    | 474    | G    |
| 25  | DA    | 479    | A    |
| 25  | DA    | 481    | G    |
| 25  | DA    | 503    | A    |
| 25  | DA    | 506    | G    |
| 25  | DA    | 527    | C    |
| 25  | DA    | 528    | A    |
| 25  | DA    | 531    | C    |
| 25  | DA    | 532    | A    |
| 25  | DA    | 555    | U    |
| 25  | DA    | 571    | A    |
| 25  | DA    | 573    | G    |
| 25  | DA    | 574    | C    |
| 25  | DA    | 587    | C    |
| 25  | DA    | 603    | A    |
| 25  | DA    | 614(A) | U    |
| 25  | DA    | 614(C) | A    |
| 25  | DA    | 620    | G    |
| 25  | DA    | 627    | A    |
| 25  | DA    | 637    | A    |
| 25  | DA    | 670    | A    |
| 25  | DA    | 685    | A    |
| 25  | DA    | 686    | G    |
| 25  | DA    | 728    | G    |
| 25  | DA    | 739    | G    |
| 25  | DA    | 752    | A    |
| 25  | DA    | 762    | U    |
| 25  | DA    | 764    | A    |
| 25  | DA    | 775    | G    |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 25  | DA    | 776     | G    |
| 25  | DA    | 788     | A    |
| 25  | DA    | 789     | A    |
| 25  | DA    | 790     | C    |
| 25  | DA    | 791     | C    |
| 25  | DA    | 792     | G    |
| 25  | DA    | 793     | A    |
| 25  | DA    | 800     | A    |
| 25  | DA    | 801     | G    |
| 25  | DA    | 805     | G    |
| 25  | DA    | 811     | U    |
| 25  | DA    | 829     | A    |
| 25  | DA    | 830     | G    |
| 25  | DA    | 845     | G    |
| 25  | DA    | 846     | C    |
| 25  | DA    | 856     | C    |
| 25  | DA    | 858     | U    |
| 25  | DA    | 865     | C    |
| 25  | DA    | 913     | U    |
| 25  | DA    | 930     | U    |
| 25  | DA    | 932     | G    |
| 25  | DA    | 957     | A    |
| 25  | DA    | 961     | C    |
| 25  | DA    | 973     | A    |
| 25  | DA    | 1008    | C    |
| 25  | DA    | 1011    | G    |
| 25  | DA    | 1020    | A    |
| 25  | DA    | 1022    | G    |
| 25  | DA    | 1025    | G    |
| 25  | DA    | 1126    | A    |
| 25  | DA    | 1130    | U    |
| 25  | DA    | 1131    | G    |
| 25  | DA    | 1142(A) | A    |
| 25  | DA    | 1143    | A    |
| 25  | DA    | 1156    | A    |
| 25  | DA    | 1175    | U    |
| 25  | DA    | 1205    | U    |
| 25  | DA    | 1210    | A    |
| 25  | DA    | 1211    | U    |
| 25  | DA    | 1236    | G    |
| 25  | DA    | 1237    | A    |
| 25  | DA    | 1247    | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 25  | DA    | 1248 | G    |
| 25  | DA    | 1250 | G    |
| 25  | DA    | 1251 | C    |
| 25  | DA    | 1252 | G    |
| 25  | DA    | 1253 | A    |
| 25  | DA    | 1265 | A    |
| 25  | DA    | 1272 | A    |
| 25  | DA    | 1275 | A    |
| 25  | DA    | 1288 | U    |
| 25  | DA    | 1300 | U    |
| 25  | DA    | 1301 | A    |
| 25  | DA    | 1302 | A    |
| 25  | DA    | 1311 | G    |
| 25  | DA    | 1312 | U    |
| 25  | DA    | 1320 | C    |
| 25  | DA    | 1324 | G    |
| 25  | DA    | 1329 | U    |
| 25  | DA    | 1340 | U    |
| 25  | DA    | 1344 | G    |
| 25  | DA    | 1359 | A    |
| 25  | DA    | 1378 | A    |
| 25  | DA    | 1385 | G    |
| 25  | DA    | 1396 | U    |
| 25  | DA    | 1428 | C    |
| 25  | DA    | 1445 | A    |
| 25  | DA    | 1453 | U    |
| 25  | DA    | 1458 | C    |
| 25  | DA    | 1493 | C    |
| 25  | DA    | 1542 | A    |
| 25  | DA    | 1554 | A    |
| 25  | DA    | 1558 | A    |
| 25  | DA    | 1559 | G    |
| 25  | DA    | 1566 | A    |
| 25  | DA    | 1567 | A    |
| 25  | DA    | 1602 | U    |
| 25  | DA    | 1607 | C    |
| 25  | DA    | 1608 | A    |
| 25  | DA    | 1610 | A    |
| 25  | DA    | 1634 | A    |
| 25  | DA    | 1653 | G    |
| 25  | DA    | 1668 | A    |
| 25  | DA    | 1674 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 25  | DA    | 1681 | G    |
| 25  | DA    | 1693 | U    |
| 25  | DA    | 1699 | G    |
| 25  | DA    | 1706 | U    |
| 25  | DA    | 1740 | G    |
| 25  | DA    | 1758 | G    |
| 25  | DA    | 1762 | A    |
| 25  | DA    | 1780 | A    |
| 25  | DA    | 1784 | A    |
| 25  | DA    | 1786 | A    |
| 25  | DA    | 1799 | G    |
| 25  | DA    | 1801 | G    |
| 25  | DA    | 1815 | A    |
| 25  | DA    | 1819 | A    |
| 25  | DA    | 1820 | U    |
| 25  | DA    | 1828 | G    |
| 25  | DA    | 1913 | A    |
| 25  | DA    | 1918 | A    |
| 25  | DA    | 1929 | G    |
| 25  | DA    | 1936 | A    |
| 25  | DA    | 1939 | U    |
| 25  | DA    | 1940 | U    |
| 25  | DA    | 1943 | U    |
| 25  | DA    | 1944 | U    |
| 25  | DA    | 1954 | G    |
| 25  | DA    | 1955 | U    |
| 25  | DA    | 1962 | C    |
| 25  | DA    | 1963 | U    |
| 25  | DA    | 1970 | A    |
| 25  | DA    | 1980 | G    |
| 25  | DA    | 1996 | C    |
| 25  | DA    | 2021 | C    |
| 25  | DA    | 2022 | U    |
| 25  | DA    | 2031 | A    |
| 25  | DA    | 2032 | G    |
| 25  | DA    | 2033 | A    |
| 25  | DA    | 2035 | G    |
| 25  | DA    | 2051 | A    |
| 25  | DA    | 2067 | G    |
| 25  | DA    | 2092 | U    |
| 25  | DA    | 2110 | G    |
| 25  | DA    | 2111 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 25  | DA    | 2116 | G    |
| 25  | DA    | 2119 | A    |
| 25  | DA    | 2126 | A    |
| 25  | DA    | 2145 | C    |
| 25  | DA    | 2146 | C    |
| 25  | DA    | 2158 | A    |
| 25  | DA    | 2171 | A    |
| 25  | DA    | 2172 | U    |
| 25  | DA    | 2198 | A    |
| 25  | DA    | 2225 | A    |
| 25  | DA    | 2238 | G    |
| 25  | DA    | 2249 | U    |
| 25  | DA    | 2250 | G    |
| 25  | DA    | 2258 | C    |
| 25  | DA    | 2266 | A    |
| 25  | DA    | 2275 | C    |
| 25  | DA    | 2282 | G    |
| 25  | DA    | 2286 | A    |
| 25  | DA    | 2287 | A    |
| 25  | DA    | 2288 | A    |
| 25  | DA    | 2296 | U    |
| 25  | DA    | 2308 | G    |
| 25  | DA    | 2318 | G    |
| 25  | DA    | 2319 | G    |
| 25  | DA    | 2334 | G    |
| 25  | DA    | 2336 | A    |
| 25  | DA    | 2344 | U    |
| 25  | DA    | 2345 | G    |
| 25  | DA    | 2384 | G    |
| 25  | DA    | 2406 | U    |
| 25  | DA    | 2422 | A    |
| 25  | DA    | 2423 | U    |
| 25  | DA    | 2425 | A    |
| 25  | DA    | 2447 | G    |
| 25  | DA    | 2448 | A    |
| 25  | DA    | 2449 | U    |
| 25  | DA    | 2481 | G    |
| 25  | DA    | 2490 | G    |
| 25  | DA    | 2497 | A    |
| 25  | DA    | 2519 | U    |
| 25  | DA    | 2581 | G    |
| 25  | DA    | 2609 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 25  | DA    | 2610 | C    |
| 25  | DA    | 2638 | G    |
| 25  | DA    | 2654 | A    |
| 25  | DA    | 2668 | G    |
| 25  | DA    | 2681 | C    |
| 25  | DA    | 2689 | U    |
| 25  | DA    | 2732 | G    |
| 25  | DA    | 2750 | A    |
| 25  | DA    | 2751 | G    |
| 25  | DA    | 2756 | U    |
| 25  | DA    | 2776 | A    |
| 25  | DA    | 2778 | A    |
| 25  | DA    | 2779 | U    |
| 25  | DA    | 2780 | G    |
| 25  | DA    | 2791 | C    |
| 25  | DA    | 2801 | A    |
| 25  | DA    | 2835 | A    |
| 25  | DA    | 2866 | U    |
| 25  | DA    | 2873 | A    |
| 25  | DA    | 2879 | C    |
| 26  | DB    | 12   | C    |
| 26  | DB    | 14   | U    |
| 26  | DB    | 15   | A    |
| 26  | DB    | 34   | U    |
| 26  | DB    | 56   | G    |
| 26  | DB    | 66   | A    |
| 26  | DB    | 88   | C    |

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 1039 ligands modelled in this entry, 1037 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$ |
| 58  | PAR  | AA    | 7111 | -    | 44,45,45     | 1.44 | 7 (15%)     | 63,67,67    | 1.18 | 4 (6%)      |
| 58  | PAR  | CA    | 1741 | -    | 44,45,45     | 1.44 | 7 (15%)     | 63,67,67    | 1.18 | 5 (7%)      |

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   |
|-----|------|-------|------|------|---------|------------|---------|
| 58  | PAR  | AA    | 7111 | -    | -       | 2/18/94/94 | 0/4/4/4 |
| 58  | PAR  | CA    | 1741 | -    | -       | 2/18/94/94 | 0/4/4/4 |

All (14) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 58  | AA    | 7111 | PAR  | O54-C14 | 3.89 | 1.51        | 1.41     |
| 58  | CA    | 1741 | PAR  | O54-C14 | 3.87 | 1.51        | 1.41     |
| 58  | CA    | 1741 | PAR  | C31-C21 | 3.20 | 1.57        | 1.53     |
| 58  | AA    | 7111 | PAR  | C31-C21 | 3.15 | 1.57        | 1.53     |
| 58  | AA    | 7111 | PAR  | C24-N24 | 2.87 | 1.51        | 1.47     |
| 58  | CA    | 1741 | PAR  | C24-N24 | 2.80 | 1.51        | 1.47     |
| 58  | CA    | 1741 | PAR  | O51-C11 | 2.64 | 1.48        | 1.41     |
| 58  | AA    | 7111 | PAR  | O51-C11 | 2.63 | 1.48        | 1.41     |
| 58  | CA    | 1741 | PAR  | C23-C33 | 2.44 | 1.58        | 1.53     |
| 58  | AA    | 7111 | PAR  | C23-C33 | 2.41 | 1.58        | 1.53     |
| 58  | AA    | 7111 | PAR  | O43-C13 | 2.24 | 1.45        | 1.41     |
| 58  | CA    | 1741 | PAR  | O43-C13 | 2.11 | 1.45        | 1.41     |
| 58  | AA    | 7111 | PAR  | O54-C54 | 2.08 | 1.49        | 1.44     |
| 58  | CA    | 1741 | PAR  | O54-C54 | 2.07 | 1.49        | 1.44     |

All (9) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|------|-------------|----------|
| 58  | AA    | 7111 | PAR  | O33-C14-C24 | 3.61 | 113.99      | 108.08   |
| 58  | CA    | 1741 | PAR  | O33-C14-C24 | 3.57 | 113.91      | 108.08   |
| 58  | CA    | 1741 | PAR  | C14-O54-C54 | 3.22 | 120.01      | 113.72   |
| 58  | AA    | 7111 | PAR  | C14-O54-C54 | 3.22 | 120.01      | 113.72   |
| 58  | AA    | 7111 | PAR  | O54-C54-C64 | 3.09 | 112.00      | 106.07   |
| 58  | CA    | 1741 | PAR  | O54-C54-C64 | 3.08 | 111.99      | 106.07   |
| 58  | CA    | 1741 | PAR  | O23-C23-C33 | 2.41 | 117.93      | 111.19   |
| 58  | AA    | 7111 | PAR  | O23-C23-C33 | 2.39 | 117.88      | 111.19   |
| 58  | CA    | 1741 | PAR  | C11-O51-C51 | 2.05 | 117.72      | 113.72   |

There are no chirality outliers.

All (4) torsion outliers are listed below:

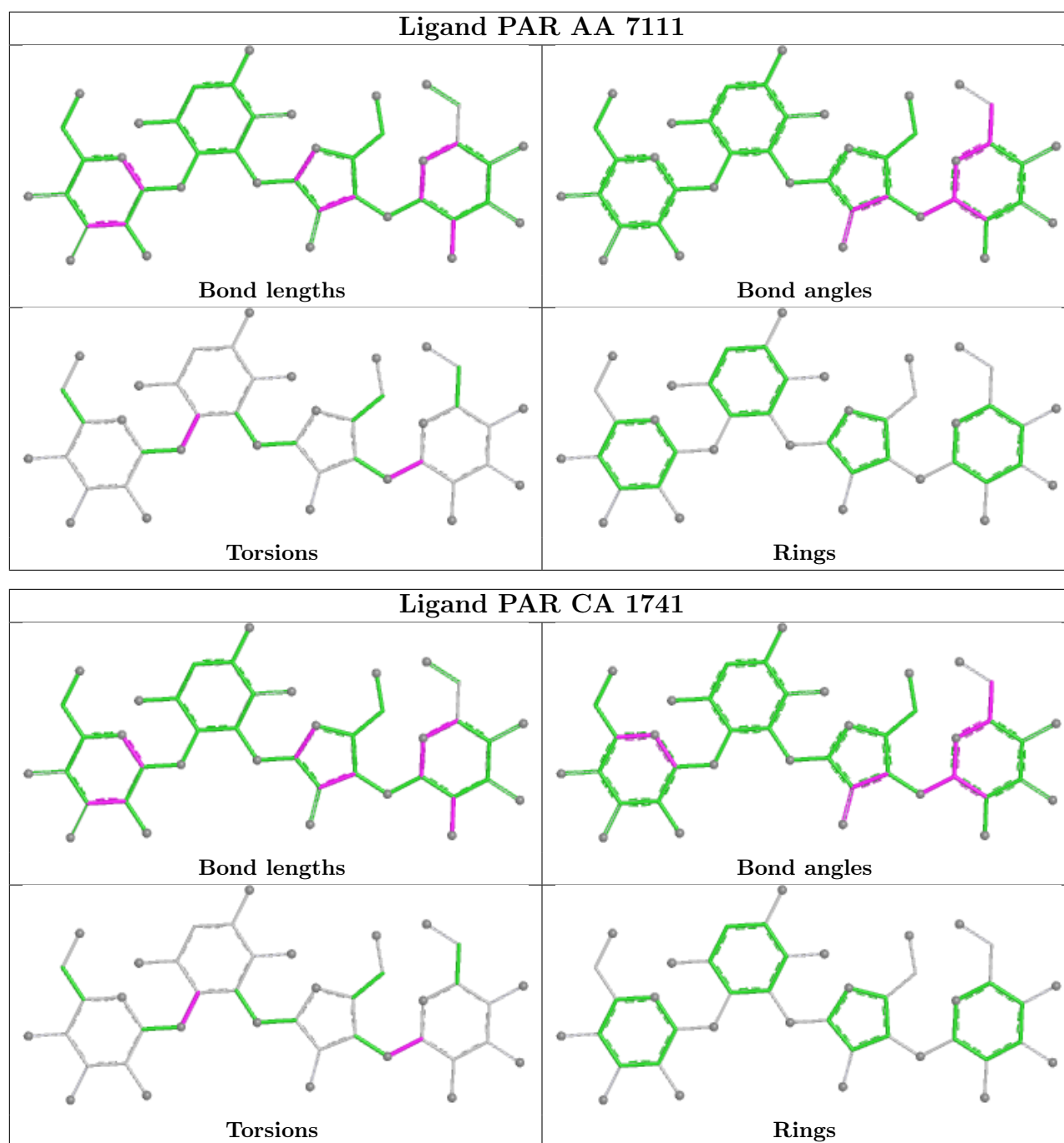
| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 58  | AA    | 7111 | PAR  | C24-C14-O33-C33 |
| 58  | CA    | 1741 | PAR  | C24-C14-O33-C33 |
| 58  | AA    | 7111 | PAR  | C52-C42-O11-C11 |
| 58  | CA    | 1741 | PAR  | C52-C42-O11-C11 |

There are no ring outliers.

2 monomers are involved in 5 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 58  | AA    | 7111 | PAR  | 3       | 0            |
| 58  | CA    | 1741 | PAR  | 2       | 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](#)

The following chains have linkage breaks:



| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 25  | BA    | 1                |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | BA    | 1453:U    | O3'    | 1455:G    | P      | 1.97         |

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ > 2 |     |     | OWAB(Å <sup>2</sup> ) | Q < 0.9 |
|-----|-------|-----------------|--------|-----------|-----|-----|-----------------------|---------|
| 1   | AA    | 1504/1522 (98%) | 0.29   | 72 (4%)   | 35  | 19  | 31, 78, 168, 331      | 0       |
| 1   | CA    | 1504/1522 (98%) | 0.30   | 69 (4%)   | 37  | 19  | 24, 68, 165, 363      | 0       |
| 2   | AB    | 235/256 (91%)   | 0.24   | 6 (2%)    | 57  | 32  | 67, 121, 201, 279     | 0       |
| 2   | CB    | 235/256 (91%)   | 0.22   | 5 (2%)    | 63  | 36  | 44, 109, 202, 287     | 0       |
| 3   | AC    | 207/239 (86%)   | 0.05   | 2 (0%)    | 79  | 54  | 44, 104, 173, 240     | 0       |
| 3   | CC    | 207/239 (86%)   | -0.03  | 2 (0%)    | 79  | 54  | 38, 90, 151, 227      | 0       |
| 4   | AD    | 208/209 (99%)   | 0.31   | 9 (4%)    | 40  | 21  | 37, 89, 153, 217      | 0       |
| 4   | CD    | 208/209 (99%)   | 0.23   | 13 (6%)   | 26  | 16  | 30, 77, 129, 209      | 0       |
| 5   | AE    | 151/162 (93%)   | 0.23   | 6 (3%)    | 42  | 23  | 44, 87, 151, 240      | 0       |
| 5   | CE    | 151/162 (93%)   | 0.18   | 7 (4%)    | 37  | 19  | 22, 71, 131, 266      | 0       |
| 6   | AF    | 101/101 (100%)  | -0.12  | 0         | 100 | 100 | 29, 74, 120, 178      | 0       |
| 6   | CF    | 101/101 (100%)  | 0.01   | 0         | 100 | 100 | 25, 68, 134, 192      | 0       |
| 7   | AG    | 155/156 (99%)   | 0.12   | 7 (4%)    | 38  | 20  | 50, 93, 149, 256      | 0       |
| 7   | CG    | 155/156 (99%)   | 0.14   | 8 (5%)    | 33  | 18  | 32, 87, 151, 269      | 0       |
| 8   | AH    | 138/138 (100%)  | -0.03  | 2 (1%)    | 73  | 46  | 41, 85, 129, 183      | 0       |
| 8   | CH    | 138/138 (100%)  | -0.02  | 2 (1%)    | 73  | 46  | 38, 75, 123, 181      | 0       |
| 9   | AI    | 127/128 (99%)   | 0.31   | 2 (1%)    | 70  | 43  | 55, 113, 161, 319     | 0       |
| 9   | CI    | 127/128 (99%)   | 0.46   | 6 (4%)    | 36  | 19  | 45, 97, 170, 245      | 0       |
| 10  | AJ    | 99/105 (94%)    | 0.54   | 5 (5%)    | 33  | 19  | 58, 124, 197, 302     | 0       |
| 10  | CJ    | 99/105 (94%)    | 0.71   | 9 (9%)    | 15  | 9   | 38, 115, 191, 204     | 0       |
| 11  | AK    | 119/129 (92%)   | 0.25   | 7 (5%)    | 28  | 16  | 41, 77, 147, 249      | 0       |
| 11  | CK    | 119/129 (92%)   | 0.11   | 5 (4%)    | 40  | 21  | 29, 73, 139, 188      | 0       |
| 12  | AL    | 125/132 (94%)   | 0.25   | 4 (3%)    | 50  | 28  | 31, 64, 129, 300      | 0       |
| 12  | CL    | 125/132 (94%)   | 0.16   | 6 (4%)    | 35  | 19  | 9, 47, 127, 252       | 0       |

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| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2        | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|----------------|-----------------------|-------|
| 13  | AM    | 125/126 (99%)   | 0.41   | 11 (8%) 15 10  | 29, 94, 148, 314      | 0     |
| 13  | CM    | 125/126 (99%)   | 0.97   | 17 (13%) 7 5   | 39, 87, 174, 274      | 0     |
| 14  | AN    | 60/61 (98%)     | 0.52   | 3 (5%) 34 19   | 53, 92, 138, 207      | 0     |
| 14  | CN    | 60/61 (98%)     | 0.28   | 4 (6%) 24 15   | 34, 71, 111, 194      | 0     |
| 15  | AO    | 88/89 (98%)     | -0.02  | 0 100 100      | 35, 80, 132, 142      | 0     |
| 15  | CO    | 88/89 (98%)     | -0.02  | 1 (1%) 78 52   | 23, 69, 122, 147      | 0     |
| 16  | AP    | 84/88 (95%)     | 0.04   | 1 (1%) 76 50   | 48, 74, 122, 182      | 0     |
| 16  | CP    | 84/88 (95%)     | 0.35   | 2 (2%) 59 34   | 44, 76, 139, 200      | 0     |
| 17  | AQ    | 100/105 (95%)   | 0.21   | 4 (4%) 42 23   | 50, 91, 141, 174      | 0     |
| 17  | CQ    | 100/105 (95%)   | 0.30   | 4 (4%) 42 23   | 38, 87, 144, 192      | 0     |
| 18  | AR    | 70/88 (79%)     | -0.11  | 0 100 100      | 35, 77, 126, 182      | 0     |
| 18  | CR    | 70/88 (79%)     | -0.00  | 1 (1%) 73 46   | 36, 70, 122, 205      | 0     |
| 19  | AS    | 79/93 (84%)     | 0.49   | 3 (3%) 44 24   | 46, 104, 202, 268     | 0     |
| 19  | CS    | 79/93 (84%)     | 0.56   | 5 (6%) 26 16   | 27, 82, 153, 206      | 0     |
| 20  | AT    | 99/106 (93%)    | 0.45   | 4 (4%) 42 23   | 42, 90, 173, 211      | 0     |
| 20  | CT    | 99/106 (93%)    | 1.04   | 16 (16%) 4 4   | 40, 97, 192, 295      | 0     |
| 21  | AU    | 25/27 (92%)     | 1.27   | 6 (24%) 2 2    | 36, 92, 165, 229      | 0     |
| 21  | CU    | 25/27 (92%)     | 1.02   | 6 (24%) 2 2    | 50, 78, 107, 150      | 0     |
| 22  | AV    | 77/77 (100%)    | 0.19   | 0 100 100      | 45, 82, 163, 276      | 0     |
| 22  | CV    | 77/77 (100%)    | 0.35   | 5 (6%) 25 15   | 32, 72, 133, 253      | 0     |
| 23  | AW    | 76/76 (100%)    | 0.68   | 4 (5%) 32 18   | 48, 175, 249, 317     | 0     |
| 23  | AY    | 17/76 (22%)     | 0.28   | 0 100 100      | 64, 94, 167, 176      | 0     |
| 23  | CW    | 76/76 (100%)    | 0.83   | 8 (10%) 11 7   | 34, 184, 271, 295     | 0     |
| 23  | CY    | 17/76 (22%)     | 0.31   | 0 100 100      | 44, 75, 149, 186      | 0     |
| 24  | AX    | 12/24 (50%)     | 1.16   | 4 (33%) 1 1    | 49, 74, 217, 234      | 0     |
| 24  | CX    | 10/24 (41%)     | 1.53   | 2 (20%) 3 3    | 42, 58, 144, 213      | 0     |
| 25  | BA    | 2810/2915 (96%) | 0.25   | 103 (3%) 45 25 | 17, 58, 187, 375      | 0     |
| 25  | DA    | 2824/2915 (96%) | 0.12   | 100 (3%) 47 26 | 6, 42, 178, 370       | 0     |
| 26  | BB    | 119/122 (97%)   | 0.36   | 3 (2%) 58 33   | 59, 94, 132, 182      | 0     |
| 26  | DB    | 119/122 (97%)   | 0.29   | 3 (2%) 58 33   | 38, 68, 113, 174      | 0     |
| 27  | BC    | 191/229 (83%)   | 0.87   | 20 (10%) 11 7  | 89, 200, 319, 378     | 0     |

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| Mol | Chain | Analysed       | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|----------------|--------|---------------|-----------------------|-------|
| 27  | DC    | 191/229 (83%)  | 0.74   | 18 (9%) 14 9  | 64, 208, 290, 334     | 0     |
| 28  | BD    | 272/276 (98%)  | 0.03   | 5 (1%) 67 40  | 9, 45, 89, 166        | 0     |
| 28  | DD    | 272/276 (98%)  | 0.01   | 9 (3%) 49 27  | 3, 33, 80, 197        | 0     |
| 29  | BE    | 205/206 (99%)  | 0.21   | 12 (5%) 28 16 | 17, 66, 128, 289      | 0     |
| 29  | DE    | 205/206 (99%)  | 0.18   | 4 (1%) 65 37  | 11, 55, 160, 338      | 0     |
| 30  | BF    | 208/210 (99%)  | 0.13   | 5 (2%) 59 34  | 14, 64, 164, 286      | 0     |
| 30  | DF    | 202/210 (96%)  | 0.40   | 9 (4%) 38 20  | 5, 51, 127, 208       | 0     |
| 31  | BG    | 181/182 (99%)  | 0.27   | 9 (4%) 34 19  | 40, 95, 175, 268      | 0     |
| 31  | DG    | 181/182 (99%)  | 0.40   | 6 (3%) 49 27  | 25, 76, 143, 219      | 0     |
| 32  | BH    | 160/180 (88%)  | 0.94   | 20 (12%) 8 6  | 85, 179, 331, 429     | 0     |
| 32  | DH    | 168/180 (93%)  | 0.69   | 13 (7%) 19 13 | 29, 81, 155, 234      | 0     |
| 33  | BI    | 145/148 (97%)  | 0.08   | 3 (2%) 63 36  | 33, 96, 156, 184      | 0     |
| 33  | DI    | 146/148 (98%)  | 0.51   | 8 (5%) 30 17  | 15, 104, 166, 207     | 0     |
| 34  | BN    | 139/140 (99%)  | 0.17   | 8 (5%) 29 17  | 36, 79, 147, 305      | 0     |
| 34  | DN    | 139/140 (99%)  | 0.26   | 4 (2%) 53 30  | 7, 61, 137, 185       | 0     |
| 35  | BO    | 122/122 (100%) | 0.02   | 1 (0%) 82 58  | 32, 65, 97, 124       | 0     |
| 35  | DO    | 122/122 (100%) | -0.29  | 0 100 100     | 10, 41, 84, 112       | 0     |
| 36  | BP    | 150/150 (100%) | 1.26   | 34 (22%) 2 2  | 27, 87, 179, 250      | 0     |
| 36  | DP    | 150/150 (100%) | 1.51   | 45 (30%) 1 2  | 23, 71, 151, 264      | 0     |
| 37  | BQ    | 141/141 (100%) | 0.20   | 9 (6%) 25 15  | 36, 74, 126, 421      | 0     |
| 37  | DQ    | 141/141 (100%) | 0.18   | 6 (4%) 40 21  | 12, 52, 108, 281      | 0     |
| 38  | BR    | 117/118 (99%)  | 0.31   | 10 (8%) 16 11 | 21, 57, 107, 148      | 0     |
| 38  | DR    | 118/118 (100%) | 0.14   | 4 (3%) 48 27  | 15, 50, 92, 126       | 0     |
| 39  | BS    | 99/112 (88%)   | 0.59   | 9 (9%) 15 9   | 38, 100, 171, 347     | 0     |
| 39  | DS    | 111/112 (99%)  | 0.49   | 6 (5%) 31 18  | 33, 73, 147, 197      | 0     |
| 40  | BT    | 138/146 (94%)  | 0.35   | 11 (7%) 18 12 | 29, 80, 225, 351      | 0     |
| 40  | DT    | 138/146 (94%)  | 0.63   | 14 (10%) 12 8 | 20, 71, 212, 304      | 0     |
| 41  | BU    | 117/118 (99%)  | 0.39   | 7 (5%) 27 16  | 29, 64, 131, 281      | 0     |
| 41  | DU    | 117/118 (99%)  | 0.27   | 3 (2%) 57 32  | 17, 52, 114, 180      | 0     |
| 42  | BV    | 101/101 (100%) | 0.12   | 1 (0%) 79 54  | 23, 90, 149, 344      | 0     |
| 42  | DV    | 101/101 (100%) | 0.54   | 6 (5%) 28 16  | 9, 70, 131, 303       | 0     |

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| Mol | Chain | Analysed          | <RSRZ> | #RSRZ>2         | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-------------------|--------|-----------------|-----------------------|-------|
| 43  | BW    | 113/113 (100%)    | -0.07  | 3 (2%) 56 32    | 19, 49, 113, 319      | 0     |
| 43  | DW    | 113/113 (100%)    | -0.04  | 0 100 100       | 14, 42, 128, 204      | 0     |
| 44  | BX    | 93/96 (96%)       | 0.07   | 2 (2%) 62 35    | 30, 63, 99, 149       | 0     |
| 44  | DX    | 93/96 (96%)       | 0.11   | 2 (2%) 62 35    | 12, 42, 87, 144       | 0     |
| 45  | BY    | 101/110 (91%)     | 1.17   | 20 (19%) 3 3    | 42, 92, 253, 363      | 0     |
| 45  | DY    | 102/110 (92%)     | 0.76   | 14 (13%) 6 5    | 28, 82, 182, 226      | 0     |
| 46  | BZ    | 177/206 (85%)     | 0.40   | 7 (3%) 42 23    | 45, 125, 202, 316     | 0     |
| 46  | DZ    | 177/206 (85%)     | 0.78   | 16 (9%) 15 9    | 29, 116, 254, 322     | 0     |
| 47  | B0    | 84/85 (98%)       | 0.34   | 9 (10%) 11 7    | 31, 69, 170, 242      | 0     |
| 47  | D0    | 84/85 (98%)       | 0.47   | 9 (10%) 11 7    | 18, 52, 136, 286      | 0     |
| 48  | B1    | 94/98 (95%)       | 0.01   | 2 (2%) 63 36    | 17, 53, 113, 219      | 0     |
| 48  | D1    | 94/98 (95%)       | 0.28   | 3 (3%) 50 28    | 7, 44, 122, 237       | 0     |
| 49  | B2    | 71/72 (98%)       | 0.19   | 1 (1%) 73 46    | 35, 77, 128, 195      | 0     |
| 49  | D2    | 71/72 (98%)       | 0.78   | 9 (12%) 8 6     | 14, 54, 137, 267      | 0     |
| 50  | B3    | 60/60 (100%)      | 0.18   | 1 (1%) 69 41    | 35, 75, 125, 382      | 0     |
| 50  | D3    | 60/60 (100%)      | 0.21   | 1 (1%) 69 41    | 20, 65, 142, 236      | 0     |
| 51  | B4    | 31/71 (43%)       | 0.15   | 2 (6%) 25 15    | 67, 121, 152, 204     | 0     |
| 51  | D4    | 40/71 (56%)       | 0.59   | 4 (10%) 12 8    | 55, 116, 173, 266     | 0     |
| 52  | B5    | 59/60 (98%)       | 0.17   | 3 (5%) 33 19    | 17, 72, 180, 340      | 0     |
| 52  | D5    | 59/60 (98%)       | 0.16   | 2 (3%) 48 27    | 12, 63, 214, 299      | 0     |
| 53  | B6    | 45/54 (83%)       | 1.18   | 9 (20%) 3 3     | 44, 138, 207, 343     | 0     |
| 53  | D6    | 45/54 (83%)       | 1.60   | 12 (26%) 1 2    | 59, 139, 235, 285     | 0     |
| 54  | B7    | 49/49 (100%)      | 0.47   | 5 (10%) 12 8    | 11, 41, 123, 149      | 0     |
| 54  | D7    | 49/49 (100%)      | 0.11   | 4 (8%) 17 12    | 1, 23, 101, 204       | 0     |
| 55  | B8    | 64/65 (98%)       | 0.70   | 8 (12%) 8 6     | 20, 60, 129, 325      | 0     |
| 55  | D8    | 64/65 (98%)       | 0.71   | 8 (12%) 8 6     | 12, 51, 115, 172      | 0     |
| 56  | B9    | 36/37 (97%)       | 3.00   | 23 (63%) 0 0    | 120, 197, 269, 389    | 0     |
| 56  | D9    | 36/37 (97%)       | 2.87   | 26 (72%) 0 0    | 115, 172, 217, 282    | 0     |
| All | All   | 21184/22210 (95%) | 0.30   | 1098 (5%) 33 18 | 1, 71, 192, 429       | 0     |

All (1098) RSRZ outliers are listed below:

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 53  | D6    | 24   | GLU  | 7.7  |
| 37  | BQ    | 140  | ALA  | 7.6  |
| 55  | B8    | 31   | HIS  | 7.4  |
| 56  | B9    | 37   | GLY  | 7.3  |
| 56  | B9    | 23   | VAL  | 7.2  |
| 13  | CM    | 123  | ALA  | 7.0  |
| 45  | BY    | 59   | GLY  | 7.0  |
| 36  | BP    | 16   | ARG  | 6.9  |
| 55  | B8    | 33   | ASN  | 6.9  |
| 7   | CG    | 32   | ARG  | 6.8  |
| 37  | DQ    | 140  | ALA  | 6.7  |
| 10  | CJ    | 59   | SER  | 6.6  |
| 36  | DP    | 11   | GLY  | 6.6  |
| 13  | CM    | 126  | LYS  | 6.5  |
| 13  | CM    | 124  | PRO  | 6.4  |
| 36  | DP    | 20   | GLY  | 6.4  |
| 40  | DT    | 24   | PRO  | 6.3  |
| 5   | CE    | 85   | GLY  | 6.1  |
| 37  | BQ    | 141  | GLN  | 6.0  |
| 56  | B9    | 22   | ARG  | 6.0  |
| 25  | DA    | 1497 | U    | 6.0  |
| 56  | D9    | 3    | VAL  | 5.9  |
| 36  | BP    | 70   | GLN  | 5.9  |
| 47  | D0    | 3    | HIS  | 5.9  |
| 56  | B9    | 14   | CYS  | 5.9  |
| 53  | D6    | 26   | ASN  | 5.8  |
| 36  | DP    | 12   | ALA  | 5.8  |
| 56  | D9    | 18   | ARG  | 5.8  |
| 39  | DS    | 2    | ALA  | 5.7  |
| 40  | DT    | 25   | GLY  | 5.7  |
| 1   | AA    | 1124 | G    | 5.6  |
| 20  | CT    | 106  | ALA  | 5.6  |
| 13  | CM    | 125  | ARG  | 5.6  |
| 9   | CI    | 106  | ALA  | 5.6  |
| 24  | AX    | 13   | A    | 5.5  |
| 36  | BP    | 56   | SER  | 5.5  |
| 7   | CG    | 84   | ASN  | 5.5  |
| 32  | BH    | 35   | VAL  | 5.4  |
| 1   | CA    | 429  | U    | 5.4  |
| 53  | B6    | 42   | TRP  | 5.3  |
| 25  | DA    | 11   | G    | 5.3  |
| 1   | CA    | 820  | U    | 5.3  |
| 45  | BY    | 49   | VAL  | 5.2  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 13  | CM    | 102  | ARG  | 5.2  |
| 24  | CX    | 13   | A    | 5.2  |
| 14  | CN    | 2    | ALA  | 5.2  |
| 56  | B9    | 24   | TYR  | 5.2  |
| 27  | DC    | 172  | HIS  | 5.2  |
| 46  | DZ    | 173  | ALA  | 5.2  |
| 36  | DP    | 70   | GLN  | 5.1  |
| 56  | D9    | 33   | LYS  | 5.1  |
| 21  | AU    | 6    | ARG  | 5.1  |
| 45  | BY    | 58   | GLY  | 5.1  |
| 19  | CS    | 81   | ARG  | 5.1  |
| 11  | AK    | 129  | SER  | 5.0  |
| 13  | CM    | 122  | LYS  | 5.0  |
| 32  | BH    | 24   | VAL  | 5.0  |
| 2   | CB    | 16   | HIS  | 5.0  |
| 56  | B9    | 3    | VAL  | 5.0  |
| 25  | DA    | 2506 | U    | 4.9  |
| 13  | AM    | 84   | ILE  | 4.9  |
| 25  | BA    | 2894 | G    | 4.9  |
| 36  | BP    | 65   | ARG  | 4.8  |
| 7   | AG    | 32   | ARG  | 4.8  |
| 12  | CL    | 28   | LYS  | 4.8  |
| 38  | BR    | 13   | HIS  | 4.8  |
| 20  | CT    | 12   | ALA  | 4.8  |
| 41  | BU    | 91   | ASP  | 4.7  |
| 8   | AH    | 1    | MET  | 4.7  |
| 25  | DA    | 2135 | A    | 4.7  |
| 1   | CA    | 48   | C    | 4.7  |
| 25  | BA    | 2504 | U    | 4.7  |
| 19  | AS    | 10   | PHE  | 4.6  |
| 28  | DD    | 34   | VAL  | 4.6  |
| 25  | DA    | 508  | G    | 4.6  |
| 27  | BC    | 45   | ALA  | 4.6  |
| 30  | BF    | 84   | VAL  | 4.6  |
| 36  | DP    | 74   | GLU  | 4.6  |
| 4   | AD    | 12   | CYS  | 4.6  |
| 4   | AD    | 3    | ARG  | 4.6  |
| 11  | AK    | 128  | ALA  | 4.5  |
| 32  | BH    | 59   | ARG  | 4.5  |
| 25  | DA    | 2802 | G    | 4.5  |
| 41  | BU    | 58   | ARG  | 4.5  |
| 47  | D0    | 2    | ALA  | 4.5  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 36         | BP           | 52         | GLU         | 4.5         |
| 56         | B9           | 34         | GLN         | 4.5         |
| 28         | BD           | 34         | VAL         | 4.5         |
| 53         | D6           | 42         | TRP         | 4.5         |
| 28         | BD           | 225        | ALA         | 4.4         |
| 20         | CT           | 83         | ARG         | 4.4         |
| 1          | CA           | 60         | A           | 4.4         |
| 45         | BY           | 2          | ARG         | 4.4         |
| 1          | AA           | 89         | C           | 4.4         |
| 39         | BS           | 54         | LEU         | 4.4         |
| 1          | AA           | 983        | A           | 4.4         |
| 27         | BC           | 166        | ASP         | 4.4         |
| 1          | CA           | 1126       | U           | 4.3         |
| 53         | B6           | 24         | GLU         | 4.3         |
| 56         | D9           | 8          | LYS         | 4.3         |
| 25         | DA           | 2690       | C           | 4.3         |
| 56         | D9           | 4          | ARG         | 4.3         |
| 1          | CA           | 1065       | U           | 4.3         |
| 53         | B6           | 12         | GLU         | 4.3         |
| 25         | BA           | 2802       | G           | 4.3         |
| 51         | D4           | 1          | MET         | 4.3         |
| 25         | DA           | 562        | U           | 4.3         |
| 36         | DP           | 43         | GLY         | 4.3         |
| 7          | AG           | 84         | ASN         | 4.3         |
| 27         | BC           | 194        | ARG         | 4.3         |
| 1          | AA           | 1067       | A           | 4.2         |
| 12         | AL           | 26         | ALA         | 4.2         |
| 49         | D2           | 72         | ALA         | 4.2         |
| 56         | B9           | 18         | ARG         | 4.2         |
| 40         | BT           | 92         | GLY         | 4.2         |
| 36         | DP           | 108        | LYS         | 4.2         |
| 36         | BP           | 58         | THR         | 4.2         |
| 14         | AN           | 2          | ALA         | 4.2         |
| 25         | BA           | 574        | C           | 4.2         |
| 36         | BP           | 71         | VAL         | 4.1         |
| 20         | CT           | 84         | LEU         | 4.1         |
| 25         | BA           | 2690       | C           | 4.1         |
| 1          | CA           | 532        | A           | 4.1         |
| 36         | DP           | 105        | LEU         | 4.1         |
| 39         | BS           | 36         | TYR         | 4.1         |
| 55         | D8           | 35         | GLN         | 4.1         |
| 56         | D9           | 30         | PRO         | 4.1         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 25         | BA           | 352        | G           | 4.1         |
| 32         | DH           | 5          | GLY         | 4.1         |
| 46         | DZ           | 39         | VAL         | 4.0         |
| 25         | BA           | 995        | C           | 4.0         |
| 11         | AK           | 117        | ASN         | 4.0         |
| 25         | BA           | 1325       | G           | 4.0         |
| 37         | DQ           | 141        | GLN         | 4.0         |
| 31         | DG           | 75         | LYS         | 4.0         |
| 49         | B2           | 52         | ASP         | 4.0         |
| 56         | B9           | 35         | ARG         | 4.0         |
| 36         | BP           | 35         | HIS         | 4.0         |
| 25         | BA           | 1049       | C           | 4.0         |
| 1          | CA           | 1190       | G           | 4.0         |
| 13         | AM           | 124        | PRO         | 4.0         |
| 45         | BY           | 28         | LYS         | 3.9         |
| 11         | AK           | 49         | GLY         | 3.9         |
| 1          | CA           | 1125       | U           | 3.9         |
| 45         | DY           | 91         | GLU         | 3.9         |
| 13         | CM           | 2          | ALA         | 3.9         |
| 29         | DE           | 76         | ARG         | 3.9         |
| 45         | BY           | 61         | ILE         | 3.9         |
| 45         | DY           | 88         | LYS         | 3.9         |
| 4          | AD           | 209        | ARG         | 3.9         |
| 38         | BR           | 4          | LEU         | 3.9         |
| 36         | DP           | 35         | HIS         | 3.9         |
| 7          | CG           | 83         | ALA         | 3.9         |
| 36         | BP           | 12         | ALA         | 3.9         |
| 1          | CA           | 1066       | C           | 3.9         |
| 56         | B9           | 2          | LYS         | 3.9         |
| 20         | AT           | 104        | LEU         | 3.9         |
| 4          | AD           | 31         | CYS         | 3.9         |
| 25         | BA           | 11         | G           | 3.9         |
| 25         | BA           | 2173       | A           | 3.9         |
| 25         | DA           | 2602       | A           | 3.9         |
| 13         | AM           | 102        | ARG         | 3.8         |
| 1          | AA           | 1125       | U           | 3.8         |
| 32         | DH           | 155        | SER         | 3.8         |
| 30         | DF           | 134        | GLY         | 3.8         |
| 36         | DP           | 21         | ARG         | 3.8         |
| 55         | B8           | 65         | GLU         | 3.8         |
| 1          | AA           | 81         | U           | 3.8         |
| 1          | CA           | 130        | A           | 3.8         |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 36  | DP    | 22   | GLY  | 3.8  |
| 39  | BS    | 12   | PHE  | 3.8  |
| 56  | D9    | 15   | LYS  | 3.8  |
| 36  | BP    | 50   | ARG  | 3.8  |
| 25  | DA    | 2258 | C    | 3.8  |
| 7   | AG    | 83   | ALA  | 3.8  |
| 10  | CJ    | 46   | ARG  | 3.7  |
| 40  | BT    | 25   | GLY  | 3.7  |
| 1   | AA    | 83   | U    | 3.7  |
| 36  | DP    | 71   | VAL  | 3.7  |
| 25  | DA    | 2402 | C    | 3.7  |
| 56  | D9    | 7    | VAL  | 3.7  |
| 45  | BY    | 60   | PHE  | 3.7  |
| 1   | CA    | 1281 | U    | 3.7  |
| 53  | D6    | 21   | TYR  | 3.7  |
| 4   | CD    | 110  | PHE  | 3.7  |
| 30  | BF    | 65   | TRP  | 3.7  |
| 1   | AA    | 1126 | U    | 3.7  |
| 36  | DP    | 64   | LYS  | 3.7  |
| 55  | D8    | 40   | GLU  | 3.7  |
| 45  | BY    | 48   | ALA  | 3.6  |
| 1   | AA    | 1049 | U    | 3.6  |
| 21  | CU    | 6    | ARG  | 3.6  |
| 56  | B9    | 25   | VAL  | 3.6  |
| 13  | CM    | 121  | LYS  | 3.6  |
| 56  | B9    | 36   | GLN  | 3.6  |
| 12  | AL    | 27   | LEU  | 3.6  |
| 25  | DA    | 2136 | C    | 3.6  |
| 25  | BA    | 2345 | G    | 3.6  |
| 25  | DA    | 1055 | G    | 3.6  |
| 45  | BY    | 88   | LYS  | 3.6  |
| 25  | DA    | 92   | A    | 3.6  |
| 46  | DZ    | 124  | ILE  | 3.6  |
| 47  | D0    | 5    | LYS  | 3.6  |
| 5   | CE    | 70   | PRO  | 3.6  |
| 31  | BG    | 142  | PRO  | 3.6  |
| 27  | BC    | 172  | HIS  | 3.6  |
| 53  | D6    | 46   | HIS  | 3.6  |
| 55  | D8    | 32   | LEU  | 3.6  |
| 11  | CK    | 129  | SER  | 3.6  |
| 8   | CH    | 1    | MET  | 3.6  |
| 36  | BP    | 120  | ALA  | 3.6  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 36         | DP           | 14         | LYS         | 3.6         |
| 45         | BY           | 3          | VAL         | 3.6         |
| 36         | BP           | 13         | ASN         | 3.6         |
| 5          | AE           | 121        | LYS         | 3.6         |
| 56         | B9           | 33         | LYS         | 3.6         |
| 21         | AU           | 9          | ARG         | 3.6         |
| 2          | CB           | 96         | ARG         | 3.5         |
| 36         | DP           | 3          | LEU         | 3.5         |
| 54         | B7           | 23         | ARG         | 3.5         |
| 36         | BP           | 24         | GLY         | 3.5         |
| 1          | CA           | 872        | A           | 3.5         |
| 25         | BA           | 1048       | A           | 3.5         |
| 31         | BG           | 98         | ARG         | 3.5         |
| 47         | B0           | 41         | ARG         | 3.5         |
| 20         | AT           | 9          | ASN         | 3.5         |
| 56         | D9           | 24         | TYR         | 3.5         |
| 25         | DA           | 529        | A           | 3.5         |
| 25         | DA           | 2021       | C           | 3.5         |
| 5          | CE           | 103        | GLY         | 3.5         |
| 1          | AA           | 84         | U           | 3.5         |
| 1          | AA           | 1503       | A           | 3.5         |
| 25         | BA           | 2506       | U           | 3.5         |
| 27         | BC           | 56         | GLN         | 3.5         |
| 23         | AW           | 34         | G           | 3.5         |
| 12         | AL           | 16         | GLU         | 3.5         |
| 56         | D9           | 35         | ARG         | 3.5         |
| 1          | CA           | 89         | C           | 3.5         |
| 25         | BA           | 2174       | C           | 3.5         |
| 25         | DA           | 2896       | C           | 3.5         |
| 46         | DZ           | 178        | GLU         | 3.4         |
| 1          | CA           | 173        | U           | 3.4         |
| 25         | BA           | 92         | A           | 3.4         |
| 25         | BA           | 1452       | A           | 3.4         |
| 25         | DA           | 2117       | A           | 3.4         |
| 1          | CA           | 1001(A)    | G           | 3.4         |
| 4          | CD           | 12         | CYS         | 3.4         |
| 46         | DZ           | 169        | GLU         | 3.4         |
| 40         | DT           | 93         | ARG         | 3.4         |
| 1          | CA           | 1503       | A           | 3.4         |
| 56         | D9           | 32         | HIS         | 3.4         |
| 56         | D9           | 22         | ARG         | 3.4         |
| 1          | AA           | 1127       | G           | 3.4         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 1          | CA           | 251        | G           | 3.4         |
| 1          | CA           | 1456       | G           | 3.4         |
| 23         | AW           | 6          | G           | 3.4         |
| 25         | DA           | 2207       | G           | 3.4         |
| 45         | BY           | 57         | GLN         | 3.4         |
| 56         | D9           | 34         | GLN         | 3.4         |
| 5          | CE           | 129        | ILE         | 3.4         |
| 36         | DP           | 60         | MET         | 3.4         |
| 25         | BA           | 1053       | C           | 3.4         |
| 55         | D8           | 64         | TYR         | 3.4         |
| 25         | DA           | 2022       | U           | 3.4         |
| 17         | CQ           | 101        | ARG         | 3.4         |
| 56         | D9           | 5          | ALA         | 3.4         |
| 36         | BP           | 19         | VAL         | 3.4         |
| 56         | B9           | 32         | HIS         | 3.4         |
| 4          | AD           | 73         | ARG         | 3.4         |
| 13         | AM           | 100        | GLY         | 3.4         |
| 39         | DS           | 20         | ARG         | 3.4         |
| 1          | AA           | 1001(A)    | G           | 3.4         |
| 10         | CJ           | 26         | ALA         | 3.4         |
| 25         | DA           | 2726       | U           | 3.4         |
| 1          | AA           | 792        | A           | 3.4         |
| 56         | D9           | 37         | GLY         | 3.3         |
| 13         | AM           | 126        | LYS         | 3.3         |
| 25         | DA           | 274        | G           | 3.3         |
| 36         | DP           | 24         | GLY         | 3.3         |
| 53         | D6           | 22         | ALA         | 3.3         |
| 44         | DX           | 12         | VAL         | 3.3         |
| 32         | DH           | 58         | GLU         | 3.3         |
| 42         | DV           | 36         | PRO         | 3.3         |
| 45         | BY           | 82         | PRO         | 3.3         |
| 47         | B0           | 55         | ARG         | 3.3         |
| 32         | BH           | 145        | ALA         | 3.3         |
| 36         | DP           | 16         | ARG         | 3.3         |
| 53         | D6           | 20         | ASN         | 3.3         |
| 2          | AB           | 18         | GLY         | 3.3         |
| 1          | AA           | 793        | U           | 3.3         |
| 25         | BA           | 1396       | U           | 3.3         |
| 39         | BS           | 11         | LYS         | 3.3         |
| 25         | DA           | 2319       | G           | 3.3         |
| 34         | BN           | 66         | LYS         | 3.3         |
| 34         | DN           | 68         | GLU         | 3.3         |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 36  | BP    | 18   | ARG  | 3.2  |
| 13  | AM    | 7    | VAL  | 3.2  |
| 36  | DP    | 19   | VAL  | 3.2  |
| 10  | CJ    | 55   | LYS  | 3.2  |
| 34  | DN    | 36   | GLY  | 3.2  |
| 1   | CA    | 1505 | G    | 3.2  |
| 51  | D4    | 34   | GLU  | 3.2  |
| 19  | CS    | 10   | PHE  | 3.2  |
| 17  | AQ    | 101  | ARG  | 3.2  |
| 46  | DZ    | 120  | ILE  | 3.2  |
| 50  | D3    | 30   | ARG  | 3.2  |
| 27  | BC    | 43   | VAL  | 3.2  |
| 45  | BY    | 53   | PRO  | 3.2  |
| 56  | B9    | 7    | VAL  | 3.2  |
| 3   | AC    | 167  | TRP  | 3.2  |
| 33  | DI    | 41   | GLU  | 3.2  |
| 27  | BC    | 58   | VAL  | 3.2  |
| 1   | CA    | 873  | A    | 3.2  |
| 25  | DA    | 1445 | A    | 3.2  |
| 25  | BA    | 10   | G    | 3.2  |
| 25  | BA    | 1816 | G    | 3.2  |
| 47  | D0    | 17   | GLN  | 3.2  |
| 42  | DV    | 37   | VAL  | 3.2  |
| 46  | BZ    | 176  | PRO  | 3.2  |
| 1   | AA    | 820  | U    | 3.2  |
| 25  | DA    | 2118 | U    | 3.2  |
| 29  | BE    | 125  | GLY  | 3.2  |
| 22  | CV    | 77   | A    | 3.2  |
| 25  | DA    | 2477 | C    | 3.2  |
| 21  | AU    | 25   | LYS  | 3.2  |
| 36  | DP    | 36   | LYS  | 3.2  |
| 56  | D9    | 6    | SER  | 3.2  |
| 1   | CA    | 976  | G    | 3.2  |
| 25  | BA    | 2732 | G    | 3.2  |
| 47  | D0    | 13   | GLY  | 3.2  |
| 20  | CT    | 9    | ASN  | 3.2  |
| 40  | DT    | 27   | THR  | 3.2  |
| 1   | AA    | 82   | U    | 3.2  |
| 23  | CW    | 20   | U    | 3.2  |
| 25  | BA    | 12   | U    | 3.2  |
| 25  | BA    | 1762 | A    | 3.1  |
| 25  | BA    | 2892 | A    | 3.1  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 25  | DA    | 945  | A    | 3.1  |
| 30  | DF    | 131  | GLY  | 3.1  |
| 49  | D2    | 31   | GLU  | 3.1  |
| 56  | D9    | 16   | VAL  | 3.1  |
| 1   | AA    | 971  | G    | 3.1  |
| 38  | BR    | 3    | HIS  | 3.1  |
| 32  | BH    | 85   | LYS  | 3.1  |
| 32  | BH    | 129  | THR  | 3.1  |
| 38  | BR    | 11   | ASN  | 3.1  |
| 56  | D9    | 14   | CYS  | 3.1  |
| 46  | BZ    | 121  | HIS  | 3.1  |
| 55  | B8    | 30   | ARG  | 3.1  |
| 45  | DY    | 83   | THR  | 3.1  |
| 12  | CL    | 16   | GLU  | 3.1  |
| 30  | BF    | 179  | GLU  | 3.1  |
| 36  | DP    | 61   | ARG  | 3.1  |
| 46  | DZ    | 80   | ARG  | 3.1  |
| 54  | B7    | 49   | ARG  | 3.1  |
| 36  | BP    | 36   | LYS  | 3.1  |
| 45  | DY    | 50   | ARG  | 3.1  |
| 25  | BA    | 1026 | U    | 3.1  |
| 27  | DC    | 56   | GLN  | 3.1  |
| 27  | DC    | 119  | VAL  | 3.1  |
| 33  | BI    | 65   | ALA  | 3.1  |
| 29  | BE    | 69   | LYS  | 3.1  |
| 25  | BA    | 2136 | C    | 3.1  |
| 45  | DY    | 79   | CYS  | 3.1  |
| 54  | B7    | 48   | LYS  | 3.0  |
| 36  | DP    | 79   | ARG  | 3.0  |
| 46  | DZ    | 76   | LEU  | 3.0  |
| 1   | CA    | 818  | G    | 3.0  |
| 5   | AE    | 85   | GLY  | 3.0  |
| 25  | BA    | 242  | G    | 3.0  |
| 25  | BA    | 508  | G    | 3.0  |
| 25  | BA    | 1114 | G    | 3.0  |
| 25  | DA    | 1799 | G    | 3.0  |
| 40  | BT    | 56   | GLY  | 3.0  |
| 38  | BR    | 8    | ARG  | 3.0  |
| 1   | AA    | 1054 | C    | 3.0  |
| 25  | BA    | 1505 | C    | 3.0  |
| 25  | BA    | 2585 | U    | 3.0  |
| 25  | DA    | 12   | U    | 3.0  |

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| Mol | Chain | Res    | Type | RSRZ |
|-----|-------|--------|------|------|
| 56  | B9    | 8      | LYS  | 3.0  |
| 31  | DG    | 80     | PHE  | 3.0  |
| 32  | DH    | 171    | LEU  | 3.0  |
| 38  | DR    | 105    | ARG  | 3.0  |
| 25  | DA    | 614(B) | G    | 3.0  |
| 25  | BA    | 2198   | A    | 3.0  |
| 25  | DA    | 603    | A    | 3.0  |
| 27  | BC    | 215    | THR  | 3.0  |
| 30  | DF    | 95     | ARG  | 3.0  |
| 49  | D2    | 49     | LYS  | 3.0  |
| 32  | BH    | 108    | GLY  | 3.0  |
| 7   | AG    | 86     | GLN  | 3.0  |
| 32  | DH    | 125    | VAL  | 3.0  |
| 20  | CT    | 66     | ALA  | 3.0  |
| 25  | DA    | 752    | A    | 3.0  |
| 25  | DA    | 896    | A    | 3.0  |
| 25  | DA    | 2119   | A    | 3.0  |
| 37  | DQ    | 139    | GLU  | 3.0  |
| 36  | DP    | 46     | LYS  | 3.0  |
| 39  | DS    | 33     | LYS  | 3.0  |
| 36  | BP    | 25     | SER  | 3.0  |
| 47  | D0    | 41     | ARG  | 3.0  |
| 53  | B6    | 22     | ALA  | 3.0  |
| 45  | DY    | 6      | HIS  | 2.9  |
| 4   | CD    | 31     | CYS  | 2.9  |
| 17  | CQ    | 99     | SER  | 2.9  |
| 1   | AA    | 1183   | A    | 2.9  |
| 1   | CA    | 1183   | A    | 2.9  |
| 1   | CA    | 1286   | A    | 2.9  |
| 30  | DF    | 130    | ALA  | 2.9  |
| 25  | DA    | 1559   | G    | 2.9  |
| 9   | AI    | 4      | TYR  | 2.9  |
| 25  | BA    | 2646   | C    | 2.9  |
| 1   | CA    | 1196   | U    | 2.9  |
| 25  | DA    | 614(A) | U    | 2.9  |
| 25  | DA    | 1033   | U    | 2.9  |
| 55  | B8    | 48     | PHE  | 2.9  |
| 36  | DP    | 107    | LYS  | 2.9  |
| 36  | DP    | 59     | LEU  | 2.9  |
| 25  | DA    | 2311   | A    | 2.9  |
| 10  | AJ    | 59     | SER  | 2.9  |
| 56  | D9    | 36     | GLN  | 2.9  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 25  | BA    | 1647 | G    | 2.9  |
| 25  | DA    | 574  | C    | 2.9  |
| 25  | DA    | 2803 | C    | 2.9  |
| 28  | DD    | 240  | ALA  | 2.9  |
| 31  | DG    | 74   | LYS  | 2.9  |
| 56  | D9    | 17   | ILE  | 2.9  |
| 45  | DY    | 89   | PHE  | 2.9  |
| 2   | CB    | 12   | GLU  | 2.9  |
| 52  | D5    | 59   | GLU  | 2.9  |
| 11  | CK    | 30   | VAL  | 2.9  |
| 41  | BU    | 90   | VAL  | 2.9  |
| 32  | BH    | 153  | LYS  | 2.9  |
| 40  | BT    | 27   | THR  | 2.9  |
| 25  | DA    | 2062 | A    | 2.9  |
| 20  | CT    | 85   | MET  | 2.9  |
| 5   | CE    | 78   | HIS  | 2.9  |
| 13  | AM    | 11   | ARG  | 2.9  |
| 31  | BG    | 35   | GLU  | 2.9  |
| 36  | DP    | 15   | ARG  | 2.9  |
| 2   | AB    | 133  | LYS  | 2.9  |
| 36  | DP    | 56   | SER  | 2.9  |
| 7   | AG    | 4    | ARG  | 2.9  |
| 27  | BC    | 190  | ARG  | 2.9  |
| 28  | DD    | 239  | ARG  | 2.9  |
| 48  | B1    | 26   | ARG  | 2.9  |
| 28  | DD    | 237  | GLU  | 2.9  |
| 39  | BS    | 34   | HIS  | 2.8  |
| 25  | BA    | 1379 | A    | 2.8  |
| 30  | DF    | 78   | ILE  | 2.8  |
| 1   | CA    | 793  | U    | 2.8  |
| 25  | BA    | 2612 | C    | 2.8  |
| 36  | DP    | 18   | ARG  | 2.8  |
| 7   | CG    | 85   | TYR  | 2.8  |
| 25  | BA    | 274  | G    | 2.8  |
| 25  | BA    | 1559 | G    | 2.8  |
| 36  | DP    | 29   | LYS  | 2.8  |
| 53  | B6    | 39   | TYR  | 2.8  |
| 53  | D6    | 39   | TYR  | 2.8  |
| 27  | BC    | 74   | VAL  | 2.8  |
| 27  | DC    | 178  | ALA  | 2.8  |
| 1   | AA    | 1279 | A    | 2.8  |
| 1   | CA    | 1067 | A    | 2.8  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 25  | DA    | 2346 | A    | 2.8  |
| 27  | DC    | 41   | VAL  | 2.8  |
| 27  | DC    | 165  | ASN  | 2.8  |
| 36  | BP    | 74   | GLU  | 2.8  |
| 36  | DP    | 62   | LEU  | 2.8  |
| 40  | BT    | 11   | GLU  | 2.8  |
| 48  | B1    | 95   | LEU  | 2.8  |
| 13  | CM    | 6    | GLY  | 2.8  |
| 1   | CA    | 1129 | C    | 2.8  |
| 25  | DA    | 34   | C    | 2.8  |
| 25  | DA    | 975  | C    | 2.8  |
| 50  | B3    | 1    | MET  | 2.8  |
| 41  | BU    | 34   | LYS  | 2.8  |
| 1   | AA    | 631  | G    | 2.8  |
| 1   | CA    | 630  | G    | 2.8  |
| 47  | B0    | 13   | GLY  | 2.8  |
| 24  | AX    | 12   | A    | 2.8  |
| 25  | BA    | 603  | A    | 2.8  |
| 27  | DC    | 25   | ALA  | 2.8  |
| 46  | DZ    | 121  | HIS  | 2.8  |
| 54  | B7    | 2    | LYS  | 2.8  |
| 28  | DD    | 244  | ARG  | 2.8  |
| 45  | DY    | 90   | LEU  | 2.8  |
| 1   | AA    | 972  | C    | 2.8  |
| 46  | DZ    | 175  | VAL  | 2.8  |
| 55  | B8    | 64   | TYR  | 2.8  |
| 13  | CM    | 100  | GLY  | 2.8  |
| 40  | DT    | 8    | LYS  | 2.8  |
| 1   | AA    | 1160 | G    | 2.8  |
| 4   | CD    | 9    | CYS  | 2.8  |
| 21  | CU    | 10   | ARG  | 2.8  |
| 36  | BP    | 61   | ARG  | 2.8  |
| 40  | DT    | 3    | ARG  | 2.8  |
| 38  | DR    | 91   | GLN  | 2.8  |
| 27  | DC    | 173  | ALA  | 2.8  |
| 1   | AA    | 1281 | U    | 2.8  |
| 25  | BA    | 1300 | U    | 2.8  |
| 21  | CU    | 15   | ARG  | 2.7  |
| 35  | BO    | 37   | ASP  | 2.7  |
| 1   | CA    | 748  | C    | 2.7  |
| 40  | BT    | 24   | PRO  | 2.7  |
| 13  | CM    | 8    | GLU  | 2.7  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 1          | AA           | 1003       | G           | 2.7         |
| 25         | BA           | 2848       | G           | 2.7         |
| 4          | AD           | 19         | LEU         | 2.7         |
| 20         | CT           | 99         | LEU         | 2.7         |
| 32         | BH           | 67         | LEU         | 2.7         |
| 40         | BT           | 115        | ARG         | 2.7         |
| 1          | AA           | 1531       | A           | 2.7         |
| 25         | DA           | 1494       | A           | 2.7         |
| 16         | AP           | 68         | ASP         | 2.7         |
| 23         | CW           | 47         | U           | 2.7         |
| 5          | CE           | 102        | ALA         | 2.7         |
| 17         | AQ           | 24         | GLU         | 2.7         |
| 23         | CW           | 62         | C           | 2.7         |
| 25         | BA           | 271(B)     | C           | 2.7         |
| 56         | B9           | 6          | SER         | 2.7         |
| 1          | AA           | 485        | G           | 2.7         |
| 25         | BA           | 75         | G           | 2.7         |
| 25         | BA           | 1992       | G           | 2.7         |
| 4          | CD           | 23         | GLY         | 2.7         |
| 36         | BP           | 26         | GLY         | 2.7         |
| 36         | DP           | 38         | GLN         | 2.7         |
| 4          | CD           | 209        | ARG         | 2.7         |
| 7          | AG           | 79         | ARG         | 2.7         |
| 41         | DU           | 58         | ARG         | 2.7         |
| 1          | CA           | 534        | U           | 2.7         |
| 45         | DY           | 46         | LYS         | 2.7         |
| 56         | D9           | 20         | HIS         | 2.7         |
| 27         | DC           | 179        | SER         | 2.7         |
| 28         | DD           | 238        | GLY         | 2.7         |
| 30         | DF           | 207        | GLY         | 2.7         |
| 36         | BP           | 107        | LYS         | 2.7         |
| 1          | AA           | 532        | A           | 2.7         |
| 1          | CA           | 533        | A           | 2.7         |
| 25         | BA           | 1786       | A           | 2.7         |
| 38         | DR           | 1          | MET         | 2.7         |
| 32         | BH           | 37         | VAL         | 2.7         |
| 52         | D5           | 60         | VAL         | 2.7         |
| 32         | DH           | 8          | PRO         | 2.7         |
| 32         | DH           | 57         | ASP         | 2.7         |
| 34         | BN           | 133        | GLN         | 2.7         |
| 37         | DQ           | 25         | ASP         | 2.7         |
| 41         | BU           | 33         | ARG         | 2.7         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 40         | DT           | 36         | GLU         | 2.7         |
| 37         | BQ           | 22         | LYS         | 2.7         |
| 49         | D2           | 71         | ASN         | 2.7         |
| 53         | D6           | 25         | LYS         | 2.7         |
| 5          | AE           | 78         | HIS         | 2.6         |
| 29         | DE           | 75         | VAL         | 2.6         |
| 56         | B9           | 20         | HIS         | 2.6         |
| 45         | BY           | 56         | PRO         | 2.6         |
| 48         | D1           | 50         | ARG         | 2.6         |
| 7          | CG           | 2          | ALA         | 2.6         |
| 1          | AA           | 130        | A           | 2.6         |
| 23         | AW           | 37         | A           | 2.6         |
| 25         | BA           | 241        | A           | 2.6         |
| 25         | BA           | 670        | A           | 2.6         |
| 25         | BA           | 2412       | A           | 2.6         |
| 1          | CA           | 871        | U           | 2.6         |
| 13         | CM           | 106        | ASN         | 2.6         |
| 25         | DA           | 1026       | U           | 2.6         |
| 1          | AA           | 1504       | G           | 2.6         |
| 23         | CW           | 6          | G           | 2.6         |
| 29         | BE           | 76         | ARG         | 2.6         |
| 54         | D7           | 47         | ARG         | 2.6         |
| 54         | D7           | 48         | LYS         | 2.6         |
| 25         | DA           | 889        | C           | 2.6         |
| 27         | DC           | 216        | THR         | 2.6         |
| 27         | DC           | 43         | VAL         | 2.6         |
| 13         | CM           | 88         | ARG         | 2.6         |
| 25         | BA           | 2135       | A           | 2.6         |
| 31         | BG           | 96         | ARG         | 2.6         |
| 45         | BY           | 50         | ARG         | 2.6         |
| 54         | B7           | 47         | ARG         | 2.6         |
| 29         | BE           | 159        | HIS         | 2.6         |
| 25         | DA           | 1453       | U           | 2.6         |
| 38         | BR           | 9          | LYS         | 2.6         |
| 47         | D0           | 4          | LYS         | 2.6         |
| 43         | BW           | 94         | ASP         | 2.6         |
| 46         | DZ           | 87         | ASP         | 2.6         |
| 25         | BA           | 1653       | G           | 2.6         |
| 45         | BY           | 45         | VAL         | 2.6         |
| 56         | D9           | 19         | ARG         | 2.6         |
| 1          | AA           | 1066       | C           | 2.6         |
| 1          | AA           | 1128       | C           | 2.6         |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 25  | DA    | 1049 | C    | 2.6  |
| 56  | B9    | 30   | PRO  | 2.6  |
| 29  | BE    | 187  | ALA  | 2.6  |
| 21  | AU    | 16   | GLY  | 2.6  |
| 1   | AA    | 1201 | A    | 2.6  |
| 1   | CA    | 389  | A    | 2.6  |
| 41  | DU    | 37   | GLU  | 2.6  |
| 1   | CA    | 427  | U    | 2.6  |
| 7   | CG    | 79   | ARG  | 2.6  |
| 29  | BE    | 59   | VAL  | 2.6  |
| 37  | BQ    | 101  | ARG  | 2.6  |
| 20  | AT    | 74   | LYS  | 2.6  |
| 36  | BP    | 59   | LEU  | 2.6  |
| 40  | DT    | 6    | LEU  | 2.6  |
| 1   | CA    | 1224 | G    | 2.6  |
| 23  | CW    | 34   | G    | 2.6  |
| 25  | BA    | 2125 | G    | 2.6  |
| 25  | DA    | 2148 | G    | 2.6  |
| 36  | BP    | 21   | ARG  | 2.6  |
| 37  | BQ    | 63   | LYS  | 2.6  |
| 40  | BT    | 91   | ARG  | 2.6  |
| 25  | DA    | 332  | A    | 2.6  |
| 11  | CK    | 118  | GLY  | 2.6  |
| 10  | AJ    | 68   | HIS  | 2.5  |
| 4   | CD    | 3    | ARG  | 2.5  |
| 20  | CT    | 8    | ARG  | 2.5  |
| 21  | AU    | 15   | ARG  | 2.5  |
| 36  | DP    | 86   | LYS  | 2.5  |
| 40  | DT    | 112  | ARG  | 2.5  |
| 49  | D2    | 27   | GLU  | 2.5  |
| 29  | BE    | 204  | ALA  | 2.5  |
| 46  | BZ    | 115  | GLY  | 2.5  |
| 2   | AB    | 16   | HIS  | 2.5  |
| 25  | DA    | 2804 | C    | 2.5  |
| 17  | CQ    | 100  | LYS  | 2.5  |
| 31  | DG    | 84   | LYS  | 2.5  |
| 7   | CG    | 4    | ARG  | 2.5  |
| 28  | DD    | 250  | TRP  | 2.5  |
| 36  | BP    | 15   | ARG  | 2.5  |
| 32  | BH    | 52   | VAL  | 2.5  |
| 1   | CA    | 1257 | U    | 2.5  |
| 25  | BA    | 1453 | U    | 2.5  |

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| Mol | Chain | Res    | Type | RSRZ |
|-----|-------|--------|------|------|
| 25  | BA    | 2132   | U    | 2.5  |
| 25  | DA    | 362(F) | A    | 2.5  |
| 25  | DA    | 887    | A    | 2.5  |
| 25  | DA    | 2629   | A    | 2.5  |
| 26  | BB    | 1      | U    | 2.5  |
| 11  | CK    | 49     | GLY  | 2.5  |
| 30  | BF    | 134    | GLY  | 2.5  |
| 37  | BQ    | 19     | GLY  | 2.5  |
| 12  | CL    | 20     | LYS  | 2.5  |
| 27  | DC    | 141    | LYS  | 2.5  |
| 39  | BS    | 33     | LYS  | 2.5  |
| 29  | BE    | 61     | ARG  | 2.5  |
| 37  | DQ    | 10     | ARG  | 2.5  |
| 10  | CJ    | 64     | GLU  | 2.5  |
| 47  | D0    | 7      | LEU  | 2.5  |
| 26  | BB    | 119    | G    | 2.5  |
| 27  | DC    | 139    | ASN  | 2.5  |
| 53  | B6    | 13     | CYS  | 2.5  |
| 1   | CA    | 1064   | G    | 2.5  |
| 25  | DA    | 989    | G    | 2.5  |
| 1   | AA    | 1129   | C    | 2.5  |
| 1   | CA    | 1030   | C    | 2.5  |
| 23  | AW    | 49     | C    | 2.5  |
| 26  | DB    | 109    | C    | 2.5  |
| 36  | BP    | 73     | GLY  | 2.5  |
| 45  | DY    | 81     | LYS  | 2.5  |
| 56  | D9    | 2      | LYS  | 2.5  |
| 1   | AA    | 871    | U    | 2.5  |
| 23  | CW    | 59     | U    | 2.5  |
| 25  | BA    | 1046   | A    | 2.5  |
| 25  | DA    | 1722   | A    | 2.5  |
| 52  | B5    | 58     | LEU  | 2.5  |
| 37  | BQ    | 139    | GLU  | 2.5  |
| 47  | B0    | 4      | LYS  | 2.5  |
| 36  | DP    | 26     | GLY  | 2.5  |
| 56  | B9    | 21     | GLY  | 2.5  |
| 56  | B9    | 4      | ARG  | 2.5  |
| 2   | AB    | 81     | VAL  | 2.5  |
| 32  | BH    | 65     | HIS  | 2.5  |
| 51  | D4    | 40     | HIS  | 2.5  |
| 1   | CA    | 63     | C    | 2.5  |
| 1   | CA    | 174    | C    | 2.5  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 1          | CA           | 345        | C           | 2.5         |
| 1          | AA           | 1034       | G           | 2.5         |
| 1          | AA           | 1094       | G           | 2.5         |
| 32         | BH           | 32         | GLU         | 2.5         |
| 41         | DU           | 89         | GLU         | 2.5         |
| 1          | CA           | 1364       | U           | 2.5         |
| 25         | BA           | 1272       | A           | 2.5         |
| 31         | DG           | 82         | LEU         | 2.5         |
| 4          | CD           | 22         | LYS         | 2.4         |
| 56         | D9           | 31         | LYS         | 2.4         |
| 10         | CJ           | 4          | ILE         | 2.4         |
| 27         | BC           | 174        | PRO         | 2.4         |
| 27         | DC           | 140        | PRO         | 2.4         |
| 49         | D2           | 51         | ARG         | 2.4         |
| 9          | CI           | 105        | ASP         | 2.4         |
| 25         | DA           | 886        | C           | 2.4         |
| 25         | DA           | 2108       | C           | 2.4         |
| 4          | AD           | 26         | CYS         | 2.4         |
| 36         | BP           | 57         | THR         | 2.4         |
| 1          | AA           | 1068       | G           | 2.4         |
| 1          | CA           | 1094       | G           | 2.4         |
| 24         | AX           | 14         | A           | 2.4         |
| 25         | BA           | 196        | A           | 2.4         |
| 25         | BA           | 1051       | G           | 2.4         |
| 25         | BA           | 1332       | G           | 2.4         |
| 25         | BA           | 2288       | A           | 2.4         |
| 25         | BA           | 2311       | A           | 2.4         |
| 25         | BA           | 2382       | G           | 2.4         |
| 25         | DA           | 530        | G           | 2.4         |
| 25         | DA           | 1110       | G           | 2.4         |
| 25         | DA           | 2713       | A           | 2.4         |
| 32         | BH           | 141        | VAL         | 2.4         |
| 14         | AN           | 49         | HIS         | 2.4         |
| 33         | DI           | 122        | GLU         | 2.4         |
| 20         | CT           | 72         | LEU         | 2.4         |
| 47         | B0           | 7          | LEU         | 2.4         |
| 37         | BQ           | 59         | ARG         | 2.4         |
| 53         | D6           | 47         | THR         | 2.4         |
| 46         | BZ           | 175        | VAL         | 2.4         |
| 3          | CC           | 161        | GLU         | 2.4         |
| 32         | DH           | 86         | GLU         | 2.4         |
| 25         | BA           | 562        | U           | 2.4         |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 15  | CO    | 62   | GLN  | 2.4  |
| 25  | BA    | 2896 | C    | 2.4  |
| 25  | DA    | 2107 | C    | 2.4  |
| 25  | DA    | 2473 | U    | 2.4  |
| 25  | DA    | 2612 | C    | 2.4  |
| 40  | BT    | 112  | ARG  | 2.4  |
| 1   | CA    | 794  | A    | 2.4  |
| 25  | BA    | 331  | A    | 2.4  |
| 25  | BA    | 1301 | A    | 2.4  |
| 36  | DP    | 13   | ASN  | 2.4  |
| 7   | CG    | 82   | GLY  | 2.4  |
| 47  | D0    | 8    | GLY  | 2.4  |
| 1   | AA    | 1202 | G    | 2.4  |
| 25  | BA    | 363  | G    | 2.4  |
| 25  | DA    | 2751 | G    | 2.4  |
| 11  | AK    | 127  | LYS  | 2.4  |
| 38  | BR    | 14   | SER  | 2.4  |
| 41  | BU    | 93   | LYS  | 2.4  |
| 3   | AC    | 188  | LEU  | 2.4  |
| 44  | DX    | 92   | LEU  | 2.4  |
| 4   | AD    | 24   | GLU  | 2.4  |
| 34  | BN    | 1    | MET  | 2.4  |
| 11  | AK    | 26   | ASN  | 2.4  |
| 25  | BA    | 2172 | U    | 2.4  |
| 25  | DA    | 913  | U    | 2.4  |
| 25  | DA    | 2150 | U    | 2.4  |
| 12  | CL    | 27   | LEU  | 2.4  |
| 25  | BA    | 587  | C    | 2.4  |
| 25  | DA    | 1532 | C    | 2.4  |
| 38  | BR    | 72   | ASP  | 2.4  |
| 1   | AA    | 88   | A    | 2.4  |
| 25  | BA    | 1490 | A    | 2.4  |
| 25  | BA    | 2117 | A    | 2.4  |
| 9   | CI    | 12   | GLU  | 2.4  |
| 21  | AU    | 24   | ARG  | 2.4  |
| 32  | DH    | 69   | ARG  | 2.4  |
| 40  | DT    | 23   | ARG  | 2.4  |
| 48  | D1    | 26   | ARG  | 2.4  |
| 49  | D2    | 56   | GLN  | 2.4  |
| 25  | BA    | 669  | G    | 2.4  |
| 25  | DA    | 2121 | G    | 2.4  |
| 9   | CI    | 123  | PRO  | 2.4  |

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| Mol | Chain | Res    | Type | RSRZ |
|-----|-------|--------|------|------|
| 39  | DS    | 112    | PHE  | 2.4  |
| 13  | CM    | 7      | VAL  | 2.4  |
| 29  | BE    | 72     | VAL  | 2.4  |
| 32  | DH    | 122    | THR  | 2.4  |
| 36  | BP    | 95     | VAL  | 2.4  |
| 45  | BY    | 51     | VAL  | 2.4  |
| 53  | B6    | 23     | THR  | 2.4  |
| 36  | DP    | 106    | LEU  | 2.4  |
| 45  | DY    | 2      | ARG  | 2.4  |
| 32  | DH    | 18     | GLU  | 2.4  |
| 34  | BN    | 68     | GLU  | 2.4  |
| 13  | AM    | 122    | LYS  | 2.4  |
| 25  | BA    | 2712   | U    | 2.3  |
| 25  | DA    | 1693   | U    | 2.3  |
| 1   | AA    | 47     | C    | 2.3  |
| 1   | AA    | 454    | C    | 2.3  |
| 1   | CA    | 315    | A    | 2.3  |
| 1   | CA    | 975    | A    | 2.3  |
| 25  | BA    | 1395   | A    | 2.3  |
| 25  | BA    | 2175   | C    | 2.3  |
| 25  | DA    | 2173   | A    | 2.3  |
| 32  | DH    | 99     | VAL  | 2.3  |
| 29  | BE    | 151    | TYR  | 2.3  |
| 1   | AA    | 993    | G    | 2.3  |
| 7   | AG    | 36     | LYS  | 2.3  |
| 25  | BA    | 2795   | G    | 2.3  |
| 54  | D7    | 32     | LYS  | 2.3  |
| 4   | CD    | 81     | GLU  | 2.3  |
| 27  | DC    | 217    | THR  | 2.3  |
| 25  | DA    | 272(A) | U    | 2.3  |
| 36  | DP    | 65     | ARG  | 2.3  |
| 37  | BQ    | 56     | ARG  | 2.3  |
| 33  | DI    | 95     | LYS  | 2.3  |
| 1   | CA    | 197    | A    | 2.3  |
| 1   | CA    | 1054   | C    | 2.3  |
| 17  | AQ    | 96     | GLU  | 2.3  |
| 25  | DA    | 2129   | C    | 2.3  |
| 52  | B5    | 53     | ALA  | 2.3  |
| 45  | DY    | 29     | GLU  | 2.3  |
| 27  | BC    | 49     | ILE  | 2.3  |
| 32  | BH    | 171    | LEU  | 2.3  |
| 19  | CS    | 41     | VAL  | 2.3  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 27         | BC           | 139        | ASN         | 2.3         |
| 4          | CD           | 26         | CYS         | 2.3         |
| 1          | AA           | 576        | G           | 2.3         |
| 22         | CV           | 54         | G           | 2.3         |
| 25         | BA           | 1044       | G           | 2.3         |
| 27         | BC           | 173        | ALA         | 2.3         |
| 27         | DC           | 213        | TYR         | 2.3         |
| 55         | B8           | 32         | LEU         | 2.3         |
| 25         | BA           | 1420       | U           | 2.3         |
| 25         | DA           | 2689       | U           | 2.3         |
| 25         | BA           | 311        | A           | 2.3         |
| 36         | DP           | 41         | ARG         | 2.3         |
| 43         | BW           | 92         | ARG         | 2.3         |
| 1          | AA           | 979        | C           | 2.3         |
| 23         | CW           | 17         | C           | 2.3         |
| 25         | BA           | 2402       | C           | 2.3         |
| 25         | DA           | 885        | C           | 2.3         |
| 51         | B4           | 51         | TYR         | 2.3         |
| 20         | CT           | 64         | ASP         | 2.3         |
| 29         | BE           | 126        | PRO         | 2.3         |
| 2          | CB           | 40         | HIS         | 2.3         |
| 45         | BY           | 86         | ARG         | 2.3         |
| 1          | AA           | 306        | G           | 2.3         |
| 1          | AA           | 351        | G           | 2.3         |
| 1          | AA           | 1117       | G           | 2.3         |
| 25         | DA           | 411        | G           | 2.3         |
| 11         | CK           | 42         | TRP         | 2.3         |
| 36         | DP           | 115        | LEU         | 2.3         |
| 1          | AA           | 1390       | U           | 2.3         |
| 45         | BY           | 44         | ILE         | 2.3         |
| 1          | AA           | 975        | A           | 2.3         |
| 1          | CA           | 88         | A           | 2.3         |
| 22         | CV           | 36         | A           | 2.3         |
| 1          | AA           | 796        | C           | 2.3         |
| 27         | BC           | 50         | ASP         | 2.3         |
| 51         | B4           | 66         | HIS         | 2.2         |
| 45         | DY           | 48         | ALA         | 2.2         |
| 40         | DT           | 32         | TYR         | 2.2         |
| 12         | AL           | 91         | LYS         | 2.2         |
| 1          | CA           | 1030(A)    | G           | 2.2         |
| 21         | CU           | 9          | ARG         | 2.2         |
| 42         | DV           | 48         | GLY         | 2.2         |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 46  | BZ    | 139  | VAL  | 2.2  |
| 25  | BA    | 2207 | G    | 2.2  |
| 27  | DC    | 50   | ASP  | 2.2  |
| 36  | DP    | 148  | LEU  | 2.2  |
| 20  | CT    | 75   | ASN  | 2.2  |
| 2   | AB    | 70   | PHE  | 2.2  |
| 20  | CT    | 55   | ILE  | 2.2  |
| 1   | AA    | 1447 | A    | 2.2  |
| 24  | AX    | 15   | A    | 2.2  |
| 25  | BA    | 332  | A    | 2.2  |
| 25  | BA    | 529  | A    | 2.2  |
| 27  | BC    | 76   | ALA  | 2.2  |
| 19  | CS    | 18   | LYS  | 2.2  |
| 42  | DV    | 6    | LYS  | 2.2  |
| 3   | CC    | 166  | GLU  | 2.2  |
| 27  | BC    | 41   | VAL  | 2.2  |
| 49  | D2    | 12   | GLU  | 2.2  |
| 19  | CS    | 68   | GLY  | 2.2  |
| 31  | BG    | 2    | PRO  | 2.2  |
| 56  | B9    | 10   | ILE  | 2.2  |
| 1   | AA    | 90   | U    | 2.2  |
| 1   | AA    | 686  | U    | 2.2  |
| 1   | AA    | 1364 | U    | 2.2  |
| 25  | DA    | 2109 | U    | 2.2  |
| 29  | DE    | 204  | ALA  | 2.2  |
| 34  | DN    | 109  | LYS  | 2.2  |
| 1   | AA    | 425  | G    | 2.2  |
| 1   | AA    | 855  | G    | 2.2  |
| 19  | AS    | 81   | ARG  | 2.2  |
| 25  | BA    | 530  | G    | 2.2  |
| 25  | BA    | 1252 | G    | 2.2  |
| 25  | DA    | 1858 | G    | 2.2  |
| 46  | DZ    | 79   | ARG  | 2.2  |
| 13  | AM    | 119  | GLY  | 2.2  |
| 20  | CT    | 51   | GLU  | 2.2  |
| 28  | DD    | 236  | GLY  | 2.2  |
| 32  | DH    | 116  | GLU  | 2.2  |
| 36  | DP    | 116  | GLY  | 2.2  |
| 37  | DQ    | 48   | GLU  | 2.2  |
| 42  | BV    | 8    | GLY  | 2.2  |
| 56  | D9    | 21   | GLY  | 2.2  |
| 1   | AA    | 1130 | A    | 2.2  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 25  | BA    | 1286 | A    | 2.2  |
| 25  | BA    | 2062 | A    | 2.2  |
| 25  | BA    | 2448 | A    | 2.2  |
| 25  | DA    | 899  | A    | 2.2  |
| 27  | BC    | 40   | THR  | 2.2  |
| 56  | D9    | 10   | ILE  | 2.2  |
| 51  | D4    | 39   | CYS  | 2.2  |
| 10  | AJ    | 12   | ASP  | 2.2  |
| 2   | CB    | 140  | HIS  | 2.2  |
| 31  | BG    | 86   | MET  | 2.2  |
| 30  | DF    | 72   | ARG  | 2.2  |
| 31  | BG    | 113  | ARG  | 2.2  |
| 32  | BH    | 26   | VAL  | 2.2  |
| 39  | BS    | 98   | VAL  | 2.2  |
| 34  | BN    | 139  | GLU  | 2.2  |
| 43  | BW    | 6    | ILE  | 2.2  |
| 1   | CA    | 723  | U    | 2.2  |
| 36  | BP    | 29   | LYS  | 2.2  |
| 21  | CU    | 5    | ASP  | 2.2  |
| 40  | DT    | 26   | ASP  | 2.2  |
| 46  | BZ    | 113  | ALA  | 2.2  |
| 1   | AA    | 1190 | G    | 2.2  |
| 1   | CA    | 31   | G    | 2.2  |
| 1   | CA    | 306  | G    | 2.2  |
| 25  | BA    | 2833 | G    | 2.2  |
| 25  | DA    | 10   | G    | 2.2  |
| 14  | CN    | 3    | ARG  | 2.2  |
| 32  | BH    | 84   | SER  | 2.2  |
| 47  | B0    | 44   | ARG  | 2.2  |
| 4   | CD    | 38   | TYR  | 2.2  |
| 5   | AE    | 69   | VAL  | 2.2  |
| 19  | AS    | 9    | VAL  | 2.2  |
| 28  | BD    | 229  | VAL  | 2.2  |
| 1   | CA    | 121  | C    | 2.2  |
| 8   | CH    | 99   | GLU  | 2.2  |
| 10  | CJ    | 37   | PRO  | 2.2  |
| 39  | DS    | 111  | GLU  | 2.2  |
| 16  | CP    | 69   | THR  | 2.2  |
| 25  | BA    | 2849 | U    | 2.1  |
| 25  | DA    | 1820 | U    | 2.1  |
| 25  | DA    | 1991 | U    | 2.1  |
| 46  | DZ    | 137  | ILE  | 2.1  |

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| Mol | Chain | Res    | Type | RSRZ |
|-----|-------|--------|------|------|
| 5   | AE    | 83     | GLU  | 2.1  |
| 10  | CJ    | 7      | LYS  | 2.1  |
| 29  | DE    | 62     | PRO  | 2.1  |
| 53  | D6    | 31     | PRO  | 2.1  |
| 55  | B8    | 56     | GLU  | 2.1  |
| 25  | DA    | 2892   | A    | 2.1  |
| 1   | AA    | 189(G) | G    | 2.1  |
| 1   | AA    | 1181   | G    | 2.1  |
| 1   | CA    | 1002   | G    | 2.1  |
| 25  | BA    | 1112   | G    | 2.1  |
| 52  | B5    | 2      | ALA  | 2.1  |
| 44  | BX    | 60     | ARG  | 2.1  |
| 1   | AA    | 701    | C    | 2.1  |
| 1   | CA    | 92     | C    | 2.1  |
| 1   | CA    | 1226   | C    | 2.1  |
| 22  | CV    | 68     | C    | 2.1  |
| 46  | DZ    | 148    | ASP  | 2.1  |
| 47  | B0    | 3      | HIS  | 2.1  |
| 34  | BN    | 62     | VAL  | 2.1  |
| 55  | D8    | 34     | TRP  | 2.1  |
| 12  | CL    | 5      | PRO  | 2.1  |
| 13  | AM    | 113    | PRO  | 2.1  |
| 32  | BH    | 70     | THR  | 2.1  |
| 42  | DV    | 45     | THR  | 2.1  |
| 25  | DA    | 2585   | U    | 2.1  |
| 40  | DT    | 105    | LEU  | 2.1  |
| 12  | CL    | 19     | ARG  | 2.1  |
| 36  | BP    | 33     | ARG  | 2.1  |
| 46  | BZ    | 82     | ARG  | 2.1  |
| 55  | D8    | 33     | ASN  | 2.1  |
| 39  | BS    | 52     | SER  | 2.1  |
| 4   | CD    | 146    | ILE  | 2.1  |
| 10  | AJ    | 7      | LYS  | 2.1  |
| 24  | CX    | 14     | A    | 2.1  |
| 25  | BA    | 1460   | A    | 2.1  |
| 25  | DA    | 1618   | A    | 2.1  |
| 36  | DP    | 142    | GLY  | 2.1  |
| 48  | D1    | 93     | GLU  | 2.1  |
| 1   | CA    | 189(G) | G    | 2.1  |
| 1   | CA    | 1182   | G    | 2.1  |
| 1   | CA    | 1504   | G    | 2.1  |
| 25  | BA    | 932    | G    | 2.1  |

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| Mol | Chain | Res    | Type | RSRZ |
|-----|-------|--------|------|------|
| 25  | DA    | 2116   | G    | 2.1  |
| 1   | CA    | 352    | C    | 2.1  |
| 23  | CW    | 48     | C    | 2.1  |
| 39  | BS    | 30     | ARG  | 2.1  |
| 27  | BC    | 91     | ALA  | 2.1  |
| 17  | AQ    | 97     | SER  | 2.1  |
| 36  | BP    | 40     | SER  | 2.1  |
| 13  | CM    | 31     | LYS  | 2.1  |
| 47  | B0    | 17     | GLN  | 2.1  |
| 56  | B9    | 31     | LYS  | 2.1  |
| 25  | BA    | 272(A) | U    | 2.1  |
| 25  | BA    | 1033   | U    | 2.1  |
| 30  | DF    | 174    | VAL  | 2.1  |
| 27  | BC    | 219    | GLY  | 2.1  |
| 33  | BI    | 134    | PRO  | 2.1  |
| 33  | BI    | 10     | GLU  | 2.1  |
| 53  | D6    | 13     | CYS  | 2.1  |
| 31  | BG    | 128    | ARG  | 2.1  |
| 1   | AA    | 1092   | A    | 2.1  |
| 1   | AA    | 1225   | A    | 2.1  |
| 1   | AA    | 1227   | A    | 2.1  |
| 25  | BA    | 2801   | A    | 2.1  |
| 25  | DA    | 265    | A    | 2.1  |
| 25  | DA    | 1558   | A    | 2.1  |
| 26  | DB    | 52     | A    | 2.1  |
| 27  | DC    | 45     | ALA  | 2.1  |
| 38  | BR    | 109    | ALA  | 2.1  |
| 45  | DY    | 47     | LYS  | 2.1  |
| 4   | AD    | 161    | ASN  | 2.1  |
| 33  | DI    | 15     | VAL  | 2.1  |
| 53  | B6    | 52     | VAL  | 2.1  |
| 54  | D7    | 46     | VAL  | 2.1  |
| 2   | AB    | 215    | LEU  | 2.1  |
| 36  | BP    | 123    | LEU  | 2.1  |
| 1   | AA    | 366    | C    | 2.1  |
| 1   | CA    | 470    | C    | 2.1  |
| 25  | BA    | 975    | C    | 2.1  |
| 25  | BA    | 1251   | C    | 2.1  |
| 26  | BB    | 109    | C    | 2.1  |
| 34  | DN    | 101    | HIS  | 2.1  |
| 1   | AA    | 1050   | G    | 2.1  |
| 1   | CA    | 484    | G    | 2.1  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | CA    | 631  | G    | 2.1  |
| 25  | BA    | 1740 | G    | 2.1  |
| 31  | BG    | 155  | MET  | 2.1  |
| 5   | AE    | 70   | PRO  | 2.1  |
| 13  | CM    | 10   | PRO  | 2.1  |
| 29  | BE    | 127  | ASP  | 2.1  |
| 32  | BH    | 29   | PRO  | 2.1  |
| 46  | DZ    | 154  | ASP  | 2.1  |
| 33  | DI    | 7    | GLU  | 2.1  |
| 14  | CN    | 12   | ARG  | 2.1  |
| 16  | CP    | 75   | ARG  | 2.1  |
| 40  | DT    | 41   | ARG  | 2.1  |
| 1   | AA    | 723  | U    | 2.1  |
| 13  | AM    | 120  | LYS  | 2.1  |
| 25  | DA    | 1101 | U    | 2.1  |
| 41  | BU    | 19   | LYS  | 2.1  |
| 14  | AN    | 32   | SER  | 2.1  |
| 47  | B0    | 2    | ALA  | 2.1  |
| 5   | CE    | 69   | VAL  | 2.1  |
| 30  | DF    | 133  | ASN  | 2.1  |
| 28  | BD    | 147  | LEU  | 2.1  |
| 32  | BH    | 49   | VAL  | 2.1  |
| 33  | DI    | 107  | VAL  | 2.1  |
| 44  | BX    | 52   | VAL  | 2.1  |
| 1   | CA    | 965  | A    | 2.0  |
| 25  | BA    | 2169 | A    | 2.0  |
| 25  | DA    | 2476 | A    | 2.0  |
| 9   | AI    | 128  | ARG  | 2.0  |
| 13  | CM    | 105  | THR  | 2.0  |
| 10  | AJ    | 55   | LYS  | 2.0  |
| 18  | CR    | 68   | LYS  | 2.0  |
| 20  | CT    | 29   | LYS  | 2.0  |
| 36  | DP    | 92   | GLU  | 2.0  |
| 42  | DV    | 53   | GLU  | 2.0  |
| 46  | DZ    | 97   | GLU  | 2.0  |
| 36  | BP    | 51   | PHE  | 2.0  |
| 9   | CI    | 109  | VAL  | 2.0  |
| 25  | BA    | 961  | C    | 2.0  |
| 25  | DA    | 2347 | C    | 2.0  |
| 36  | BP    | 88   | LEU  | 2.0  |
| 1   | AA    | 1002 | G    | 2.0  |
| 1   | AA    | 1224 | G    | 2.0  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | CA    | 61   | G    | 2.0  |
| 25  | DA    | 1236 | G    | 2.0  |
| 25  | DA    | 1325 | G    | 2.0  |
| 25  | DA    | 1899 | G    | 2.0  |
| 25  | DA    | 2458 | G    | 2.0  |
| 26  | DB    | 119  | G    | 2.0  |
| 31  | DG    | 42   | GLY  | 2.0  |
| 36  | DP    | 69   | GLY  | 2.0  |
| 4   | CD    | 36   | ARG  | 2.0  |
| 10  | CJ    | 96   | ILE  | 2.0  |
| 20  | CT    | 58   | LYS  | 2.0  |
| 30  | BF    | 10   | PRO  | 2.0  |
| 39  | DS    | 3    | ARG  | 2.0  |
| 36  | DP    | 58   | THR  | 2.0  |
| 9   | CI    | 60   | ASP  | 2.0  |
| 40  | BT    | 26   | ASP  | 2.0  |
| 45  | BY    | 91   | GLU  | 2.0  |
| 55  | D8    | 65   | GLU  | 2.0  |
| 8   | AH    | 107  | LEU  | 2.0  |
| 28  | DD    | 33   | LEU  | 2.0  |
| 1   | AA    | 1093 | A    | 2.0  |
| 1   | CA    | 1492 | A    | 2.0  |
| 25  | DA    | 1174 | A    | 2.0  |
| 25  | DA    | 1938 | A    | 2.0  |
| 25  | DA    | 2750 | A    | 2.0  |
| 34  | BN    | 8    | GLN  | 2.0  |
| 49  | D2    | 70   | GLN  | 2.0  |
| 21  | CU    | 25   | LYS  | 2.0  |
| 28  | BD    | 43   | ARG  | 2.0  |
| 38  | DR    | 9    | LYS  | 2.0  |
| 14  | CN    | 14   | PRO  | 2.0  |
| 36  | DP    | 72   | PRO  | 2.0  |
| 53  | B6    | 41   | PRO  | 2.0  |
| 55  | D8    | 46   | ARG  | 2.0  |
| 25  | BA    | 2258 | C    | 2.0  |
| 36  | BP    | 115  | LEU  | 2.0  |
| 38  | BR    | 111  | LEU  | 2.0  |
| 40  | BT    | 105  | LEU  | 2.0  |
| 20  | AT    | 106  | ALA  | 2.0  |
| 22  | CV    | 18   | U    | 2.0  |
| 25  | BA    | 72   | U    | 2.0  |
| 25  | DA    | 2172 | U    | 2.0  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 33  | DI    | 143 | SER  | 2.0  |
| 34  | BN    | 47  | ALA  | 2.0  |
| 11  | AK    | 114 | VAL  | 2.0  |
| 17  | CQ    | 35  | VAL  | 2.0  |
| 33  | DI    | 145 | VAL  | 2.0  |

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 57  | MG   | DA    | 9660 | 1/1   | 0.30 | 0.27 | 176,176,176,176            | 0     |
| 57  | MG   | CA    | 1691 | 1/1   | 0.32 | 0.38 | 91,91,91,91                | 0     |
| 57  | MG   | BA    | 3315 | 1/1   | 0.34 | 0.15 | 84,84,84,84                | 0     |
| 57  | MG   | DA    | 9475 | 1/1   | 0.37 | 0.16 | 26,26,26,26                | 0     |
| 57  | MG   | BA    | 3086 | 1/1   | 0.38 | 0.17 | 1,1,1,1                    | 0     |
| 57  | MG   | DB    | 204  | 1/1   | 0.38 | 0.52 | 0,0,0,0                    | 1     |
| 57  | MG   | CA    | 1610 | 1/1   | 0.44 | 0.23 | 58,58,58,58                | 0     |
| 57  | MG   | BA    | 3082 | 1/1   | 0.48 | 0.27 | 23,23,23,23                | 0     |
| 57  | MG   | CA    | 1694 | 1/1   | 0.49 | 0.20 | 51,51,51,51                | 0     |
| 57  | MG   | BA    | 3322 | 1/1   | 0.51 | 0.24 | 54,54,54,54                | 0     |
| 57  | MG   | BA    | 3036 | 1/1   | 0.51 | 0.30 | 78,78,78,78                | 1     |
| 57  | MG   | DA    | 9441 | 1/1   | 0.51 | 0.24 | 31,31,31,31                | 1     |
| 57  | MG   | BA    | 3273 | 1/1   | 0.53 | 0.15 | 71,71,71,71                | 0     |
| 57  | MG   | BA    | 3033 | 1/1   | 0.55 | 0.11 | 6,6,6,6                    | 0     |
| 57  | MG   | DA    | 9600 | 1/1   | 0.55 | 0.23 | 55,55,55,55                | 0     |
| 57  | MG   | DA    | 9380 | 1/1   | 0.56 | 0.40 | 23,23,23,23                | 1     |
| 57  | MG   | BB    | 205  | 1/1   | 0.56 | 0.28 | 19,19,19,19                | 1     |
| 57  | MG   | DA    | 9402 | 1/1   | 0.57 | 0.32 | 25,25,25,25                | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | AA    | 7071 | 1/1   | 0.58 | 0.16 | 38,38,38,38                 | 0     |
| 57  | MG   | DA    | 9352 | 1/1   | 0.58 | 0.09 | 89,89,89,89                 | 0     |
| 57  | MG   | BA    | 3265 | 1/1   | 0.58 | 0.37 | 43,43,43,43                 | 0     |
| 57  | MG   | BA    | 3286 | 1/1   | 0.59 | 0.15 | 22,22,22,22                 | 0     |
| 57  | MG   | DA    | 9367 | 1/1   | 0.61 | 0.25 | 35,35,35,35                 | 0     |
| 57  | MG   | CA    | 1716 | 1/1   | 0.62 | 0.15 | 26,26,26,26                 | 0     |
| 57  | MG   | DA    | 9666 | 1/1   | 0.63 | 0.21 | 7,7,7,7                     | 0     |
| 57  | MG   | BA    | 3037 | 1/1   | 0.64 | 0.23 | 83,83,83,83                 | 0     |
| 57  | MG   | DA    | 9638 | 1/1   | 0.65 | 0.09 | 8,8,8,8                     | 1     |
| 57  | MG   | DA    | 9685 | 1/1   | 0.65 | 0.26 | 22,22,22,22                 | 0     |
| 57  | MG   | CA    | 1736 | 1/1   | 0.65 | 0.11 | 6,6,6,6                     | 0     |
| 57  | MG   | D1    | 101  | 1/1   | 0.65 | 0.16 | 55,55,55,55                 | 0     |
| 57  | MG   | AX    | 101  | 1/1   | 0.66 | 0.21 | 43,43,43,43                 | 0     |
| 57  | MG   | BP    | 201  | 1/1   | 0.66 | 0.28 | 166,166,166,166             | 0     |
| 57  | MG   | BB    | 202  | 1/1   | 0.67 | 0.13 | 62,62,62,62                 | 0     |
| 57  | MG   | CA    | 1719 | 1/1   | 0.67 | 0.19 | 10,10,10,10                 | 0     |
| 57  | MG   | BA    | 3320 | 1/1   | 0.67 | 0.34 | 54,54,54,54                 | 0     |
| 57  | MG   | AA    | 7076 | 1/1   | 0.67 | 0.27 | 60,60,60,60                 | 0     |
| 57  | MG   | DA    | 9655 | 1/1   | 0.68 | 0.35 | 35,35,35,35                 | 0     |
| 57  | MG   | BA    | 3063 | 1/1   | 0.68 | 0.21 | 55,55,55,55                 | 0     |
| 57  | MG   | DA    | 9350 | 1/1   | 0.69 | 0.20 | 48,48,48,48                 | 1     |
| 57  | MG   | DA    | 9661 | 1/1   | 0.69 | 0.29 | 57,57,57,57                 | 0     |
| 57  | MG   | BA    | 3076 | 1/1   | 0.70 | 0.16 | 18,18,18,18                 | 0     |
| 57  | MG   | DA    | 9425 | 1/1   | 0.70 | 0.31 | 37,37,37,37                 | 0     |
| 57  | MG   | BA    | 3137 | 1/1   | 0.70 | 0.40 | 1,1,1,1                     | 1     |
| 57  | MG   | DA    | 9658 | 1/1   | 0.70 | 0.13 | 36,36,36,36                 | 0     |
| 57  | MG   | DB    | 205  | 1/1   | 0.70 | 0.14 | 6,6,6,6                     | 1     |
| 57  | MG   | DW    | 201  | 1/1   | 0.70 | 0.23 | 27,27,27,27                 | 0     |
| 57  | MG   | AA    | 7057 | 1/1   | 0.70 | 0.12 | 44,44,44,44                 | 0     |
| 57  | MG   | CA    | 1739 | 1/1   | 0.71 | 0.23 | 36,36,36,36                 | 0     |
| 57  | MG   | DA    | 9644 | 1/1   | 0.71 | 0.16 | 25,25,25,25                 | 0     |
| 57  | MG   | BA    | 3196 | 1/1   | 0.71 | 0.39 | 30,30,30,30                 | 0     |
| 57  | MG   | BA    | 3101 | 1/1   | 0.72 | 0.46 | 27,27,27,27                 | 1     |
| 57  | MG   | DA    | 9674 | 1/1   | 0.72 | 0.25 | 17,17,17,17                 | 0     |
| 57  | MG   | BA    | 3028 | 1/1   | 0.72 | 0.19 | 44,44,44,44                 | 0     |
| 57  | MG   | DA    | 9429 | 1/1   | 0.72 | 0.32 | 51,51,51,51                 | 0     |
| 57  | MG   | BA    | 3053 | 1/1   | 0.72 | 0.16 | 17,17,17,17                 | 0     |
| 57  | MG   | BA    | 3242 | 1/1   | 0.72 | 0.26 | 44,44,44,44                 | 0     |
| 57  | MG   | DA    | 9399 | 1/1   | 0.72 | 0.47 | 52,52,52,52                 | 0     |
| 57  | MG   | DA    | 9630 | 1/1   | 0.73 | 0.18 | 16,16,16,16                 | 1     |
| 57  | MG   | BA    | 3093 | 1/1   | 0.73 | 0.25 | 49,49,49,49                 | 0     |
| 57  | MG   | CA    | 1672 | 1/1   | 0.73 | 0.26 | 62,62,62,62                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | DA    | 9467 | 1/1   | 0.73 | 0.18 | 53,53,53,53                 | 1     |
| 57  | MG   | CA    | 1674 | 1/1   | 0.73 | 0.20 | 89,89,89,89                 | 0     |
| 57  | MG   | DA    | 9494 | 1/1   | 0.73 | 0.27 | 39,39,39,39                 | 0     |
| 57  | MG   | AV    | 105  | 1/1   | 0.73 | 0.25 | 54,54,54,54                 | 0     |
| 57  | MG   | DA    | 9688 | 1/1   | 0.74 | 0.30 | 78,78,78,78                 | 0     |
| 57  | MG   | CA    | 1609 | 1/1   | 0.74 | 0.16 | 30,30,30,30                 | 0     |
| 57  | MG   | DA    | 9671 | 1/1   | 0.74 | 0.31 | 45,45,45,45                 | 0     |
| 57  | MG   | BA    | 3149 | 1/1   | 0.74 | 0.11 | 27,27,27,27                 | 0     |
| 57  | MG   | AA    | 7090 | 1/1   | 0.74 | 0.41 | 69,69,69,69                 | 0     |
| 57  | MG   | CA    | 1708 | 1/1   | 0.75 | 0.16 | 34,34,34,34                 | 0     |
| 57  | MG   | DB    | 202  | 1/1   | 0.75 | 0.10 | 28,28,28,28                 | 0     |
| 57  | MG   | BA    | 3173 | 1/1   | 0.75 | 0.29 | 27,27,27,27                 | 0     |
| 57  | MG   | BA    | 3313 | 1/1   | 0.75 | 0.12 | 42,42,42,42                 | 0     |
| 57  | MG   | CA    | 1722 | 1/1   | 0.75 | 0.23 | 27,27,27,27                 | 0     |
| 57  | MG   | DA    | 9634 | 1/1   | 0.75 | 0.20 | 44,44,44,44                 | 0     |
| 57  | MG   | DA    | 9501 | 1/1   | 0.76 | 0.30 | 42,42,42,42                 | 0     |
| 57  | MG   | DA    | 9567 | 1/1   | 0.76 | 0.16 | 31,31,31,31                 | 0     |
| 57  | MG   | DA    | 9693 | 1/1   | 0.76 | 0.34 | 47,47,47,47                 | 0     |
| 57  | MG   | AA    | 7088 | 1/1   | 0.76 | 0.14 | 60,60,60,60                 | 0     |
| 57  | MG   | CA    | 1680 | 1/1   | 0.76 | 0.17 | 49,49,49,49                 | 0     |
| 57  | MG   | CW    | 101  | 1/1   | 0.76 | 0.07 | 29,29,29,29                 | 1     |
| 57  | MG   | BA    | 3248 | 1/1   | 0.76 | 0.22 | 49,49,49,49                 | 0     |
| 57  | MG   | BA    | 3227 | 1/1   | 0.76 | 0.22 | 40,40,40,40                 | 0     |
| 57  | MG   | AA    | 7059 | 1/1   | 0.77 | 0.29 | 96,96,96,96                 | 0     |
| 57  | MG   | DA    | 9396 | 1/1   | 0.77 | 0.19 | 26,26,26,26                 | 0     |
| 57  | MG   | DA    | 9503 | 1/1   | 0.77 | 0.20 | 66,66,66,66                 | 0     |
| 57  | MG   | DA    | 9530 | 1/1   | 0.77 | 0.38 | 41,41,41,41                 | 0     |
| 57  | MG   | AA    | 7083 | 1/1   | 0.77 | 0.22 | 18,18,18,18                 | 0     |
| 57  | MG   | DA    | 9574 | 1/1   | 0.77 | 0.16 | 14,14,14,14                 | 1     |
| 57  | MG   | BA    | 3133 | 1/1   | 0.77 | 0.14 | 43,43,43,43                 | 0     |
| 57  | MG   | CA    | 1707 | 1/1   | 0.77 | 0.40 | 1,1,1,1                     | 1     |
| 57  | MG   | DA    | 9695 | 1/1   | 0.77 | 0.34 | 63,63,63,63                 | 0     |
| 57  | MG   | AA    | 7060 | 1/1   | 0.77 | 0.09 | 8,8,8,8                     | 0     |
| 57  | MG   | AA    | 7008 | 1/1   | 0.77 | 0.40 | 35,35,35,35                 | 0     |
| 57  | MG   | DA    | 9358 | 1/1   | 0.77 | 0.48 | 5,5,5,5                     | 0     |
| 57  | MG   | AA    | 7074 | 1/1   | 0.77 | 0.32 | 26,26,26,26                 | 0     |
| 57  | MG   | DA    | 9490 | 1/1   | 0.77 | 0.27 | 39,39,39,39                 | 0     |
| 57  | MG   | CA    | 1614 | 1/1   | 0.78 | 0.28 | 38,38,38,38                 | 0     |
| 57  | MG   | BA    | 3319 | 1/1   | 0.78 | 0.08 | 27,27,27,27                 | 0     |
| 57  | MG   | BA    | 3262 | 1/1   | 0.78 | 0.22 | 39,39,39,39                 | 0     |
| 57  | MG   | DA    | 9477 | 1/1   | 0.78 | 0.26 | 36,36,36,36                 | 0     |
| 57  | MG   | AA    | 7023 | 1/1   | 0.79 | 0.10 | 56,56,56,56                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | AA    | 7070 | 1/1   | 0.79 | 0.15 | 61,61,61,61                 | 0     |
| 57  | MG   | BA    | 3109 | 1/1   | 0.79 | 0.26 | 66,66,66,66                 | 0     |
| 57  | MG   | DA    | 9453 | 1/1   | 0.79 | 0.39 | 4,4,4,4                     | 1     |
| 57  | MG   | DA    | 9333 | 1/1   | 0.79 | 0.15 | 31,31,31,31                 | 0     |
| 57  | MG   | DA    | 9347 | 1/1   | 0.79 | 0.18 | 22,22,22,22                 | 0     |
| 57  | MG   | BA    | 3231 | 1/1   | 0.79 | 0.17 | 90,90,90,90                 | 0     |
| 57  | MG   | BA    | 3236 | 1/1   | 0.79 | 0.23 | 17,17,17,17                 | 0     |
| 57  | MG   | DA    | 9493 | 1/1   | 0.79 | 0.17 | 1,1,1,1                     | 0     |
| 57  | MG   | BA    | 3126 | 1/1   | 0.79 | 0.25 | 44,44,44,44                 | 0     |
| 57  | MG   | AA    | 7109 | 1/1   | 0.79 | 0.18 | 33,33,33,33                 | 0     |
| 57  | MG   | BA    | 3252 | 1/1   | 0.79 | 0.30 | 56,56,56,56                 | 0     |
| 57  | MG   | DA    | 9388 | 1/1   | 0.79 | 0.12 | 28,28,28,28                 | 0     |
| 57  | MG   | BA    | 3030 | 1/1   | 0.79 | 0.28 | 22,22,22,22                 | 0     |
| 57  | MG   | DA    | 9397 | 1/1   | 0.79 | 0.31 | 25,25,25,25                 | 1     |
| 57  | MG   | BA    | 3088 | 1/1   | 0.79 | 0.20 | 43,43,43,43                 | 0     |
| 57  | MG   | BA    | 3167 | 1/1   | 0.79 | 0.16 | 30,30,30,30                 | 0     |
| 57  | MG   | DA    | 9419 | 1/1   | 0.79 | 0.19 | 10,10,10,10                 | 1     |
| 57  | MG   | CA    | 1641 | 1/1   | 0.80 | 0.14 | 40,40,40,40                 | 0     |
| 57  | MG   | CA    | 1697 | 1/1   | 0.80 | 0.13 | 49,49,49,49                 | 0     |
| 57  | MG   | CA    | 1643 | 1/1   | 0.80 | 0.28 | 40,40,40,40                 | 1     |
| 57  | MG   | BA    | 3128 | 1/1   | 0.80 | 0.14 | 57,57,57,57                 | 0     |
| 57  | MG   | CA    | 1673 | 1/1   | 0.80 | 0.14 | 18,18,18,18                 | 0     |
| 57  | MG   | AA    | 7029 | 1/1   | 0.80 | 0.22 | 41,41,41,41                 | 0     |
| 57  | MG   | BA    | 3062 | 1/1   | 0.80 | 0.08 | 27,27,27,27                 | 0     |
| 57  | MG   | CA    | 1687 | 1/1   | 0.80 | 0.21 | 47,47,47,47                 | 0     |
| 57  | MG   | CA    | 1737 | 1/1   | 0.80 | 0.29 | 28,28,28,28                 | 0     |
| 57  | MG   | BA    | 3095 | 1/1   | 0.80 | 0.31 | 35,35,35,35                 | 0     |
| 57  | MG   | CA    | 1650 | 1/1   | 0.81 | 0.29 | 34,34,34,34                 | 0     |
| 57  | MG   | AA    | 7002 | 1/1   | 0.81 | 0.15 | 35,35,35,35                 | 0     |
| 57  | MG   | BA    | 3145 | 1/1   | 0.81 | 0.18 | 22,22,22,22                 | 0     |
| 57  | MG   | CA    | 1728 | 1/1   | 0.81 | 0.11 | 59,59,59,59                 | 0     |
| 57  | MG   | BB    | 203  | 1/1   | 0.81 | 0.31 | 16,16,16,16                 | 1     |
| 57  | MG   | AA    | 7101 | 1/1   | 0.81 | 0.16 | 22,22,22,22                 | 0     |
| 57  | MG   | BA    | 3312 | 1/1   | 0.81 | 0.19 | 45,45,45,45                 | 0     |
| 57  | MG   | DA    | 9415 | 1/1   | 0.81 | 0.32 | 0,0,0,0                     | 0     |
| 57  | MG   | BA    | 3001 | 1/1   | 0.81 | 0.23 | 38,38,38,38                 | 0     |
| 57  | MG   | AA    | 7005 | 1/1   | 0.81 | 0.26 | 45,45,45,45                 | 0     |
| 57  | MG   | BA    | 3318 | 1/1   | 0.81 | 0.27 | 37,37,37,37                 | 0     |
| 57  | MG   | DA    | 9439 | 1/1   | 0.81 | 0.10 | 32,32,32,32                 | 0     |
| 57  | MG   | CA    | 1704 | 1/1   | 0.81 | 0.31 | 28,28,28,28                 | 0     |
| 57  | MG   | BA    | 3079 | 1/1   | 0.81 | 0.26 | 29,29,29,29                 | 1     |
| 57  | MG   | BA    | 3216 | 1/1   | 0.81 | 0.24 | 48,48,48,48                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | DA    | 9651 | 1/1   | 0.81 | 0.10 | 81,81,81,81                 | 0     |
| 57  | MG   | D5    | 102  | 1/1   | 0.81 | 0.14 | 32,32,32,32                 | 1     |
| 57  | MG   | AA    | 7016 | 1/1   | 0.82 | 0.20 | 45,45,45,45                 | 0     |
| 57  | MG   | AA    | 7069 | 1/1   | 0.82 | 0.13 | 11,11,11,11                 | 1     |
| 57  | MG   | DA    | 9458 | 1/1   | 0.82 | 0.13 | 22,22,22,22                 | 0     |
| 57  | MG   | BA    | 3077 | 1/1   | 0.82 | 0.15 | 21,21,21,21                 | 0     |
| 57  | MG   | BA    | 3203 | 1/1   | 0.82 | 0.15 | 37,37,37,37                 | 0     |
| 57  | MG   | BA    | 3115 | 1/1   | 0.82 | 0.19 | 33,33,33,33                 | 0     |
| 57  | MG   | CA    | 1621 | 1/1   | 0.82 | 0.10 | 52,52,52,52                 | 0     |
| 57  | MG   | BA    | 3147 | 1/1   | 0.82 | 0.28 | 48,48,48,48                 | 0     |
| 57  | MG   | DA    | 9412 | 1/1   | 0.82 | 0.17 | 27,27,27,27                 | 0     |
| 57  | MG   | CA    | 1702 | 1/1   | 0.82 | 0.08 | 49,49,49,49                 | 0     |
| 57  | MG   | DA    | 9416 | 1/1   | 0.82 | 0.20 | 38,38,38,38                 | 0     |
| 57  | MG   | DA    | 9523 | 1/1   | 0.82 | 0.33 | 9,9,9,9                     | 0     |
| 57  | MG   | DA    | 9526 | 1/1   | 0.82 | 0.24 | 12,12,12,12                 | 0     |
| 57  | MG   | BA    | 3228 | 1/1   | 0.82 | 0.24 | 13,13,13,13                 | 0     |
| 57  | MG   | BA    | 3282 | 1/1   | 0.82 | 0.10 | 24,24,24,24                 | 0     |
| 57  | MG   | DA    | 9569 | 1/1   | 0.82 | 0.17 | 54,54,54,54                 | 0     |
| 57  | MG   | CA    | 1651 | 1/1   | 0.82 | 0.34 | 39,39,39,39                 | 0     |
| 57  | MG   | DA    | 9431 | 1/1   | 0.82 | 0.29 | 12,12,12,12                 | 0     |
| 57  | MG   | DA    | 9602 | 1/1   | 0.82 | 0.17 | 37,37,37,37                 | 0     |
| 57  | MG   | DA    | 9603 | 1/1   | 0.82 | 0.21 | 33,33,33,33                 | 0     |
| 57  | MG   | AA    | 7035 | 1/1   | 0.82 | 0.20 | 42,42,42,42                 | 0     |
| 57  | MG   | CA    | 1675 | 1/1   | 0.83 | 0.12 | 55,55,55,55                 | 0     |
| 57  | MG   | BA    | 3245 | 1/1   | 0.83 | 0.17 | 45,45,45,45                 | 0     |
| 57  | MG   | CA    | 1684 | 1/1   | 0.83 | 0.17 | 41,41,41,41                 | 0     |
| 57  | MG   | AA    | 7102 | 1/1   | 0.83 | 0.29 | 38,38,38,38                 | 0     |
| 57  | MG   | CA    | 1637 | 1/1   | 0.83 | 0.27 | 57,57,57,57                 | 0     |
| 57  | MG   | CE    | 202  | 1/1   | 0.83 | 0.08 | 34,34,34,34                 | 0     |
| 57  | MG   | BA    | 3306 | 1/1   | 0.83 | 0.23 | 48,48,48,48                 | 0     |
| 57  | MG   | AA    | 7084 | 1/1   | 0.83 | 0.14 | 49,49,49,49                 | 0     |
| 57  | MG   | CA    | 1699 | 1/1   | 0.83 | 0.30 | 45,45,45,45                 | 1     |
| 57  | MG   | BA    | 3255 | 1/1   | 0.83 | 0.23 | 45,45,45,45                 | 0     |
| 57  | MG   | BD    | 301  | 1/1   | 0.83 | 0.32 | 7,7,7,7                     | 0     |
| 57  | MG   | DA    | 9536 | 1/1   | 0.83 | 0.34 | 0,0,0,0                     | 0     |
| 57  | MG   | DA    | 9677 | 1/1   | 0.83 | 0.25 | 27,27,27,27                 | 0     |
| 57  | MG   | DA    | 9681 | 1/1   | 0.83 | 0.17 | 13,13,13,13                 | 0     |
| 57  | MG   | DA    | 9543 | 1/1   | 0.83 | 0.21 | 5,5,5,5                     | 0     |
| 57  | MG   | DA    | 9687 | 1/1   | 0.83 | 0.11 | 12,12,12,12                 | 0     |
| 57  | MG   | DA    | 9545 | 1/1   | 0.83 | 0.21 | 1,1,1,1                     | 0     |
| 57  | MG   | DA    | 9553 | 1/1   | 0.83 | 0.22 | 20,20,20,20                 | 0     |
| 57  | MG   | DA    | 9434 | 1/1   | 0.83 | 0.21 | 4,4,4,4                     | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | CA    | 1654 | 1/1   | 0.83 | 0.10 | 31,31,31,31                 | 0     |
| 57  | MG   | DA    | 9440 | 1/1   | 0.83 | 0.18 | 25,25,25,25                 | 0     |
| 57  | MG   | BA    | 3087 | 1/1   | 0.83 | 0.15 | 21,21,21,21                 | 0     |
| 57  | MG   | BA    | 3039 | 1/1   | 0.83 | 0.20 | 30,30,30,30                 | 0     |
| 57  | MG   | BA    | 3154 | 1/1   | 0.83 | 0.25 | 17,17,17,17                 | 0     |
| 57  | MG   | DA    | 9621 | 1/1   | 0.83 | 0.33 | 0,0,0,0                     | 1     |
| 57  | MG   | BA    | 3121 | 1/1   | 0.84 | 0.27 | 1,1,1,1                     | 0     |
| 57  | MG   | CA    | 1640 | 1/1   | 0.84 | 0.33 | 49,49,49,49                 | 0     |
| 57  | MG   | DA    | 9337 | 1/1   | 0.84 | 0.39 | 45,45,45,45                 | 0     |
| 57  | MG   | DA    | 9573 | 1/1   | 0.84 | 0.22 | 45,45,45,45                 | 0     |
| 57  | MG   | BA    | 3058 | 1/1   | 0.84 | 0.23 | 1,1,1,1                     | 0     |
| 57  | MG   | DA    | 9577 | 1/1   | 0.84 | 0.31 | 102,102,102,102             | 0     |
| 57  | MG   | BA    | 3106 | 1/1   | 0.84 | 0.23 | 34,34,34,34                 | 0     |
| 57  | MG   | BA    | 3003 | 1/1   | 0.84 | 0.13 | 33,33,33,33                 | 0     |
| 57  | MG   | BA    | 3136 | 1/1   | 0.84 | 0.17 | 46,46,46,46                 | 1     |
| 57  | MG   | DA    | 9615 | 1/1   | 0.84 | 0.19 | 45,45,45,45                 | 0     |
| 57  | MG   | BA    | 3195 | 1/1   | 0.84 | 0.19 | 3,3,3,3                     | 0     |
| 57  | MG   | DA    | 9689 | 1/1   | 0.84 | 0.29 | 25,25,25,25                 | 0     |
| 57  | MG   | DA    | 9692 | 1/1   | 0.84 | 0.25 | 30,30,30,30                 | 0     |
| 57  | MG   | DA    | 9629 | 1/1   | 0.84 | 0.10 | 52,52,52,52                 | 0     |
| 57  | MG   | DA    | 9377 | 1/1   | 0.84 | 0.17 | 19,19,19,19                 | 0     |
| 57  | MG   | BA    | 3110 | 1/1   | 0.84 | 0.38 | 23,23,23,23                 | 1     |
| 57  | MG   | AA    | 7036 | 1/1   | 0.84 | 0.18 | 42,42,42,42                 | 0     |
| 57  | MG   | CA    | 1625 | 1/1   | 0.84 | 0.18 | 26,26,26,26                 | 0     |
| 57  | MG   | DA    | 9645 | 1/1   | 0.84 | 0.23 | 4,4,4,4                     | 0     |
| 57  | MG   | CV    | 103  | 1/1   | 0.84 | 0.16 | 43,43,43,43                 | 1     |
| 57  | MG   | CV    | 105  | 1/1   | 0.84 | 0.11 | 69,69,69,69                 | 0     |
| 57  | MG   | DA    | 9385 | 1/1   | 0.85 | 0.11 | 5,5,5,5                     | 0     |
| 57  | MG   | CA    | 1676 | 1/1   | 0.85 | 0.52 | 88,88,88,88                 | 0     |
| 57  | MG   | CA    | 1729 | 1/1   | 0.85 | 0.22 | 35,35,35,35                 | 0     |
| 57  | MG   | BA    | 3111 | 1/1   | 0.85 | 0.23 | 35,35,35,35                 | 0     |
| 57  | MG   | CA    | 1682 | 1/1   | 0.85 | 0.11 | 60,60,60,60                 | 0     |
| 57  | MG   | BA    | 3278 | 1/1   | 0.85 | 0.27 | 22,22,22,22                 | 0     |
| 57  | MG   | CA    | 1639 | 1/1   | 0.85 | 0.19 | 55,55,55,55                 | 0     |
| 57  | MG   | BA    | 3130 | 1/1   | 0.85 | 0.12 | 3,3,3,3                     | 0     |
| 57  | MG   | CV    | 104  | 1/1   | 0.85 | 0.21 | 22,22,22,22                 | 1     |
| 57  | MG   | DA    | 9539 | 1/1   | 0.85 | 0.37 | 35,35,35,35                 | 0     |
| 57  | MG   | BA    | 3160 | 1/1   | 0.85 | 0.26 | 22,22,22,22                 | 0     |
| 57  | MG   | BA    | 3162 | 1/1   | 0.85 | 0.14 | 4,4,4,4                     | 0     |
| 57  | MG   | BA    | 3222 | 1/1   | 0.85 | 0.23 | 5,5,5,5                     | 0     |
| 57  | MG   | BA    | 3131 | 1/1   | 0.85 | 0.18 | 38,38,38,38                 | 0     |
| 57  | MG   | CA    | 1605 | 1/1   | 0.85 | 0.17 | 32,32,32,32                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | CA    | 1664 | 1/1   | 0.85 | 0.17 | 24,24,24,24                 | 0     |
| 57  | MG   | BA    | 3168 | 1/1   | 0.85 | 0.25 | 36,36,36,36                 | 0     |
| 57  | MG   | BA    | 3316 | 1/1   | 0.85 | 0.29 | 7,7,7,7                     | 0     |
| 57  | MG   | DA    | 9578 | 1/1   | 0.85 | 0.25 | 44,44,44,44                 | 0     |
| 57  | MG   | DA    | 9448 | 1/1   | 0.85 | 0.18 | 18,18,18,18                 | 0     |
| 57  | MG   | BA    | 3061 | 1/1   | 0.85 | 0.17 | 32,32,32,32                 | 0     |
| 57  | MG   | DA    | 9371 | 1/1   | 0.85 | 0.20 | 29,29,29,29                 | 0     |
| 57  | MG   | DA    | 9607 | 1/1   | 0.85 | 0.26 | 49,49,49,49                 | 0     |
| 57  | MG   | BA    | 3267 | 1/1   | 0.85 | 0.18 | 41,41,41,41                 | 0     |
| 57  | MG   | CA    | 1725 | 1/1   | 0.85 | 0.25 | 29,29,29,29                 | 0     |
| 57  | MG   | D0    | 101  | 1/1   | 0.85 | 0.28 | 27,27,27,27                 | 0     |
| 57  | MG   | DA    | 9383 | 1/1   | 0.85 | 0.29 | 18,18,18,18                 | 0     |
| 57  | MG   | DA    | 9486 | 1/1   | 0.85 | 0.23 | 21,21,21,21                 | 0     |
| 57  | MG   | DA    | 9487 | 1/1   | 0.86 | 0.29 | 71,71,71,71                 | 0     |
| 57  | MG   | CA    | 1740 | 1/1   | 0.86 | 0.21 | 48,48,48,48                 | 0     |
| 57  | MG   | BA    | 3113 | 1/1   | 0.86 | 0.17 | 49,49,49,49                 | 0     |
| 57  | MG   | DA    | 9643 | 1/1   | 0.86 | 0.33 | 34,34,34,34                 | 1     |
| 57  | MG   | CA    | 1696 | 1/1   | 0.86 | 0.20 | 49,49,49,49                 | 0     |
| 57  | MG   | AA    | 7063 | 1/1   | 0.86 | 0.20 | 31,31,31,31                 | 0     |
| 57  | MG   | DA    | 9405 | 1/1   | 0.86 | 0.11 | 5,5,5,5                     | 0     |
| 57  | MG   | BU    | 201  | 1/1   | 0.86 | 0.28 | 170,170,170,170             | 1     |
| 57  | MG   | DA    | 9657 | 1/1   | 0.86 | 0.16 | 29,29,29,29                 | 0     |
| 57  | MG   | CA    | 1659 | 1/1   | 0.86 | 0.25 | 28,28,28,28                 | 0     |
| 57  | MG   | CY    | 101  | 1/1   | 0.86 | 0.30 | 33,33,33,33                 | 0     |
| 57  | MG   | DA    | 9321 | 1/1   | 0.86 | 0.21 | 35,35,35,35                 | 0     |
| 57  | MG   | DA    | 9421 | 1/1   | 0.86 | 0.21 | 28,28,28,28                 | 0     |
| 57  | MG   | CA    | 1661 | 1/1   | 0.86 | 0.08 | 50,50,50,50                 | 0     |
| 57  | MG   | BA    | 3181 | 1/1   | 0.86 | 0.20 | 1,1,1,1                     | 0     |
| 57  | MG   | AA    | 7078 | 1/1   | 0.86 | 0.12 | 30,30,30,30                 | 0     |
| 57  | MG   | BA    | 3122 | 1/1   | 0.86 | 0.11 | 13,13,13,13                 | 0     |
| 57  | MG   | AA    | 7086 | 1/1   | 0.86 | 0.27 | 30,30,30,30                 | 0     |
| 57  | MG   | DA    | 9570 | 1/1   | 0.86 | 0.12 | 61,61,61,61                 | 0     |
| 57  | MG   | BA    | 3153 | 1/1   | 0.86 | 0.31 | 0,0,0,0                     | 0     |
| 57  | MG   | CA    | 1723 | 1/1   | 0.86 | 0.15 | 15,15,15,15                 | 0     |
| 57  | MG   | AA    | 7080 | 1/1   | 0.86 | 0.14 | 8,8,8,8                     | 1     |
| 57  | MG   | AV    | 101  | 1/1   | 0.86 | 0.09 | 2,2,2,2                     | 0     |
| 57  | MG   | DA    | 9579 | 1/1   | 0.86 | 0.32 | 38,38,38,38                 | 0     |
| 57  | MG   | DA    | 9379 | 1/1   | 0.86 | 0.11 | 41,41,41,41                 | 0     |
| 57  | MG   | DA    | 9460 | 1/1   | 0.86 | 0.06 | 40,40,40,40                 | 0     |
| 57  | MG   | DA    | 9466 | 1/1   | 0.86 | 0.20 | 36,36,36,36                 | 0     |
| 57  | MG   | BA    | 3066 | 1/1   | 0.86 | 0.49 | 48,48,48,48                 | 0     |
| 57  | MG   | BA    | 3274 | 1/1   | 0.86 | 0.07 | 8,8,8,8                     | 1     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | BA    | 3067 | 1/1   | 0.86 | 0.19 | 2,2,2,2                     | 0     |
| 57  | MG   | BA    | 3233 | 1/1   | 0.86 | 0.19 | 19,19,19,19                 | 0     |
| 58  | PAR  | CA    | 1741 | 42/42 | 0.86 | 0.18 | 55,55,55,55                 | 0     |
| 57  | MG   | BA    | 3258 | 1/1   | 0.87 | 0.30 | 19,19,19,19                 | 0     |
| 57  | MG   | AA    | 7027 | 1/1   | 0.87 | 0.15 | 28,28,28,28                 | 0     |
| 57  | MG   | CA    | 1657 | 1/1   | 0.87 | 0.11 | 30,30,30,30                 | 0     |
| 57  | MG   | BA    | 3031 | 1/1   | 0.87 | 0.29 | 44,44,44,44                 | 0     |
| 57  | MG   | AA    | 7004 | 1/1   | 0.87 | 0.16 | 30,30,30,30                 | 0     |
| 57  | MG   | BA    | 3268 | 1/1   | 0.87 | 0.24 | 13,13,13,13                 | 1     |
| 57  | MG   | BA    | 3164 | 1/1   | 0.87 | 0.25 | 39,39,39,39                 | 0     |
| 57  | MG   | AA    | 7020 | 1/1   | 0.87 | 0.20 | 33,33,33,33                 | 0     |
| 57  | MG   | DA    | 9648 | 1/1   | 0.87 | 0.14 | 34,34,34,34                 | 0     |
| 57  | MG   | DA    | 9650 | 1/1   | 0.87 | 0.21 | 7,7,7,7                     | 0     |
| 57  | MG   | BA    | 3276 | 1/1   | 0.87 | 0.24 | 31,31,31,31                 | 0     |
| 57  | MG   | DA    | 9404 | 1/1   | 0.87 | 0.20 | 12,12,12,12                 | 0     |
| 57  | MG   | AA    | 7011 | 1/1   | 0.87 | 0.11 | 43,43,43,43                 | 0     |
| 57  | MG   | CA    | 1607 | 1/1   | 0.87 | 0.26 | 32,32,32,32                 | 0     |
| 57  | MG   | DA    | 9659 | 1/1   | 0.87 | 0.18 | 52,52,52,52                 | 0     |
| 57  | MG   | BA    | 3117 | 1/1   | 0.87 | 0.29 | 11,11,11,11                 | 1     |
| 57  | MG   | BA    | 3119 | 1/1   | 0.87 | 0.18 | 42,42,42,42                 | 0     |
| 57  | MG   | BA    | 3299 | 1/1   | 0.87 | 0.26 | 10,10,10,10                 | 0     |
| 57  | MG   | CA    | 1617 | 1/1   | 0.87 | 0.24 | 16,16,16,16                 | 0     |
| 57  | MG   | BA    | 3102 | 1/1   | 0.87 | 0.28 | 1,1,1,1                     | 0     |
| 57  | MG   | DA    | 9676 | 1/1   | 0.87 | 0.14 | 13,13,13,13                 | 0     |
| 57  | MG   | DA    | 9550 | 1/1   | 0.87 | 0.21 | 55,55,55,55                 | 0     |
| 57  | MG   | BA    | 3308 | 1/1   | 0.87 | 0.12 | 37,37,37,37                 | 0     |
| 57  | MG   | DA    | 9555 | 1/1   | 0.87 | 0.32 | 39,39,39,39                 | 0     |
| 57  | MG   | BA    | 3247 | 1/1   | 0.87 | 0.25 | 55,55,55,55                 | 0     |
| 57  | MG   | DA    | 9433 | 1/1   | 0.87 | 0.11 | 13,13,13,13                 | 0     |
| 57  | MG   | AA    | 7054 | 1/1   | 0.87 | 0.22 | 29,29,29,29                 | 0     |
| 57  | MG   | DA    | 9436 | 1/1   | 0.87 | 0.27 | 3,3,3,3                     | 0     |
| 57  | MG   | BA    | 3108 | 1/1   | 0.87 | 0.20 | 27,27,27,27                 | 0     |
| 57  | MG   | CA    | 1700 | 1/1   | 0.87 | 0.15 | 20,20,20,20                 | 0     |
| 57  | MG   | BA    | 3254 | 1/1   | 0.87 | 0.26 | 54,54,54,54                 | 0     |
| 57  | MG   | DA    | 9445 | 1/1   | 0.87 | 0.18 | 22,22,22,22                 | 0     |
| 57  | MG   | BA    | 3205 | 1/1   | 0.87 | 0.23 | 0,0,0,0                     | 0     |
| 57  | MG   | DA    | 9601 | 1/1   | 0.87 | 0.22 | 31,31,31,31                 | 0     |
| 57  | MG   | CA    | 1644 | 1/1   | 0.87 | 0.07 | 45,45,45,45                 | 0     |
| 57  | MG   | BA    | 3257 | 1/1   | 0.87 | 0.08 | 21,21,21,21                 | 0     |
| 57  | MG   | CA    | 1709 | 1/1   | 0.87 | 0.40 | 68,68,68,68                 | 0     |
| 57  | MG   | CA    | 1711 | 1/1   | 0.87 | 0.16 | 26,26,26,26                 | 0     |
| 59  | ZN   | AD    | 301  | 1/1   | 0.87 | 0.21 | 41,41,41,41                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | ZN   | CN    | 101  | 1/1   | 0.87 | 0.10 | 171,171,171,171             | 0     |
| 57  | MG   | BA    | 3253 | 1/1   | 0.88 | 0.18 | 34,34,34,34                 | 0     |
| 57  | MG   | BA    | 3212 | 1/1   | 0.88 | 0.17 | 8,8,8,8                     | 0     |
| 57  | MG   | AA    | 7081 | 1/1   | 0.88 | 0.21 | 44,44,44,44                 | 0     |
| 57  | MG   | BA    | 3219 | 1/1   | 0.88 | 0.13 | 19,19,19,19                 | 0     |
| 57  | MG   | BA    | 3114 | 1/1   | 0.88 | 0.17 | 41,41,41,41                 | 0     |
| 57  | MG   | BA    | 3055 | 1/1   | 0.88 | 0.12 | 11,11,11,11                 | 0     |
| 57  | MG   | DA    | 9443 | 1/1   | 0.88 | 0.28 | 37,37,37,37                 | 0     |
| 57  | MG   | BA    | 3264 | 1/1   | 0.88 | 0.24 | 36,36,36,36                 | 0     |
| 57  | MG   | CA    | 1681 | 1/1   | 0.88 | 0.28 | 18,18,18,18                 | 1     |
| 57  | MG   | CA    | 1627 | 1/1   | 0.88 | 0.26 | 22,22,22,22                 | 0     |
| 57  | MG   | CA    | 1683 | 1/1   | 0.88 | 0.32 | 29,29,29,29                 | 0     |
| 57  | MG   | BA    | 3134 | 1/1   | 0.88 | 0.13 | 21,21,21,21                 | 0     |
| 57  | MG   | DA    | 9462 | 1/1   | 0.88 | 0.14 | 30,30,30,30                 | 0     |
| 57  | MG   | BA    | 3116 | 1/1   | 0.88 | 0.07 | 38,38,38,38                 | 0     |
| 57  | MG   | CA    | 1690 | 1/1   | 0.88 | 0.30 | 17,17,17,17                 | 0     |
| 57  | MG   | AA    | 7018 | 1/1   | 0.88 | 0.26 | 27,27,27,27                 | 0     |
| 57  | MG   | DA    | 9476 | 1/1   | 0.88 | 0.28 | 2,2,2,2                     | 0     |
| 57  | MG   | BA    | 3271 | 1/1   | 0.88 | 0.28 | 52,52,52,52                 | 0     |
| 57  | MG   | BA    | 3323 | 1/1   | 0.88 | 0.21 | 26,26,26,26                 | 0     |
| 57  | MG   | AA    | 7062 | 1/1   | 0.88 | 0.13 | 31,31,31,31                 | 0     |
| 57  | MG   | DA    | 9610 | 1/1   | 0.88 | 0.22 | 19,19,19,19                 | 0     |
| 57  | MG   | AA    | 7100 | 1/1   | 0.88 | 0.21 | 21,21,21,21                 | 0     |
| 57  | MG   | BA    | 3025 | 1/1   | 0.88 | 0.09 | 37,37,37,37                 | 0     |
| 57  | MG   | BA    | 3202 | 1/1   | 0.88 | 0.21 | 7,7,7,7                     | 0     |
| 57  | MG   | DA    | 9329 | 1/1   | 0.88 | 0.26 | 21,21,21,21                 | 0     |
| 57  | MG   | AV    | 103  | 1/1   | 0.88 | 0.18 | 7,7,7,7                     | 1     |
| 57  | MG   | DA    | 9504 | 1/1   | 0.88 | 0.12 | 27,27,27,27                 | 0     |
| 57  | MG   | BA    | 3044 | 1/1   | 0.88 | 0.17 | 18,18,18,18                 | 0     |
| 57  | MG   | DA    | 9340 | 1/1   | 0.88 | 0.27 | 1,1,1,1                     | 0     |
| 57  | MG   | DA    | 9528 | 1/1   | 0.88 | 0.24 | 6,6,6,6                     | 0     |
| 57  | MG   | BA    | 3294 | 1/1   | 0.88 | 0.14 | 15,15,15,15                 | 1     |
| 57  | MG   | CA    | 1653 | 1/1   | 0.89 | 0.15 | 29,29,29,29                 | 0     |
| 57  | MG   | BA    | 3232 | 1/1   | 0.89 | 0.17 | 44,44,44,44                 | 0     |
| 57  | MG   | BA    | 3184 | 1/1   | 0.89 | 0.30 | 22,22,22,22                 | 0     |
| 57  | MG   | BA    | 3187 | 1/1   | 0.89 | 0.15 | 24,24,24,24                 | 0     |
| 57  | MG   | DA    | 9376 | 1/1   | 0.89 | 0.10 | 26,26,26,26                 | 0     |
| 57  | MG   | BA    | 3193 | 1/1   | 0.89 | 0.16 | 12,12,12,12                 | 0     |
| 57  | MG   | BA    | 3052 | 1/1   | 0.89 | 0.12 | 40,40,40,40                 | 0     |
| 57  | MG   | DA    | 9616 | 1/1   | 0.89 | 0.29 | 54,54,54,54                 | 0     |
| 57  | MG   | BA    | 3284 | 1/1   | 0.89 | 0.07 | 21,21,21,21                 | 0     |
| 57  | MG   | DA    | 9470 | 1/1   | 0.89 | 0.23 | 0,0,0,0                     | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | DA    | 9471 | 1/1   | 0.89 | 0.15 | 50,50,50,50                 | 1     |
| 57  | MG   | AA    | 7009 | 1/1   | 0.89 | 0.15 | 18,18,18,18                 | 0     |
| 57  | MG   | BA    | 3103 | 1/1   | 0.89 | 0.14 | 31,31,31,31                 | 0     |
| 57  | MG   | DA    | 9387 | 1/1   | 0.89 | 0.26 | 1,1,1,1                     | 0     |
| 57  | MG   | CA    | 1608 | 1/1   | 0.89 | 0.18 | 16,16,16,16                 | 0     |
| 57  | MG   | BA    | 3296 | 1/1   | 0.89 | 0.32 | 0,0,0,0                     | 1     |
| 57  | MG   | CA    | 1731 | 1/1   | 0.89 | 0.10 | 30,30,30,30                 | 0     |
| 57  | MG   | CA    | 1735 | 1/1   | 0.89 | 0.20 | 29,29,29,29                 | 0     |
| 57  | MG   | BA    | 3297 | 1/1   | 0.89 | 0.54 | 46,46,46,46                 | 0     |
| 57  | MG   | DA    | 9652 | 1/1   | 0.89 | 0.17 | 44,44,44,44                 | 0     |
| 57  | MG   | AA    | 7046 | 1/1   | 0.89 | 0.28 | 35,35,35,35                 | 0     |
| 57  | MG   | CA    | 1616 | 1/1   | 0.89 | 0.15 | 44,44,44,44                 | 0     |
| 57  | MG   | AA    | 7073 | 1/1   | 0.89 | 0.08 | 29,29,29,29                 | 0     |
| 57  | MG   | BA    | 3206 | 1/1   | 0.89 | 0.23 | 29,29,29,29                 | 0     |
| 57  | MG   | BA    | 3085 | 1/1   | 0.89 | 0.19 | 29,29,29,29                 | 0     |
| 57  | MG   | DA    | 9418 | 1/1   | 0.89 | 0.33 | 61,61,61,61                 | 0     |
| 57  | MG   | CA    | 1688 | 1/1   | 0.89 | 0.13 | 16,16,16,16                 | 0     |
| 57  | MG   | AA    | 7052 | 1/1   | 0.89 | 0.14 | 74,74,74,74                 | 0     |
| 57  | MG   | DA    | 9422 | 1/1   | 0.89 | 0.14 | 56,56,56,56                 | 0     |
| 57  | MG   | DA    | 9540 | 1/1   | 0.89 | 0.20 | 0,0,0,0                     | 0     |
| 57  | MG   | AA    | 7031 | 1/1   | 0.89 | 0.25 | 44,44,44,44                 | 0     |
| 57  | MG   | CA    | 1693 | 1/1   | 0.89 | 0.14 | 24,24,24,24                 | 0     |
| 57  | MG   | BA    | 3220 | 1/1   | 0.89 | 0.45 | 56,56,56,56                 | 0     |
| 57  | MG   | DA    | 9686 | 1/1   | 0.89 | 0.15 | 11,11,11,11                 | 0     |
| 57  | MG   | DA    | 9432 | 1/1   | 0.89 | 0.22 | 38,38,38,38                 | 0     |
| 57  | MG   | BA    | 3221 | 1/1   | 0.89 | 0.19 | 17,17,17,17                 | 0     |
| 57  | MG   | DA    | 9559 | 1/1   | 0.89 | 0.22 | 58,58,58,58                 | 0     |
| 57  | MG   | DA    | 9563 | 1/1   | 0.89 | 0.12 | 3,3,3,3                     | 0     |
| 57  | MG   | DA    | 9565 | 1/1   | 0.89 | 0.22 | 11,11,11,11                 | 0     |
| 57  | MG   | BA    | 3021 | 1/1   | 0.89 | 0.15 | 49,49,49,49                 | 0     |
| 57  | MG   | BA    | 3022 | 1/1   | 0.89 | 0.17 | 40,40,40,40                 | 0     |
| 57  | MG   | DA    | 9437 | 1/1   | 0.89 | 0.10 | 14,14,14,14                 | 0     |
| 57  | MG   | BA    | 3321 | 1/1   | 0.89 | 0.25 | 35,35,35,35                 | 0     |
| 57  | MG   | DD    | 7101 | 1/1   | 0.89 | 0.31 | 3,3,3,3                     | 0     |
| 57  | MG   | AA    | 7010 | 1/1   | 0.89 | 0.10 | 30,30,30,30                 | 0     |
| 57  | MG   | DA    | 9576 | 1/1   | 0.89 | 0.10 | 22,22,22,22                 | 0     |
| 57  | MG   | DA    | 9348 | 1/1   | 0.89 | 0.38 | 47,47,47,47                 | 0     |
| 57  | MG   | D1    | 102  | 1/1   | 0.89 | 0.09 | 9,9,9,9                     | 1     |
| 57  | MG   | BA    | 3096 | 1/1   | 0.89 | 0.25 | 12,12,12,12                 | 0     |
| 58  | PAR  | AA    | 7111 | 42/42 | 0.89 | 0.15 | 58,58,58,58                 | 0     |
| 57  | MG   | DA    | 9444 | 1/1   | 0.89 | 0.16 | 42,42,42,42                 | 0     |
| 57  | MG   | DA    | 9595 | 1/1   | 0.89 | 0.17 | 49,49,49,49                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | DA    | 9596 | 1/1   | 0.89 | 0.10 | 27,27,27,27                 | 0     |
| 57  | MG   | DA    | 9633 | 1/1   | 0.90 | 0.48 | 30,30,30,30                 | 0     |
| 57  | MG   | DA    | 9374 | 1/1   | 0.90 | 0.15 | 28,28,28,28                 | 0     |
| 57  | MG   | BA    | 3159 | 1/1   | 0.90 | 0.20 | 9,9,9,9                     | 0     |
| 57  | MG   | DA    | 9639 | 1/1   | 0.90 | 0.19 | 57,57,57,57                 | 0     |
| 57  | MG   | CA    | 1734 | 1/1   | 0.90 | 0.12 | 22,22,22,22                 | 0     |
| 57  | MG   | CA    | 1692 | 1/1   | 0.90 | 0.25 | 28,28,28,28                 | 0     |
| 57  | MG   | BA    | 3198 | 1/1   | 0.90 | 0.24 | 0,0,0,0                     | 0     |
| 57  | MG   | DA    | 9544 | 1/1   | 0.90 | 0.18 | 10,10,10,10                 | 0     |
| 57  | MG   | BA    | 3050 | 1/1   | 0.90 | 0.16 | 4,4,4,4                     | 0     |
| 57  | MG   | AA    | 7006 | 1/1   | 0.90 | 0.24 | 20,20,20,20                 | 0     |
| 57  | MG   | BA    | 3204 | 1/1   | 0.90 | 0.21 | 3,3,3,3                     | 0     |
| 57  | MG   | BA    | 3314 | 1/1   | 0.90 | 0.10 | 42,42,42,42                 | 0     |
| 57  | MG   | DA    | 9656 | 1/1   | 0.90 | 0.15 | 58,58,58,58                 | 0     |
| 57  | MG   | AA    | 7053 | 1/1   | 0.90 | 0.18 | 32,32,32,32                 | 0     |
| 57  | MG   | DA    | 9561 | 1/1   | 0.90 | 0.10 | 10,10,10,10                 | 0     |
| 57  | MG   | AA    | 7013 | 1/1   | 0.90 | 0.19 | 27,27,27,27                 | 0     |
| 57  | MG   | AA    | 7050 | 1/1   | 0.90 | 0.28 | 29,29,29,29                 | 0     |
| 57  | MG   | DA    | 9465 | 1/1   | 0.90 | 0.17 | 34,34,34,34                 | 0     |
| 57  | MG   | BA    | 3141 | 1/1   | 0.90 | 0.22 | 18,18,18,18                 | 0     |
| 57  | MG   | BA    | 3250 | 1/1   | 0.90 | 0.14 | 18,18,18,18                 | 0     |
| 57  | MG   | CA    | 1626 | 1/1   | 0.90 | 0.23 | 28,28,28,28                 | 0     |
| 57  | MG   | DA    | 9411 | 1/1   | 0.90 | 0.12 | 2,2,2,2                     | 0     |
| 57  | MG   | DA    | 9325 | 1/1   | 0.90 | 0.15 | 32,32,32,32                 | 0     |
| 57  | MG   | DA    | 9680 | 1/1   | 0.90 | 0.21 | 24,24,24,24                 | 0     |
| 57  | MG   | DA    | 9327 | 1/1   | 0.90 | 0.17 | 20,20,20,20                 | 0     |
| 57  | MG   | CA    | 1710 | 1/1   | 0.90 | 0.23 | 19,19,19,19                 | 0     |
| 57  | MG   | DA    | 9479 | 1/1   | 0.90 | 0.33 | 0,0,0,0                     | 0     |
| 57  | MG   | DA    | 9582 | 1/1   | 0.90 | 0.33 | 21,21,21,21                 | 0     |
| 57  | MG   | DA    | 9586 | 1/1   | 0.90 | 0.24 | 3,3,3,3                     | 0     |
| 57  | MG   | DA    | 9590 | 1/1   | 0.90 | 0.30 | 1,1,1,1                     | 0     |
| 57  | MG   | DA    | 9591 | 1/1   | 0.90 | 0.10 | 52,52,52,52                 | 0     |
| 57  | MG   | DA    | 9484 | 1/1   | 0.90 | 0.20 | 5,5,5,5                     | 0     |
| 57  | MG   | BA    | 3217 | 1/1   | 0.90 | 0.10 | 28,28,28,28                 | 0     |
| 57  | MG   | DA    | 9597 | 1/1   | 0.90 | 0.13 | 12,12,12,12                 | 0     |
| 57  | MG   | CA    | 1713 | 1/1   | 0.90 | 0.26 | 31,31,31,31                 | 0     |
| 57  | MG   | AA    | 7064 | 1/1   | 0.90 | 0.13 | 50,50,50,50                 | 0     |
| 57  | MG   | AA    | 7108 | 1/1   | 0.90 | 0.10 | 27,27,27,27                 | 0     |
| 57  | MG   | DQ    | 201  | 1/1   | 0.90 | 0.15 | 36,36,36,36                 | 0     |
| 57  | MG   | BA    | 3290 | 1/1   | 0.90 | 0.29 | 19,19,19,19                 | 1     |
| 57  | MG   | DX    | 101  | 1/1   | 0.90 | 0.08 | 6,6,6,6                     | 0     |
| 57  | MG   | BA    | 3004 | 1/1   | 0.90 | 0.24 | 1,1,1,1                     | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | AA    | 7065 | 1/1   | 0.90 | 0.17 | 23,23,23,23                 | 0     |
| 57  | MG   | AA    | 7110 | 1/1   | 0.90 | 0.14 | 31,31,31,31                 | 0     |
| 57  | MG   | DA    | 9515 | 1/1   | 0.90 | 0.20 | 10,10,10,10                 | 0     |
| 57  | MG   | DA    | 9618 | 1/1   | 0.90 | 0.37 | 28,28,28,28                 | 1     |
| 57  | MG   | DA    | 9361 | 1/1   | 0.90 | 0.20 | 5,5,5,5                     | 0     |
| 57  | MG   | BA    | 3298 | 1/1   | 0.90 | 0.30 | 18,18,18,18                 | 0     |
| 57  | MG   | CA    | 1730 | 1/1   | 0.90 | 0.10 | 49,49,49,49                 | 0     |
| 57  | MG   | DA    | 9464 | 1/1   | 0.91 | 0.10 | 25,25,25,25                 | 0     |
| 57  | MG   | DA    | 9366 | 1/1   | 0.91 | 0.27 | 1,1,1,1                     | 0     |
| 57  | MG   | BA    | 3178 | 1/1   | 0.91 | 0.15 | 28,28,28,28                 | 0     |
| 57  | MG   | BA    | 3135 | 1/1   | 0.91 | 0.28 | 43,43,43,43                 | 0     |
| 57  | MG   | DA    | 9605 | 1/1   | 0.91 | 0.08 | 19,19,19,19                 | 0     |
| 57  | MG   | CA    | 1655 | 1/1   | 0.91 | 0.18 | 24,24,24,24                 | 0     |
| 57  | MG   | BA    | 3183 | 1/1   | 0.91 | 0.27 | 56,56,56,56                 | 0     |
| 57  | MG   | AA    | 7066 | 1/1   | 0.91 | 0.25 | 36,36,36,36                 | 0     |
| 57  | MG   | DA    | 9378 | 1/1   | 0.91 | 0.12 | 29,29,29,29                 | 0     |
| 57  | MG   | BB    | 204  | 1/1   | 0.91 | 0.16 | 23,23,23,23                 | 0     |
| 57  | MG   | BA    | 3185 | 1/1   | 0.91 | 0.17 | 14,14,14,14                 | 0     |
| 57  | MG   | DA    | 9622 | 1/1   | 0.91 | 0.18 | 36,36,36,36                 | 0     |
| 57  | MG   | DA    | 9628 | 1/1   | 0.91 | 0.19 | 35,35,35,35                 | 1     |
| 57  | MG   | DA    | 9483 | 1/1   | 0.91 | 0.27 | 0,0,0,0                     | 0     |
| 57  | MG   | CA    | 1724 | 1/1   | 0.91 | 0.07 | 5,5,5,5                     | 0     |
| 57  | MG   | CA    | 1665 | 1/1   | 0.91 | 0.26 | 16,16,16,16                 | 0     |
| 57  | MG   | CA    | 1727 | 1/1   | 0.91 | 0.15 | 27,27,27,27                 | 0     |
| 57  | MG   | DA    | 9637 | 1/1   | 0.91 | 0.17 | 18,18,18,18                 | 0     |
| 57  | MG   | CA    | 1666 | 1/1   | 0.91 | 0.09 | 66,66,66,66                 | 0     |
| 57  | MG   | DA    | 9392 | 1/1   | 0.91 | 0.29 | 12,12,12,12                 | 0     |
| 57  | MG   | DA    | 9394 | 1/1   | 0.91 | 0.19 | 16,16,16,16                 | 0     |
| 57  | MG   | CA    | 1671 | 1/1   | 0.91 | 0.09 | 38,38,38,38                 | 0     |
| 57  | MG   | AA    | 7055 | 1/1   | 0.91 | 0.15 | 29,29,29,29                 | 0     |
| 57  | MG   | BO    | 201  | 1/1   | 0.91 | 0.22 | 45,45,45,45                 | 0     |
| 57  | MG   | DA    | 9649 | 1/1   | 0.91 | 0.24 | 1,1,1,1                     | 0     |
| 57  | MG   | BA    | 3241 | 1/1   | 0.91 | 0.19 | 4,4,4,4                     | 0     |
| 57  | MG   | DA    | 9517 | 1/1   | 0.91 | 0.11 | 0,0,0,0                     | 0     |
| 57  | MG   | BA    | 3189 | 1/1   | 0.91 | 0.12 | 1,1,1,1                     | 0     |
| 57  | MG   | AA    | 7077 | 1/1   | 0.91 | 0.09 | 22,22,22,22                 | 0     |
| 57  | MG   | CA    | 1606 | 1/1   | 0.91 | 0.11 | 8,8,8,8                     | 0     |
| 57  | MG   | BA    | 3295 | 1/1   | 0.91 | 0.13 | 27,27,27,27                 | 0     |
| 57  | MG   | BA    | 3143 | 1/1   | 0.91 | 0.18 | 7,7,7,7                     | 0     |
| 57  | MG   | AV    | 102  | 1/1   | 0.91 | 0.20 | 25,25,25,25                 | 1     |
| 57  | MG   | CV    | 101  | 1/1   | 0.91 | 0.15 | 12,12,12,12                 | 1     |
| 57  | MG   | AA    | 7045 | 1/1   | 0.91 | 0.26 | 38,38,38,38                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | DA    | 9420 | 1/1   | 0.91 | 0.28 | 6,6,6,6                     | 0     |
| 57  | MG   | AA    | 7097 | 1/1   | 0.91 | 0.15 | 20,20,20,20                 | 0     |
| 57  | MG   | DA    | 9549 | 1/1   | 0.91 | 0.26 | 44,44,44,44                 | 0     |
| 57  | MG   | BA    | 3301 | 1/1   | 0.91 | 0.19 | 20,20,20,20                 | 0     |
| 57  | MG   | BA    | 3302 | 1/1   | 0.91 | 0.17 | 8,8,8,8                     | 0     |
| 57  | MG   | AA    | 7033 | 1/1   | 0.91 | 0.13 | 35,35,35,35                 | 0     |
| 57  | MG   | DA    | 9557 | 1/1   | 0.91 | 0.13 | 25,25,25,25                 | 0     |
| 57  | MG   | DA    | 9304 | 1/1   | 0.91 | 0.14 | 27,27,27,27                 | 0     |
| 57  | MG   | DA    | 9313 | 1/1   | 0.91 | 0.15 | 18,18,18,18                 | 0     |
| 57  | MG   | AA    | 7072 | 1/1   | 0.91 | 0.12 | 23,23,23,23                 | 0     |
| 57  | MG   | BA    | 3310 | 1/1   | 0.91 | 0.11 | 35,35,35,35                 | 0     |
| 57  | MG   | BA    | 3158 | 1/1   | 0.91 | 0.10 | 29,29,29,29                 | 0     |
| 57  | MG   | CA    | 1628 | 1/1   | 0.91 | 0.08 | 9,9,9,9                     | 0     |
| 57  | MG   | DA    | 9330 | 1/1   | 0.91 | 0.19 | 0,0,0,0                     | 0     |
| 57  | MG   | BA    | 3072 | 1/1   | 0.91 | 0.15 | 25,25,25,25                 | 0     |
| 57  | MG   | BA    | 3075 | 1/1   | 0.91 | 0.23 | 12,12,12,12                 | 0     |
| 57  | MG   | BA    | 3105 | 1/1   | 0.91 | 0.18 | 26,26,26,26                 | 0     |
| 57  | MG   | AA    | 7082 | 1/1   | 0.91 | 0.22 | 24,24,24,24                 | 0     |
| 57  | MG   | CA    | 1703 | 1/1   | 0.91 | 0.28 | 9,9,9,9                     | 0     |
| 57  | MG   | DF    | 301  | 1/1   | 0.91 | 0.08 | 20,20,20,20                 | 0     |
| 57  | MG   | DP    | 203  | 1/1   | 0.91 | 0.16 | 11,11,11,11                 | 0     |
| 57  | MG   | AA    | 7105 | 1/1   | 0.91 | 0.24 | 42,42,42,42                 | 0     |
| 57  | MG   | DA    | 9581 | 1/1   | 0.91 | 0.12 | 4,4,4,4                     | 0     |
| 57  | MG   | BA    | 3014 | 1/1   | 0.91 | 0.17 | 33,33,33,33                 | 0     |
| 57  | MG   | DA    | 9454 | 1/1   | 0.91 | 0.31 | 34,34,34,34                 | 0     |
| 57  | MG   | DA    | 9588 | 1/1   | 0.91 | 0.06 | 16,16,16,16                 | 0     |
| 57  | MG   | AA    | 7034 | 1/1   | 0.91 | 0.22 | 43,43,43,43                 | 0     |
| 57  | MG   | DA    | 9360 | 1/1   | 0.91 | 0.29 | 7,7,7,7                     | 0     |
| 57  | MG   | DA    | 9592 | 1/1   | 0.91 | 0.18 | 36,36,36,36                 | 0     |
| 57  | MG   | DA    | 9461 | 1/1   | 0.91 | 0.11 | 13,13,13,13                 | 0     |
| 57  | MG   | BA    | 3177 | 1/1   | 0.91 | 0.17 | 0,0,0,0                     | 0     |
| 57  | MG   | DA    | 9463 | 1/1   | 0.91 | 0.08 | 12,12,12,12                 | 0     |
| 57  | MG   | BA    | 3038 | 1/1   | 0.92 | 0.07 | 31,31,31,31                 | 0     |
| 57  | MG   | CA    | 1685 | 1/1   | 0.92 | 0.11 | 41,41,41,41                 | 0     |
| 57  | MG   | CA    | 1686 | 1/1   | 0.92 | 0.17 | 77,77,77,77                 | 0     |
| 57  | MG   | AA    | 7068 | 1/1   | 0.92 | 0.09 | 34,34,34,34                 | 0     |
| 57  | MG   | BA    | 3190 | 1/1   | 0.92 | 0.17 | 8,8,8,8                     | 0     |
| 57  | MG   | CA    | 1689 | 1/1   | 0.92 | 0.07 | 15,15,15,15                 | 0     |
| 57  | MG   | DA    | 9619 | 1/1   | 0.92 | 0.06 | 0,0,0,0                     | 0     |
| 57  | MG   | DA    | 9620 | 1/1   | 0.92 | 0.09 | 26,26,26,26                 | 0     |
| 57  | MG   | DA    | 9499 | 1/1   | 0.92 | 0.12 | 29,29,29,29                 | 0     |
| 57  | MG   | CA    | 1633 | 1/1   | 0.92 | 0.12 | 9,9,9,9                     | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | DA    | 9502 | 1/1   | 0.92 | 0.23 | 3,3,3,3                     | 0     |
| 57  | MG   | CA    | 1634 | 1/1   | 0.92 | 0.14 | 43,43,43,43                 | 0     |
| 57  | MG   | BA    | 3041 | 1/1   | 0.92 | 0.23 | 7,7,7,7                     | 0     |
| 57  | MG   | DA    | 9510 | 1/1   | 0.92 | 0.23 | 1,1,1,1                     | 0     |
| 57  | MG   | CA    | 1638 | 1/1   | 0.92 | 0.22 | 24,24,24,24                 | 0     |
| 57  | MG   | DA    | 9636 | 1/1   | 0.92 | 0.16 | 16,16,16,16                 | 0     |
| 57  | MG   | DA    | 9306 | 1/1   | 0.92 | 0.18 | 4,4,4,4                     | 0     |
| 57  | MG   | DA    | 9519 | 1/1   | 0.92 | 0.23 | 1,1,1,1                     | 0     |
| 57  | MG   | BA    | 3097 | 1/1   | 0.92 | 0.13 | 43,43,43,43                 | 0     |
| 57  | MG   | DA    | 9315 | 1/1   | 0.92 | 0.11 | 26,26,26,26                 | 0     |
| 57  | MG   | BA    | 3281 | 1/1   | 0.92 | 0.64 | 53,53,53,53                 | 0     |
| 57  | MG   | BA    | 3070 | 1/1   | 0.92 | 0.32 | 34,34,34,34                 | 0     |
| 57  | MG   | DA    | 9531 | 1/1   | 0.92 | 0.26 | 1,1,1,1                     | 0     |
| 57  | MG   | BB    | 201  | 1/1   | 0.92 | 0.12 | 34,34,34,34                 | 0     |
| 57  | MG   | AA    | 7037 | 1/1   | 0.92 | 0.18 | 7,7,7,7                     | 0     |
| 57  | MG   | DA    | 9430 | 1/1   | 0.92 | 0.24 | 0,0,0,0                     | 0     |
| 57  | MG   | DA    | 9542 | 1/1   | 0.92 | 0.20 | 6,6,6,6                     | 0     |
| 57  | MG   | CA    | 1645 | 1/1   | 0.92 | 0.24 | 20,20,20,20                 | 0     |
| 57  | MG   | BA    | 3073 | 1/1   | 0.92 | 0.17 | 8,8,8,8                     | 0     |
| 57  | MG   | BA    | 3161 | 1/1   | 0.92 | 0.15 | 11,11,11,11                 | 0     |
| 57  | MG   | CA    | 1706 | 1/1   | 0.92 | 0.17 | 32,32,32,32                 | 0     |
| 57  | MG   | DA    | 9344 | 1/1   | 0.92 | 0.21 | 33,33,33,33                 | 0     |
| 57  | MG   | DA    | 9551 | 1/1   | 0.92 | 0.13 | 48,48,48,48                 | 0     |
| 57  | MG   | BA    | 3129 | 1/1   | 0.92 | 0.27 | 1,1,1,1                     | 0     |
| 57  | MG   | DA    | 9663 | 1/1   | 0.92 | 0.25 | 7,7,7,7                     | 0     |
| 57  | MG   | DA    | 9664 | 1/1   | 0.92 | 0.26 | 1,1,1,1                     | 0     |
| 57  | MG   | DA    | 9665 | 1/1   | 0.92 | 0.31 | 9,9,9,9                     | 0     |
| 57  | MG   | DA    | 9438 | 1/1   | 0.92 | 0.06 | 21,21,21,21                 | 0     |
| 57  | MG   | DA    | 9667 | 1/1   | 0.92 | 0.23 | 10,10,10,10                 | 0     |
| 57  | MG   | BA    | 3251 | 1/1   | 0.92 | 0.06 | 34,34,34,34                 | 0     |
| 57  | MG   | BD    | 302  | 1/1   | 0.92 | 0.10 | 4,4,4,4                     | 0     |
| 57  | MG   | CA    | 1656 | 1/1   | 0.92 | 0.16 | 22,22,22,22                 | 0     |
| 57  | MG   | DA    | 9355 | 1/1   | 0.92 | 0.28 | 0,0,0,0                     | 0     |
| 57  | MG   | DA    | 9564 | 1/1   | 0.92 | 0.20 | 17,17,17,17                 | 0     |
| 57  | MG   | BF    | 301  | 1/1   | 0.92 | 0.10 | 39,39,39,39                 | 0     |
| 57  | MG   | DA    | 9684 | 1/1   | 0.92 | 0.12 | 8,8,8,8                     | 0     |
| 57  | MG   | CA    | 1658 | 1/1   | 0.92 | 0.09 | 44,44,44,44                 | 0     |
| 57  | MG   | DA    | 9446 | 1/1   | 0.92 | 0.10 | 13,13,13,13                 | 0     |
| 57  | MG   | BA    | 3045 | 1/1   | 0.92 | 0.36 | 2,2,2,2                     | 0     |
| 57  | MG   | DA    | 9450 | 1/1   | 0.92 | 0.26 | 2,2,2,2                     | 1     |
| 57  | MG   | DA    | 9362 | 1/1   | 0.92 | 0.21 | 5,5,5,5                     | 0     |
| 57  | MG   | CA    | 1718 | 1/1   | 0.92 | 0.14 | 27,27,27,27                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | AA    | 7091 | 1/1   | 0.92 | 0.12 | 22,22,22,22                 | 0     |
| 57  | MG   | DA    | 9369 | 1/1   | 0.92 | 0.23 | 0,0,0,0                     | 0     |
| 57  | MG   | DB    | 201  | 1/1   | 0.92 | 0.25 | 22,22,22,22                 | 0     |
| 57  | MG   | BA    | 3051 | 1/1   | 0.92 | 0.23 | 6,6,6,6                     | 0     |
| 57  | MG   | CA    | 1604 | 1/1   | 0.92 | 0.22 | 15,15,15,15                 | 0     |
| 57  | MG   | AA    | 7048 | 1/1   | 0.92 | 0.18 | 27,27,27,27                 | 0     |
| 57  | MG   | BA    | 3300 | 1/1   | 0.92 | 0.21 | 1,1,1,1                     | 0     |
| 57  | MG   | BA    | 3006 | 1/1   | 0.92 | 0.17 | 38,38,38,38                 | 0     |
| 57  | MG   | BA    | 3032 | 1/1   | 0.92 | 0.12 | 18,18,18,18                 | 0     |
| 57  | MG   | BA    | 3180 | 1/1   | 0.92 | 0.26 | 2,2,2,2                     | 0     |
| 57  | MG   | BA    | 3263 | 1/1   | 0.92 | 0.17 | 16,16,16,16                 | 1     |
| 57  | MG   | BA    | 3112 | 1/1   | 0.92 | 0.28 | 14,14,14,14                 | 0     |
| 57  | MG   | DA    | 9474 | 1/1   | 0.92 | 0.15 | 28,28,28,28                 | 0     |
| 57  | MG   | BA    | 3009 | 1/1   | 0.92 | 0.06 | 2,2,2,2                     | 0     |
| 57  | MG   | DA    | 9598 | 1/1   | 0.92 | 0.22 | 14,14,14,14                 | 0     |
| 57  | MG   | D2    | 101  | 1/1   | 0.92 | 0.17 | 34,34,34,34                 | 0     |
| 57  | MG   | AV    | 104  | 1/1   | 0.92 | 0.19 | 16,16,16,16                 | 0     |
| 57  | MG   | DA    | 9390 | 1/1   | 0.92 | 0.21 | 0,0,0,0                     | 0     |
| 57  | MG   | AA    | 7017 | 1/1   | 0.92 | 0.17 | 29,29,29,29                 | 0     |
| 57  | MG   | BA    | 3270 | 1/1   | 0.92 | 0.28 | 0,0,0,0                     | 1     |
| 57  | MG   | DA    | 9604 | 1/1   | 0.92 | 0.13 | 21,21,21,21                 | 0     |
| 57  | MG   | BA    | 3150 | 1/1   | 0.93 | 0.15 | 1,1,1,1                     | 0     |
| 57  | MG   | DA    | 9640 | 1/1   | 0.93 | 0.20 | 42,42,42,42                 | 0     |
| 57  | MG   | BA    | 3269 | 1/1   | 0.93 | 0.22 | 20,20,20,20                 | 0     |
| 57  | MG   | DA    | 9316 | 1/1   | 0.93 | 0.24 | 0,0,0,0                     | 0     |
| 57  | MG   | BA    | 3186 | 1/1   | 0.93 | 0.21 | 2,2,2,2                     | 0     |
| 57  | MG   | AA    | 7098 | 1/1   | 0.93 | 0.20 | 28,28,28,28                 | 0     |
| 57  | MG   | BA    | 3081 | 1/1   | 0.93 | 0.41 | 24,24,24,24                 | 1     |
| 57  | MG   | DA    | 9468 | 1/1   | 0.93 | 0.43 | 2,2,2,2                     | 1     |
| 57  | MG   | BA    | 3155 | 1/1   | 0.93 | 0.17 | 33,33,33,33                 | 0     |
| 57  | MG   | AA    | 7003 | 1/1   | 0.93 | 0.14 | 27,27,27,27                 | 0     |
| 57  | MG   | DA    | 9408 | 1/1   | 0.93 | 0.24 | 3,3,3,3                     | 0     |
| 57  | MG   | DA    | 9332 | 1/1   | 0.93 | 0.14 | 34,34,34,34                 | 0     |
| 57  | MG   | BA    | 3084 | 1/1   | 0.93 | 0.20 | 1,1,1,1                     | 0     |
| 57  | MG   | DA    | 9334 | 1/1   | 0.93 | 0.20 | 27,27,27,27                 | 0     |
| 57  | MG   | CA    | 1629 | 1/1   | 0.93 | 0.23 | 37,37,37,37                 | 0     |
| 57  | MG   | DA    | 9339 | 1/1   | 0.93 | 0.25 | 13,13,13,13                 | 0     |
| 57  | MG   | CA    | 1630 | 1/1   | 0.93 | 0.11 | 34,34,34,34                 | 0     |
| 57  | MG   | BA    | 3243 | 1/1   | 0.93 | 0.26 | 5,5,5,5                     | 0     |
| 57  | MG   | AA    | 7028 | 1/1   | 0.93 | 0.29 | 30,30,30,30                 | 0     |
| 57  | MG   | DA    | 9489 | 1/1   | 0.93 | 0.28 | 37,37,37,37                 | 0     |
| 57  | MG   | BA    | 3246 | 1/1   | 0.93 | 0.24 | 33,33,33,33                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | DA    | 9589 | 1/1   | 0.93 | 0.18 | 32,32,32,32                 | 0     |
| 57  | MG   | DA    | 9669 | 1/1   | 0.93 | 0.13 | 5,5,5,5                     | 0     |
| 57  | MG   | BA    | 3132 | 1/1   | 0.93 | 0.20 | 51,51,51,51                 | 0     |
| 57  | MG   | DA    | 9427 | 1/1   | 0.93 | 0.16 | 91,91,91,91                 | 0     |
| 57  | MG   | BA    | 3026 | 1/1   | 0.93 | 0.22 | 29,29,29,29                 | 0     |
| 57  | MG   | BA    | 3042 | 1/1   | 0.93 | 0.20 | 8,8,8,8                     | 0     |
| 57  | MG   | DA    | 9678 | 1/1   | 0.93 | 0.14 | 33,33,33,33                 | 0     |
| 57  | MG   | AA    | 7061 | 1/1   | 0.93 | 0.07 | 19,19,19,19                 | 0     |
| 57  | MG   | BA    | 3069 | 1/1   | 0.93 | 0.21 | 5,5,5,5                     | 0     |
| 57  | MG   | BA    | 3171 | 1/1   | 0.93 | 0.12 | 7,7,7,7                     | 0     |
| 57  | MG   | DA    | 9505 | 1/1   | 0.93 | 0.15 | 0,0,0,0                     | 0     |
| 57  | MG   | BN    | 201  | 1/1   | 0.93 | 0.21 | 125,125,125,125             | 1     |
| 57  | MG   | DA    | 9365 | 1/1   | 0.93 | 0.16 | 1,1,1,1                     | 0     |
| 57  | MG   | CA    | 1648 | 1/1   | 0.93 | 0.11 | 23,23,23,23                 | 0     |
| 57  | MG   | BA    | 3029 | 1/1   | 0.93 | 0.15 | 24,24,24,24                 | 0     |
| 57  | MG   | BA    | 3174 | 1/1   | 0.93 | 0.10 | 31,31,31,31                 | 0     |
| 57  | MG   | DA    | 9525 | 1/1   | 0.93 | 0.19 | 4,4,4,4                     | 0     |
| 57  | MG   | DA    | 9608 | 1/1   | 0.93 | 0.12 | 19,19,19,19                 | 0     |
| 57  | MG   | DA    | 9370 | 1/1   | 0.93 | 0.33 | 0,0,0,0                     | 0     |
| 57  | MG   | DA    | 9614 | 1/1   | 0.93 | 0.16 | 12,12,12,12                 | 0     |
| 57  | MG   | BA    | 3138 | 1/1   | 0.93 | 0.26 | 15,15,15,15                 | 0     |
| 57  | MG   | AA    | 7092 | 1/1   | 0.93 | 0.06 | 37,37,37,37                 | 0     |
| 57  | MG   | BA    | 3259 | 1/1   | 0.93 | 0.12 | 18,18,18,18                 | 0     |
| 57  | MG   | BA    | 3008 | 1/1   | 0.93 | 0.24 | 2,2,2,2                     | 0     |
| 57  | MG   | DA    | 9538 | 1/1   | 0.93 | 0.22 | 1,1,1,1                     | 0     |
| 57  | MG   | AA    | 7106 | 1/1   | 0.93 | 0.09 | 12,12,12,12                 | 0     |
| 57  | MG   | BA    | 3012 | 1/1   | 0.93 | 0.24 | 29,29,29,29                 | 0     |
| 57  | MG   | DA    | 9624 | 1/1   | 0.93 | 0.09 | 18,18,18,18                 | 1     |
| 57  | MG   | DA    | 9626 | 1/1   | 0.93 | 0.09 | 8,8,8,8                     | 1     |
| 57  | MG   | BA    | 3226 | 1/1   | 0.93 | 0.31 | 36,36,36,36                 | 0     |
| 57  | MG   | DA    | 9302 | 1/1   | 0.93 | 0.17 | 34,34,34,34                 | 0     |
| 57  | MG   | AA    | 7087 | 1/1   | 0.93 | 0.07 | 24,24,24,24                 | 0     |
| 57  | MG   | DA    | 9455 | 1/1   | 0.93 | 0.23 | 0,0,0,0                     | 0     |
| 57  | MG   | DA    | 9456 | 1/1   | 0.93 | 0.24 | 19,19,19,19                 | 0     |
| 57  | MG   | CA    | 1612 | 1/1   | 0.93 | 0.17 | 31,31,31,31                 | 0     |
| 57  | MG   | DA    | 9310 | 1/1   | 0.93 | 0.14 | 0,0,0,0                     | 0     |
| 57  | MG   | DA    | 9312 | 1/1   | 0.93 | 0.19 | 4,4,4,4                     | 0     |
| 57  | MG   | DA    | 9423 | 1/1   | 0.94 | 0.05 | 1,1,1,1                     | 0     |
| 57  | MG   | BA    | 3277 | 1/1   | 0.94 | 0.32 | 2,2,2,2                     | 1     |
| 57  | MG   | AA    | 7104 | 1/1   | 0.94 | 0.16 | 33,33,33,33                 | 0     |
| 57  | MG   | DA    | 9512 | 1/1   | 0.94 | 0.24 | 2,2,2,2                     | 0     |
| 57  | MG   | DA    | 9513 | 1/1   | 0.94 | 0.11 | 22,22,22,22                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | DA    | 9428 | 1/1   | 0.94 | 0.12 | 15,15,15,15                 | 0     |
| 57  | MG   | DA    | 9346 | 1/1   | 0.94 | 0.19 | 0,0,0,0                     | 0     |
| 57  | MG   | BA    | 3210 | 1/1   | 0.94 | 0.33 | 11,11,11,11                 | 0     |
| 57  | MG   | DA    | 9520 | 1/1   | 0.94 | 0.22 | 2,2,2,2                     | 0     |
| 57  | MG   | DA    | 9521 | 1/1   | 0.94 | 0.26 | 2,2,2,2                     | 0     |
| 57  | MG   | CA    | 1726 | 1/1   | 0.94 | 0.10 | 38,38,38,38                 | 0     |
| 57  | MG   | AA    | 7021 | 1/1   | 0.94 | 0.21 | 25,25,25,25                 | 0     |
| 57  | MG   | DA    | 9351 | 1/1   | 0.94 | 0.15 | 2,2,2,2                     | 0     |
| 57  | MG   | BA    | 3249 | 1/1   | 0.94 | 0.21 | 25,25,25,25                 | 0     |
| 57  | MG   | CA    | 1632 | 1/1   | 0.94 | 0.13 | 18,18,18,18                 | 0     |
| 57  | MG   | BA    | 3214 | 1/1   | 0.94 | 0.14 | 39,39,39,39                 | 0     |
| 57  | MG   | BA    | 3120 | 1/1   | 0.94 | 0.29 | 24,24,24,24                 | 0     |
| 57  | MG   | CA    | 1636 | 1/1   | 0.94 | 0.11 | 19,19,19,19                 | 0     |
| 57  | MG   | BA    | 3292 | 1/1   | 0.94 | 0.11 | 28,28,28,28                 | 0     |
| 57  | MG   | BA    | 3046 | 1/1   | 0.94 | 0.26 | 1,1,1,1                     | 0     |
| 57  | MG   | DA    | 9442 | 1/1   | 0.94 | 0.20 | 36,36,36,36                 | 0     |
| 57  | MG   | DA    | 9647 | 1/1   | 0.94 | 0.25 | 1,1,1,1                     | 0     |
| 57  | MG   | BA    | 3218 | 1/1   | 0.94 | 0.18 | 24,24,24,24                 | 0     |
| 57  | MG   | CA    | 1738 | 1/1   | 0.94 | 0.30 | 49,49,49,49                 | 0     |
| 57  | MG   | AA    | 7051 | 1/1   | 0.94 | 0.23 | 22,22,22,22                 | 0     |
| 57  | MG   | DA    | 9548 | 1/1   | 0.94 | 0.19 | 26,26,26,26                 | 0     |
| 57  | MG   | BA    | 3123 | 1/1   | 0.94 | 0.08 | 14,14,14,14                 | 0     |
| 57  | MG   | DA    | 9447 | 1/1   | 0.94 | 0.27 | 68,68,68,68                 | 0     |
| 57  | MG   | CA    | 1642 | 1/1   | 0.94 | 0.09 | 54,54,54,54                 | 0     |
| 57  | MG   | DA    | 9552 | 1/1   | 0.94 | 0.30 | 58,58,58,58                 | 0     |
| 57  | MG   | DA    | 9372 | 1/1   | 0.94 | 0.17 | 8,8,8,8                     | 0     |
| 57  | MG   | DA    | 9451 | 1/1   | 0.94 | 0.10 | 35,35,35,35                 | 0     |
| 57  | MG   | AA    | 7043 | 1/1   | 0.94 | 0.11 | 16,16,16,16                 | 0     |
| 57  | MG   | AA    | 7026 | 1/1   | 0.94 | 0.26 | 30,30,30,30                 | 0     |
| 57  | MG   | BA    | 3225 | 1/1   | 0.94 | 0.20 | 2,2,2,2                     | 0     |
| 57  | MG   | CA    | 1601 | 1/1   | 0.94 | 0.12 | 39,39,39,39                 | 0     |
| 57  | MG   | DA    | 9457 | 1/1   | 0.94 | 0.18 | 13,13,13,13                 | 0     |
| 57  | MG   | CA    | 1602 | 1/1   | 0.94 | 0.18 | 14,14,14,14                 | 0     |
| 57  | MG   | DA    | 9459 | 1/1   | 0.94 | 0.16 | 3,3,3,3                     | 0     |
| 57  | MG   | DA    | 9568 | 1/1   | 0.94 | 0.25 | 3,3,3,3                     | 0     |
| 57  | MG   | CX    | 101  | 1/1   | 0.94 | 0.16 | 25,25,25,25                 | 0     |
| 57  | MG   | DA    | 9382 | 1/1   | 0.94 | 0.28 | 0,0,0,0                     | 0     |
| 57  | MG   | DA    | 9572 | 1/1   | 0.94 | 0.15 | 4,4,4,4                     | 0     |
| 57  | MG   | AA    | 7030 | 1/1   | 0.94 | 0.17 | 2,2,2,2                     | 0     |
| 57  | MG   | BA    | 3054 | 1/1   | 0.94 | 0.20 | 14,14,14,14                 | 0     |
| 57  | MG   | DA    | 9575 | 1/1   | 0.94 | 0.08 | 35,35,35,35                 | 0     |
| 57  | MG   | CA    | 1701 | 1/1   | 0.94 | 0.18 | 1,1,1,1                     | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | AE    | 201  | 1/1   | 0.94 | 0.15 | 45,45,45,45                 | 0     |
| 57  | MG   | AA    | 7047 | 1/1   | 0.94 | 0.12 | 41,41,41,41                 | 0     |
| 57  | MG   | BA    | 3083 | 1/1   | 0.94 | 0.20 | 27,27,27,27                 | 1     |
| 57  | MG   | DA    | 9393 | 1/1   | 0.94 | 0.21 | 24,24,24,24                 | 0     |
| 57  | MG   | CA    | 1705 | 1/1   | 0.94 | 0.05 | 15,15,15,15                 | 0     |
| 57  | MG   | DA    | 9395 | 1/1   | 0.94 | 0.15 | 29,29,29,29                 | 0     |
| 57  | MG   | DA    | 9314 | 1/1   | 0.94 | 0.17 | 1,1,1,1                     | 0     |
| 57  | MG   | AA    | 7099 | 1/1   | 0.94 | 0.21 | 6,6,6,6                     | 0     |
| 57  | MG   | DA    | 9694 | 1/1   | 0.94 | 0.19 | 25,25,25,25                 | 0     |
| 57  | MG   | BA    | 3235 | 1/1   | 0.94 | 0.21 | 25,25,25,25                 | 0     |
| 57  | MG   | DA    | 9696 | 1/1   | 0.94 | 0.31 | 34,34,34,34                 | 0     |
| 57  | MG   | DA    | 9401 | 1/1   | 0.94 | 0.35 | 21,21,21,21                 | 1     |
| 57  | MG   | DA    | 9478 | 1/1   | 0.94 | 0.24 | 13,13,13,13                 | 0     |
| 57  | MG   | DA    | 9593 | 1/1   | 0.94 | 0.32 | 25,25,25,25                 | 0     |
| 57  | MG   | BA    | 3017 | 1/1   | 0.94 | 0.16 | 22,22,22,22                 | 0     |
| 57  | MG   | AA    | 7056 | 1/1   | 0.94 | 0.21 | 12,12,12,12                 | 0     |
| 57  | MG   | DD    | 7102 | 1/1   | 0.94 | 0.13 | 0,0,0,0                     | 0     |
| 57  | MG   | DA    | 9326 | 1/1   | 0.94 | 0.16 | 1,1,1,1                     | 0     |
| 57  | MG   | DP    | 202  | 1/1   | 0.94 | 0.26 | 173,173,173,173             | 0     |
| 57  | MG   | CA    | 1662 | 1/1   | 0.94 | 0.10 | 29,29,29,29                 | 0     |
| 57  | MG   | DA    | 9599 | 1/1   | 0.94 | 0.24 | 20,20,20,20                 | 0     |
| 57  | MG   | DU    | 201  | 1/1   | 0.94 | 0.15 | 30,30,30,30                 | 1     |
| 57  | MG   | BA    | 3064 | 1/1   | 0.94 | 0.19 | 29,29,29,29                 | 1     |
| 57  | MG   | AA    | 7075 | 1/1   | 0.94 | 0.33 | 53,53,53,53                 | 0     |
| 57  | MG   | DA    | 9331 | 1/1   | 0.94 | 0.06 | 8,8,8,8                     | 0     |
| 57  | MG   | D0    | 102  | 1/1   | 0.94 | 0.18 | 15,15,15,15                 | 0     |
| 57  | MG   | CA    | 1714 | 1/1   | 0.94 | 0.14 | 53,53,53,53                 | 0     |
| 57  | MG   | BA    | 3275 | 1/1   | 0.94 | 0.07 | 1,1,1,1                     | 1     |
| 57  | MG   | DA    | 9496 | 1/1   | 0.94 | 0.09 | 26,26,26,26                 | 0     |
| 57  | MG   | DA    | 9497 | 1/1   | 0.94 | 0.22 | 29,29,29,29                 | 0     |
| 57  | MG   | CA    | 1622 | 1/1   | 0.94 | 0.04 | 37,37,37,37                 | 0     |
| 57  | MG   | CA    | 1624 | 1/1   | 0.94 | 0.22 | 18,18,18,18                 | 0     |
| 57  | MG   | DA    | 9338 | 1/1   | 0.94 | 0.26 | 58,58,58,58                 | 0     |
| 57  | MG   | AA    | 7022 | 1/1   | 0.94 | 0.13 | 32,32,32,32                 | 0     |
| 57  | MG   | DA    | 9508 | 1/1   | 0.95 | 0.15 | 0,0,0,0                     | 0     |
| 57  | MG   | DA    | 9342 | 1/1   | 0.95 | 0.08 | 0,0,0,0                     | 0     |
| 57  | MG   | CA    | 1668 | 1/1   | 0.95 | 0.19 | 56,56,56,56                 | 0     |
| 57  | MG   | BA    | 3307 | 1/1   | 0.95 | 0.17 | 25,25,25,25                 | 0     |
| 57  | MG   | BA    | 3024 | 1/1   | 0.95 | 0.25 | 22,22,22,22                 | 0     |
| 57  | MG   | DA    | 9516 | 1/1   | 0.95 | 0.28 | 1,1,1,1                     | 0     |
| 57  | MG   | BA    | 3261 | 1/1   | 0.95 | 0.14 | 10,10,10,10                 | 0     |
| 57  | MG   | BA    | 3311 | 1/1   | 0.95 | 0.16 | 13,13,13,13                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | BA    | 3035 | 1/1   | 0.95 | 0.18 | 0,0,0,0                     | 0     |
| 57  | MG   | BA    | 3010 | 1/1   | 0.95 | 0.36 | 28,28,28,28                 | 0     |
| 57  | MG   | DA    | 9522 | 1/1   | 0.95 | 0.25 | 2,2,2,2                     | 0     |
| 57  | MG   | DA    | 9353 | 1/1   | 0.95 | 0.15 | 24,24,24,24                 | 0     |
| 57  | MG   | DA    | 9524 | 1/1   | 0.95 | 0.22 | 2,2,2,2                     | 0     |
| 57  | MG   | DA    | 9632 | 1/1   | 0.95 | 0.28 | 12,12,12,12                 | 1     |
| 57  | MG   | DA    | 9435 | 1/1   | 0.95 | 0.43 | 30,30,30,30                 | 0     |
| 57  | MG   | BA    | 3139 | 1/1   | 0.95 | 0.22 | 0,0,0,0                     | 0     |
| 57  | MG   | DA    | 9356 | 1/1   | 0.95 | 0.17 | 1,1,1,1                     | 0     |
| 57  | MG   | DA    | 9529 | 1/1   | 0.95 | 0.23 | 0,0,0,0                     | 0     |
| 57  | MG   | BA    | 3078 | 1/1   | 0.95 | 0.14 | 2,2,2,2                     | 0     |
| 57  | MG   | DA    | 9359 | 1/1   | 0.95 | 0.20 | 0,0,0,0                     | 0     |
| 57  | MG   | BA    | 3118 | 1/1   | 0.95 | 0.25 | 28,28,28,28                 | 0     |
| 57  | MG   | BA    | 3317 | 1/1   | 0.95 | 0.34 | 21,21,21,21                 | 0     |
| 57  | MG   | BA    | 3182 | 1/1   | 0.95 | 0.21 | 2,2,2,2                     | 0     |
| 57  | MG   | BA    | 3100 | 1/1   | 0.95 | 0.05 | 21,21,21,21                 | 0     |
| 57  | MG   | AA    | 7049 | 1/1   | 0.95 | 0.15 | 41,41,41,41                 | 0     |
| 57  | MG   | BA    | 3005 | 1/1   | 0.95 | 0.13 | 22,22,22,22                 | 0     |
| 57  | MG   | CA    | 1742 | 1/1   | 0.95 | 0.22 | 10,10,10,10                 | 0     |
| 57  | MG   | BA    | 3230 | 1/1   | 0.95 | 0.16 | 22,22,22,22                 | 0     |
| 57  | MG   | DA    | 9546 | 1/1   | 0.95 | 0.24 | 2,2,2,2                     | 0     |
| 57  | MG   | DA    | 9547 | 1/1   | 0.95 | 0.13 | 3,3,3,3                     | 0     |
| 57  | MG   | DA    | 9653 | 1/1   | 0.95 | 0.19 | 5,5,5,5                     | 0     |
| 57  | MG   | CA    | 1635 | 1/1   | 0.95 | 0.19 | 4,4,4,4                     | 0     |
| 57  | MG   | DA    | 9449 | 1/1   | 0.95 | 0.23 | 0,0,0,0                     | 0     |
| 57  | MG   | AA    | 7040 | 1/1   | 0.95 | 0.12 | 36,36,36,36                 | 0     |
| 57  | MG   | BA    | 3151 | 1/1   | 0.95 | 0.07 | 12,12,12,12                 | 0     |
| 57  | MG   | DA    | 9375 | 1/1   | 0.95 | 0.25 | 0,0,0,0                     | 0     |
| 57  | MG   | BA    | 3188 | 1/1   | 0.95 | 0.10 | 0,0,0,0                     | 0     |
| 57  | MG   | DA    | 9554 | 1/1   | 0.95 | 0.16 | 10,10,10,10                 | 0     |
| 57  | MG   | DA    | 9662 | 1/1   | 0.95 | 0.29 | 2,2,2,2                     | 0     |
| 57  | MG   | BA    | 3104 | 1/1   | 0.95 | 0.07 | 16,16,16,16                 | 0     |
| 57  | MG   | BA    | 3125 | 1/1   | 0.95 | 0.22 | 20,20,20,20                 | 0     |
| 57  | MG   | CA    | 1695 | 1/1   | 0.95 | 0.15 | 15,15,15,15                 | 0     |
| 57  | MG   | BA    | 3068 | 1/1   | 0.95 | 0.06 | 11,11,11,11                 | 0     |
| 57  | MG   | DA    | 9303 | 1/1   | 0.95 | 0.13 | 42,42,42,42                 | 0     |
| 57  | MG   | BA    | 3194 | 1/1   | 0.95 | 0.18 | 1,1,1,1                     | 0     |
| 57  | MG   | DA    | 9670 | 1/1   | 0.95 | 0.17 | 11,11,11,11                 | 0     |
| 57  | MG   | DA    | 9384 | 1/1   | 0.95 | 0.23 | 16,16,16,16                 | 0     |
| 57  | MG   | DA    | 9673 | 1/1   | 0.95 | 0.10 | 8,8,8,8                     | 0     |
| 57  | MG   | DA    | 9305 | 1/1   | 0.95 | 0.25 | 0,0,0,0                     | 0     |
| 57  | MG   | BA    | 3127 | 1/1   | 0.95 | 0.20 | 8,8,8,8                     | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | DA    | 9308 | 1/1   | 0.95 | 0.24 | 2,2,2,2                     | 0     |
| 57  | MG   | BE    | 302  | 1/1   | 0.95 | 0.17 | 74,74,74,74                 | 0     |
| 57  | MG   | DA    | 9679 | 1/1   | 0.95 | 0.13 | 16,16,16,16                 | 0     |
| 57  | MG   | BA    | 3019 | 1/1   | 0.95 | 0.17 | 44,44,44,44                 | 0     |
| 57  | MG   | CA    | 1646 | 1/1   | 0.95 | 0.26 | 7,7,7,7                     | 0     |
| 57  | MG   | DA    | 9682 | 1/1   | 0.95 | 0.14 | 20,20,20,20                 | 0     |
| 57  | MG   | BA    | 3287 | 1/1   | 0.95 | 0.18 | 30,30,30,30                 | 0     |
| 57  | MG   | CA    | 1649 | 1/1   | 0.95 | 0.08 | 33,33,33,33                 | 0     |
| 57  | MG   | BA    | 3107 | 1/1   | 0.95 | 0.20 | 36,36,36,36                 | 0     |
| 57  | MG   | DA    | 9472 | 1/1   | 0.95 | 0.20 | 16,16,16,16                 | 0     |
| 57  | MG   | DA    | 9320 | 1/1   | 0.95 | 0.14 | 10,10,10,10                 | 0     |
| 57  | MG   | BA    | 3291 | 1/1   | 0.95 | 0.08 | 22,22,22,22                 | 0     |
| 57  | MG   | DA    | 9323 | 1/1   | 0.95 | 0.25 | 33,33,33,33                 | 0     |
| 57  | MG   | AA    | 7014 | 1/1   | 0.95 | 0.26 | 20,20,20,20                 | 0     |
| 57  | MG   | DA    | 9584 | 1/1   | 0.95 | 0.28 | 0,0,0,0                     | 0     |
| 57  | MG   | DA    | 9403 | 1/1   | 0.95 | 0.16 | 0,0,0,0                     | 0     |
| 57  | MG   | DA    | 9587 | 1/1   | 0.95 | 0.19 | 2,2,2,2                     | 0     |
| 57  | MG   | BA    | 3057 | 1/1   | 0.95 | 0.18 | 2,2,2,2                     | 0     |
| 57  | MG   | AA    | 7039 | 1/1   | 0.95 | 0.22 | 11,11,11,11                 | 0     |
| 57  | MG   | DA    | 9407 | 1/1   | 0.95 | 0.09 | 2,2,2,2                     | 0     |
| 57  | MG   | BA    | 3165 | 1/1   | 0.95 | 0.24 | 0,0,0,0                     | 0     |
| 57  | MG   | DA    | 9409 | 1/1   | 0.95 | 0.23 | 4,4,4,4                     | 0     |
| 57  | MG   | DA    | 9410 | 1/1   | 0.95 | 0.13 | 4,4,4,4                     | 0     |
| 57  | MG   | DE    | 301  | 1/1   | 0.95 | 0.16 | 1,1,1,1                     | 0     |
| 57  | MG   | BA    | 3074 | 1/1   | 0.95 | 0.34 | 34,34,34,34                 | 0     |
| 57  | MG   | DA    | 9492 | 1/1   | 0.95 | 0.06 | 76,76,76,76                 | 0     |
| 57  | MG   | BA    | 3089 | 1/1   | 0.95 | 0.23 | 18,18,18,18                 | 0     |
| 57  | MG   | BA    | 3211 | 1/1   | 0.95 | 0.09 | 2,2,2,2                     | 0     |
| 57  | MG   | BA    | 3169 | 1/1   | 0.95 | 0.26 | 3,3,3,3                     | 0     |
| 57  | MG   | CA    | 1717 | 1/1   | 0.95 | 0.10 | 11,11,11,11                 | 0     |
| 57  | MG   | DA    | 9498 | 1/1   | 0.95 | 0.22 | 2,2,2,2                     | 0     |
| 57  | MG   | DA    | 9335 | 1/1   | 0.95 | 0.21 | 21,21,21,21                 | 0     |
| 57  | MG   | BA    | 3213 | 1/1   | 0.95 | 0.22 | 8,8,8,8                     | 0     |
| 57  | MG   | BA    | 3092 | 1/1   | 0.95 | 0.11 | 1,1,1,1                     | 0     |
| 57  | MG   | BA    | 3172 | 1/1   | 0.95 | 0.24 | 58,58,58,58                 | 0     |
| 57  | MG   | DA    | 9606 | 1/1   | 0.95 | 0.29 | 4,4,4,4                     | 0     |
| 57  | MG   | D5    | 101  | 1/1   | 0.95 | 0.16 | 7,7,7,7                     | 0     |
| 57  | MG   | CA    | 1613 | 1/1   | 0.95 | 0.23 | 31,31,31,31                 | 0     |
| 57  | MG   | DA    | 9424 | 1/1   | 0.95 | 0.19 | 5,5,5,5                     | 0     |
| 57  | MG   | DA    | 9507 | 1/1   | 0.95 | 0.26 | 2,2,2,2                     | 0     |
| 57  | MG   | DA    | 9611 | 1/1   | 0.95 | 0.17 | 8,8,8,8                     | 0     |
| 57  | MG   | DA    | 9612 | 1/1   | 0.95 | 0.17 | 1,1,1,1                     | 1     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | BA    | 3065 | 1/1   | 0.96 | 0.36 | 2,2,2,2                     | 0     |
| 57  | MG   | CA    | 1677 | 1/1   | 0.96 | 0.08 | 22,22,22,22                 | 0     |
| 57  | MG   | CA    | 1678 | 1/1   | 0.96 | 0.11 | 17,17,17,17                 | 0     |
| 57  | MG   | DA    | 9482 | 1/1   | 0.96 | 0.06 | 12,12,12,12                 | 0     |
| 57  | MG   | CA    | 1732 | 1/1   | 0.96 | 0.27 | 27,27,27,27                 | 0     |
| 57  | MG   | CA    | 1733 | 1/1   | 0.96 | 0.14 | 11,11,11,11                 | 0     |
| 57  | MG   | DA    | 9485 | 1/1   | 0.96 | 0.17 | 15,15,15,15                 | 0     |
| 57  | MG   | DA    | 9566 | 1/1   | 0.96 | 0.22 | 18,18,18,18                 | 0     |
| 57  | MG   | AA    | 7096 | 1/1   | 0.96 | 0.23 | 31,31,31,31                 | 0     |
| 57  | MG   | DA    | 9349 | 1/1   | 0.96 | 0.33 | 3,3,3,3                     | 0     |
| 57  | MG   | AA    | 7032 | 1/1   | 0.96 | 0.15 | 24,24,24,24                 | 0     |
| 57  | MG   | BA    | 3047 | 1/1   | 0.96 | 0.18 | 0,0,0,0                     | 0     |
| 57  | MG   | DA    | 9571 | 1/1   | 0.96 | 0.23 | 0,0,0,0                     | 0     |
| 57  | MG   | DA    | 9491 | 1/1   | 0.96 | 0.11 | 11,11,11,11                 | 0     |
| 57  | MG   | BA    | 3229 | 1/1   | 0.96 | 0.12 | 19,19,19,19                 | 0     |
| 57  | MG   | CA    | 1631 | 1/1   | 0.96 | 0.36 | 22,22,22,22                 | 0     |
| 57  | MG   | DA    | 9354 | 1/1   | 0.96 | 0.25 | 2,2,2,2                     | 0     |
| 57  | MG   | BA    | 3191 | 1/1   | 0.96 | 0.19 | 2,2,2,2                     | 0     |
| 57  | MG   | BA    | 3192 | 1/1   | 0.96 | 0.22 | 2,2,2,2                     | 0     |
| 57  | MG   | BA    | 3020 | 1/1   | 0.96 | 0.16 | 1,1,1,1                     | 0     |
| 57  | MG   | CE    | 201  | 1/1   | 0.96 | 0.11 | 16,16,16,16                 | 0     |
| 57  | MG   | BA    | 3163 | 1/1   | 0.96 | 0.16 | 28,28,28,28                 | 0     |
| 57  | MG   | BA    | 3034 | 1/1   | 0.96 | 0.15 | 7,7,7,7                     | 0     |
| 57  | MG   | DA    | 9583 | 1/1   | 0.96 | 0.15 | 1,1,1,1                     | 0     |
| 57  | MG   | AA    | 7079 | 1/1   | 0.96 | 0.13 | 35,35,35,35                 | 0     |
| 57  | MG   | DA    | 9585 | 1/1   | 0.96 | 0.11 | 18,18,18,18                 | 0     |
| 57  | MG   | BA    | 3279 | 1/1   | 0.96 | 0.24 | 31,31,31,31                 | 0     |
| 57  | MG   | BA    | 3280 | 1/1   | 0.96 | 0.24 | 19,19,19,19                 | 1     |
| 57  | MG   | BA    | 3238 | 1/1   | 0.96 | 0.24 | 9,9,9,9                     | 0     |
| 57  | MG   | BA    | 3166 | 1/1   | 0.96 | 0.27 | 40,40,40,40                 | 0     |
| 57  | MG   | BA    | 3200 | 1/1   | 0.96 | 0.14 | 5,5,5,5                     | 0     |
| 57  | MG   | DA    | 9511 | 1/1   | 0.96 | 0.30 | 7,7,7,7                     | 0     |
| 57  | MG   | AA    | 7107 | 1/1   | 0.96 | 0.24 | 24,24,24,24                 | 0     |
| 57  | MG   | AA    | 7019 | 1/1   | 0.96 | 0.14 | 16,16,16,16                 | 0     |
| 57  | MG   | DA    | 9514 | 1/1   | 0.96 | 0.38 | 19,19,19,19                 | 0     |
| 57  | MG   | BA    | 3289 | 1/1   | 0.96 | 0.20 | 21,21,21,21                 | 0     |
| 57  | MG   | AA    | 7085 | 1/1   | 0.96 | 0.06 | 15,15,15,15                 | 0     |
| 57  | MG   | CA    | 1647 | 1/1   | 0.96 | 0.15 | 6,6,6,6                     | 0     |
| 57  | MG   | BA    | 3140 | 1/1   | 0.96 | 0.11 | 40,40,40,40                 | 0     |
| 57  | MG   | DA    | 9309 | 1/1   | 0.96 | 0.16 | 6,6,6,6                     | 0     |
| 57  | MG   | BA    | 3099 | 1/1   | 0.96 | 0.09 | 30,30,30,30                 | 0     |
| 57  | MG   | BA    | 3209 | 1/1   | 0.96 | 0.13 | 1,1,1,1                     | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | DA    | 9690 | 1/1   | 0.96 | 0.07 | 5,5,5,5                     | 0     |
| 57  | MG   | BA    | 3056 | 1/1   | 0.96 | 0.11 | 5,5,5,5                     | 0     |
| 57  | MG   | BA    | 3144 | 1/1   | 0.96 | 0.40 | 41,41,41,41                 | 0     |
| 57  | MG   | BA    | 3176 | 1/1   | 0.96 | 0.16 | 0,0,0,0                     | 0     |
| 57  | MG   | AA    | 7058 | 1/1   | 0.96 | 0.10 | 13,13,13,13                 | 0     |
| 57  | MG   | DA    | 9527 | 1/1   | 0.96 | 0.22 | 1,1,1,1                     | 0     |
| 57  | MG   | DA    | 9317 | 1/1   | 0.96 | 0.07 | 18,18,18,18                 | 0     |
| 57  | MG   | DA    | 9318 | 1/1   | 0.96 | 0.17 | 2,2,2,2                     | 0     |
| 57  | MG   | DA    | 9389 | 1/1   | 0.96 | 0.06 | 11,11,11,11                 | 0     |
| 57  | MG   | DA    | 9319 | 1/1   | 0.96 | 0.20 | 30,30,30,30                 | 0     |
| 57  | MG   | DA    | 9533 | 1/1   | 0.96 | 0.19 | 0,0,0,0                     | 0     |
| 57  | MG   | DA    | 9534 | 1/1   | 0.96 | 0.21 | 1,1,1,1                     | 0     |
| 57  | MG   | DD    | 7103 | 1/1   | 0.96 | 0.15 | 0,0,0,0                     | 0     |
| 57  | MG   | BA    | 3040 | 1/1   | 0.96 | 0.23 | 0,0,0,0                     | 0     |
| 57  | MG   | DA    | 9537 | 1/1   | 0.96 | 0.25 | 0,0,0,0                     | 0     |
| 57  | MG   | BA    | 3215 | 1/1   | 0.96 | 0.21 | 1,1,1,1                     | 0     |
| 57  | MG   | BA    | 3059 | 1/1   | 0.96 | 0.07 | 0,0,0,0                     | 0     |
| 57  | MG   | BA    | 3080 | 1/1   | 0.96 | 0.17 | 0,0,0,0                     | 0     |
| 57  | MG   | BA    | 3304 | 1/1   | 0.96 | 0.18 | 13,13,13,13                 | 0     |
| 57  | MG   | DU    | 202  | 1/1   | 0.96 | 0.06 | 6,6,6,6                     | 0     |
| 57  | MG   | BA    | 3305 | 1/1   | 0.96 | 0.15 | 24,24,24,24                 | 0     |
| 57  | MG   | DA    | 9328 | 1/1   | 0.96 | 0.17 | 1,1,1,1                     | 0     |
| 57  | MG   | CA    | 1663 | 1/1   | 0.96 | 0.23 | 11,11,11,11                 | 0     |
| 57  | MG   | BA    | 3013 | 1/1   | 0.96 | 0.13 | 16,16,16,16                 | 0     |
| 57  | MG   | BA    | 3152 | 1/1   | 0.96 | 0.14 | 18,18,18,18                 | 0     |
| 57  | MG   | DA    | 9631 | 1/1   | 0.96 | 0.19 | 21,21,21,21                 | 0     |
| 57  | MG   | AA    | 7093 | 1/1   | 0.96 | 0.21 | 30,30,30,30                 | 0     |
| 57  | MG   | BA    | 3309 | 1/1   | 0.96 | 0.34 | 25,25,25,25                 | 0     |
| 57  | MG   | CA    | 1618 | 1/1   | 0.96 | 0.11 | 31,31,31,31                 | 0     |
| 57  | MG   | BA    | 3043 | 1/1   | 0.96 | 0.11 | 8,8,8,8                     | 0     |
| 57  | MG   | BA    | 3016 | 1/1   | 0.96 | 0.16 | 8,8,8,8                     | 0     |
| 57  | MG   | BA    | 3223 | 1/1   | 0.96 | 0.09 | 9,9,9,9                     | 0     |
| 57  | MG   | BA    | 3266 | 1/1   | 0.96 | 0.19 | 33,33,33,33                 | 0     |
| 57  | MG   | DA    | 9336 | 1/1   | 0.97 | 0.16 | 52,52,52,52                 | 0     |
| 57  | MG   | BA    | 3197 | 1/1   | 0.97 | 0.12 | 1,1,1,1                     | 0     |
| 57  | MG   | BA    | 3244 | 1/1   | 0.97 | 0.05 | 1,1,1,1                     | 0     |
| 57  | MG   | CA    | 1623 | 1/1   | 0.97 | 0.12 | 19,19,19,19                 | 0     |
| 57  | MG   | DA    | 9654 | 1/1   | 0.97 | 0.14 | 15,15,15,15                 | 0     |
| 57  | MG   | DA    | 9452 | 1/1   | 0.97 | 0.24 | 10,10,10,10                 | 0     |
| 57  | MG   | CA    | 1660 | 1/1   | 0.97 | 0.13 | 9,9,9,9                     | 0     |
| 57  | MG   | AA    | 7067 | 1/1   | 0.97 | 0.16 | 28,28,28,28                 | 0     |
| 57  | MG   | DA    | 9398 | 1/1   | 0.97 | 0.19 | 0,0,0,0                     | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | BA    | 3048 | 1/1   | 0.97 | 0.14 | 17,17,17,17                 | 0     |
| 57  | MG   | DA    | 9400 | 1/1   | 0.97 | 0.15 | 0,0,0,0                     | 0     |
| 57  | MG   | BA    | 3094 | 1/1   | 0.97 | 0.19 | 7,7,7,7                     | 0     |
| 57  | MG   | BA    | 3148 | 1/1   | 0.97 | 0.07 | 16,16,16,16                 | 0     |
| 57  | MG   | BA    | 3002 | 1/1   | 0.97 | 0.21 | 53,53,53,53                 | 0     |
| 57  | MG   | BA    | 3303 | 1/1   | 0.97 | 0.04 | 19,19,19,19                 | 0     |
| 57  | MG   | BE    | 303  | 1/1   | 0.97 | 0.12 | 1,1,1,1                     | 0     |
| 57  | MG   | DA    | 9301 | 1/1   | 0.97 | 0.18 | 32,32,32,32                 | 0     |
| 57  | MG   | CA    | 1669 | 1/1   | 0.97 | 0.08 | 10,10,10,10                 | 0     |
| 57  | MG   | DA    | 9668 | 1/1   | 0.97 | 0.30 | 4,4,4,4                     | 0     |
| 57  | MG   | CA    | 1670 | 1/1   | 0.97 | 0.07 | 2,2,2,2                     | 0     |
| 57  | MG   | AA    | 7042 | 1/1   | 0.97 | 0.05 | 31,31,31,31                 | 0     |
| 57  | MG   | CA    | 1712 | 1/1   | 0.97 | 0.17 | 34,34,34,34                 | 1     |
| 57  | MG   | AA    | 7095 | 1/1   | 0.97 | 0.08 | 17,17,17,17                 | 0     |
| 57  | MG   | DA    | 9469 | 1/1   | 0.97 | 0.17 | 17,17,17,17                 | 0     |
| 57  | MG   | DA    | 9413 | 1/1   | 0.97 | 0.21 | 3,3,3,3                     | 0     |
| 57  | MG   | DA    | 9535 | 1/1   | 0.97 | 0.19 | 14,14,14,14                 | 0     |
| 57  | MG   | DA    | 9307 | 1/1   | 0.97 | 0.16 | 12,12,12,12                 | 0     |
| 57  | MG   | BA    | 3208 | 1/1   | 0.97 | 0.12 | 8,8,8,8                     | 0     |
| 57  | MG   | BA    | 3023 | 1/1   | 0.97 | 0.10 | 4,4,4,4                     | 0     |
| 57  | MG   | BA    | 3170 | 1/1   | 0.97 | 0.26 | 1,1,1,1                     | 0     |
| 57  | MG   | DA    | 9311 | 1/1   | 0.97 | 0.25 | 29,29,29,29                 | 0     |
| 57  | MG   | DA    | 9683 | 1/1   | 0.97 | 0.21 | 19,19,19,19                 | 0     |
| 57  | MG   | DA    | 9541 | 1/1   | 0.97 | 0.25 | 2,2,2,2                     | 0     |
| 57  | MG   | DA    | 9363 | 1/1   | 0.97 | 0.08 | 1,1,1,1                     | 0     |
| 57  | MG   | DA    | 9609 | 1/1   | 0.97 | 0.14 | 2,2,2,2                     | 0     |
| 57  | MG   | B5    | 101  | 1/1   | 0.97 | 0.11 | 2,2,2,2                     | 0     |
| 57  | MG   | B7    | 101  | 1/1   | 0.97 | 0.18 | 13,13,13,13                 | 0     |
| 57  | MG   | DA    | 9480 | 1/1   | 0.97 | 0.05 | 30,30,30,30                 | 0     |
| 57  | MG   | DA    | 9613 | 1/1   | 0.97 | 0.08 | 5,5,5,5                     | 0     |
| 57  | MG   | DA    | 9691 | 1/1   | 0.97 | 0.17 | 12,12,12,12                 | 0     |
| 57  | MG   | CA    | 1720 | 1/1   | 0.97 | 0.19 | 2,2,2,2                     | 0     |
| 57  | MG   | DA    | 9368 | 1/1   | 0.97 | 0.10 | 1,1,1,1                     | 0     |
| 57  | MG   | CA    | 1721 | 1/1   | 0.97 | 0.12 | 1,1,1,1                     | 0     |
| 57  | MG   | BA    | 3124 | 1/1   | 0.97 | 0.09 | 17,17,17,17                 | 0     |
| 57  | MG   | BA    | 3256 | 1/1   | 0.97 | 0.03 | 13,13,13,13                 | 0     |
| 57  | MG   | AA    | 7089 | 1/1   | 0.97 | 0.04 | 21,21,21,21                 | 0     |
| 57  | MG   | BA    | 3283 | 1/1   | 0.97 | 0.13 | 22,22,22,22                 | 0     |
| 57  | MG   | BA    | 3015 | 1/1   | 0.97 | 0.18 | 3,3,3,3                     | 0     |
| 57  | MG   | BA    | 3285 | 1/1   | 0.97 | 0.40 | 32,32,32,32                 | 1     |
| 57  | MG   | DA    | 9625 | 1/1   | 0.97 | 0.18 | 26,26,26,26                 | 0     |
| 57  | MG   | BA    | 3234 | 1/1   | 0.97 | 0.35 | 10,10,10,10                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | DA    | 9556 | 1/1   | 0.97 | 0.04 | 23,23,23,23                 | 0     |
| 57  | MG   | BA    | 3260 | 1/1   | 0.97 | 0.17 | 8,8,8,8                     | 0     |
| 57  | MG   | AA    | 7001 | 1/1   | 0.97 | 0.17 | 26,26,26,26                 | 0     |
| 57  | MG   | DA    | 9495 | 1/1   | 0.97 | 0.23 | 3,3,3,3                     | 0     |
| 57  | MG   | DA    | 9562 | 1/1   | 0.97 | 0.38 | 2,2,2,2                     | 0     |
| 57  | MG   | CA    | 1611 | 1/1   | 0.97 | 0.20 | 0,0,0,0                     | 0     |
| 57  | MG   | DA    | 9381 | 1/1   | 0.97 | 0.08 | 12,12,12,12                 | 0     |
| 57  | MG   | DA    | 9635 | 1/1   | 0.97 | 0.19 | 24,24,24,24                 | 0     |
| 57  | MG   | BA    | 3175 | 1/1   | 0.97 | 0.12 | 4,4,4,4                     | 0     |
| 57  | MG   | AA    | 7012 | 1/1   | 0.97 | 0.28 | 12,12,12,12                 | 0     |
| 57  | MG   | DA    | 9500 | 1/1   | 0.97 | 0.11 | 1,1,1,1                     | 0     |
| 57  | MG   | BA    | 3240 | 1/1   | 0.97 | 0.10 | 21,21,21,21                 | 0     |
| 57  | MG   | CA    | 1615 | 1/1   | 0.97 | 0.17 | 0,0,0,0                     | 0     |
| 57  | MG   | DA    | 9642 | 1/1   | 0.97 | 0.12 | 1,1,1,1                     | 0     |
| 57  | MG   | DA    | 9386 | 1/1   | 0.97 | 0.19 | 2,2,2,2                     | 0     |
| 57  | MG   | BA    | 3293 | 1/1   | 0.97 | 0.09 | 1,1,1,1                     | 0     |
| 57  | MG   | BA    | 3142 | 1/1   | 0.97 | 0.18 | 10,10,10,10                 | 0     |
| 57  | MG   | D8    | 101  | 1/1   | 0.97 | 0.04 | 3,3,3,3                     | 0     |
| 57  | MG   | DA    | 9646 | 1/1   | 0.97 | 0.12 | 31,31,31,31                 | 0     |
| 57  | MG   | BA    | 3090 | 1/1   | 0.97 | 0.19 | 2,2,2,2                     | 0     |
| 57  | MG   | CA    | 1619 | 1/1   | 0.97 | 0.18 | 11,11,11,11                 | 0     |
| 57  | MG   | DA    | 9509 | 1/1   | 0.97 | 0.10 | 17,17,17,17                 | 0     |
| 57  | MG   | BA    | 3156 | 1/1   | 0.98 | 0.15 | 19,19,19,19                 | 0     |
| 57  | MG   | DA    | 9345 | 1/1   | 0.98 | 0.23 | 19,19,19,19                 | 0     |
| 57  | MG   | CA    | 1620 | 1/1   | 0.98 | 0.08 | 1,1,1,1                     | 0     |
| 57  | MG   | BA    | 3288 | 1/1   | 0.98 | 0.10 | 18,18,18,18                 | 0     |
| 57  | MG   | BA    | 3224 | 1/1   | 0.98 | 0.07 | 5,5,5,5                     | 0     |
| 57  | MG   | BA    | 3018 | 1/1   | 0.98 | 0.13 | 37,37,37,37                 | 0     |
| 57  | MG   | BA    | 3207 | 1/1   | 0.98 | 0.16 | 1,1,1,1                     | 0     |
| 57  | MG   | BA    | 3027 | 1/1   | 0.98 | 0.18 | 4,4,4,4                     | 0     |
| 57  | MG   | BA    | 3091 | 1/1   | 0.98 | 0.12 | 0,0,0,0                     | 0     |
| 57  | MG   | DA    | 9426 | 1/1   | 0.98 | 0.21 | 9,9,9,9                     | 1     |
| 57  | MG   | CA    | 1679 | 1/1   | 0.98 | 0.13 | 9,9,9,9                     | 0     |
| 57  | MG   | CA    | 1652 | 1/1   | 0.98 | 0.24 | 6,6,6,6                     | 0     |
| 57  | MG   | BA    | 3011 | 1/1   | 0.98 | 0.24 | 36,36,36,36                 | 0     |
| 57  | MG   | DA    | 9391 | 1/1   | 0.98 | 0.12 | 1,1,1,1                     | 0     |
| 57  | MG   | BA    | 3272 | 1/1   | 0.98 | 0.12 | 10,10,10,10                 | 0     |
| 57  | MG   | DA    | 9357 | 1/1   | 0.98 | 0.12 | 0,0,0,0                     | 0     |
| 57  | MG   | BA    | 3146 | 1/1   | 0.98 | 0.34 | 0,0,0,0                     | 0     |
| 57  | MG   | AA    | 7038 | 1/1   | 0.98 | 0.25 | 10,10,10,10                 | 0     |
| 57  | MG   | DA    | 9558 | 1/1   | 0.98 | 0.04 | 6,6,6,6                     | 0     |
| 57  | MG   | DA    | 9473 | 1/1   | 0.98 | 0.34 | 0,0,0,0                     | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | AA    | 7044 | 1/1   | 0.98 | 0.09 | 21,21,21,21                 | 0     |
| 57  | MG   | CA    | 1715 | 1/1   | 0.98 | 0.20 | 12,12,12,12                 | 0     |
| 57  | MG   | DA    | 9518 | 1/1   | 0.98 | 0.14 | 0,0,0,0                     | 0     |
| 57  | MG   | BA    | 3049 | 1/1   | 0.98 | 0.08 | 30,30,30,30                 | 0     |
| 57  | MG   | BA    | 3071 | 1/1   | 0.98 | 0.19 | 0,0,0,0                     | 0     |
| 57  | MG   | BA    | 3060 | 1/1   | 0.98 | 0.30 | 1,1,1,1                     | 0     |
| 57  | MG   | DE    | 302  | 1/1   | 0.98 | 0.06 | 35,35,35,35                 | 0     |
| 57  | MG   | BA    | 3199 | 1/1   | 0.98 | 0.08 | 1,1,1,1                     | 0     |
| 57  | MG   | DP    | 201  | 1/1   | 0.98 | 0.05 | 7,7,7,7                     | 0     |
| 57  | MG   | BA    | 3237 | 1/1   | 0.98 | 0.12 | 43,43,43,43                 | 0     |
| 57  | MG   | DA    | 9481 | 1/1   | 0.98 | 0.07 | 0,0,0,0                     | 0     |
| 57  | MG   | BA    | 3007 | 1/1   | 0.98 | 0.25 | 4,4,4,4                     | 0     |
| 57  | MG   | BA    | 3239 | 1/1   | 0.98 | 0.16 | 1,1,1,1                     | 0     |
| 57  | MG   | BA    | 3201 | 1/1   | 0.98 | 0.17 | 6,6,6,6                     | 0     |
| 57  | MG   | DA    | 9406 | 1/1   | 0.98 | 0.20 | 32,32,32,32                 | 0     |
| 57  | MG   | AA    | 7041 | 1/1   | 0.98 | 0.17 | 20,20,20,20                 | 0     |
| 57  | MG   | CA    | 1667 | 1/1   | 0.98 | 0.13 | 12,12,12,12                 | 0     |
| 57  | MG   | DA    | 9488 | 1/1   | 0.98 | 0.26 | 0,0,0,0                     | 0     |
| 57  | MG   | DA    | 9623 | 1/1   | 0.98 | 0.15 | 13,13,13,13                 | 0     |
| 57  | MG   | DA    | 9373 | 1/1   | 0.98 | 0.10 | 0,0,0,0                     | 0     |
| 57  | MG   | BE    | 301  | 1/1   | 0.98 | 0.09 | 0,0,0,0                     | 0     |
| 57  | MG   | DA    | 9672 | 1/1   | 0.98 | 0.12 | 5,5,5,5                     | 0     |
| 57  | MG   | AA    | 7094 | 1/1   | 0.98 | 0.26 | 8,8,8,8                     | 0     |
| 57  | MG   | CA    | 1698 | 1/1   | 0.98 | 0.15 | 1,1,1,1                     | 1     |
| 57  | MG   | DA    | 9675 | 1/1   | 0.98 | 0.13 | 11,11,11,11                 | 0     |
| 57  | MG   | DA    | 9341 | 1/1   | 0.98 | 0.25 | 11,11,11,11                 | 0     |
| 57  | MG   | DA    | 9414 | 1/1   | 0.98 | 0.27 | 16,16,16,16                 | 0     |
| 59  | ZN   | AN    | 101  | 1/1   | 0.98 | 0.04 | 147,147,147,147             | 0     |
| 59  | ZN   | CD    | 301  | 1/1   | 0.98 | 0.20 | 44,44,44,44                 | 0     |
| 57  | MG   | AA    | 7015 | 1/1   | 0.98 | 0.14 | 4,4,4,4                     | 0     |
| 57  | MG   | DA    | 9627 | 1/1   | 0.99 | 0.09 | 0,0,0,0                     | 1     |
| 57  | MG   | DA    | 9364 | 1/1   | 0.99 | 0.36 | 1,1,1,1                     | 0     |
| 57  | MG   | DA    | 9322 | 1/1   | 0.99 | 0.05 | 8,8,8,8                     | 0     |
| 57  | MG   | DA    | 9594 | 1/1   | 0.99 | 0.31 | 19,19,19,19                 | 0     |
| 57  | MG   | DA    | 9343 | 1/1   | 0.99 | 0.15 | 2,2,2,2                     | 0     |
| 57  | MG   | DA    | 9506 | 1/1   | 0.99 | 0.09 | 0,0,0,0                     | 0     |
| 57  | MG   | DU    | 203  | 1/1   | 0.99 | 0.07 | 0,0,0,0                     | 1     |
| 57  | MG   | DA    | 9580 | 1/1   | 0.99 | 0.26 | 0,0,0,0                     | 0     |
| 57  | MG   | BA    | 3179 | 1/1   | 0.99 | 0.10 | 10,10,10,10                 | 0     |
| 57  | MG   | DA    | 9324 | 1/1   | 0.99 | 0.20 | 2,2,2,2                     | 0     |
| 57  | MG   | DA    | 9617 | 1/1   | 0.99 | 0.10 | 11,11,11,11                 | 0     |
| 57  | MG   | DA    | 9697 | 1/1   | 0.99 | 0.07 | 41,41,41,41                 | 0     |

*Continued on next page...*



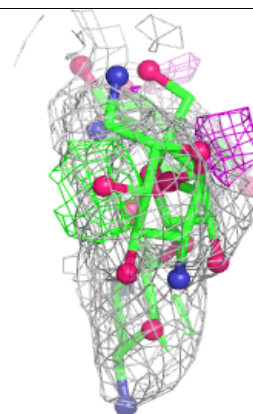
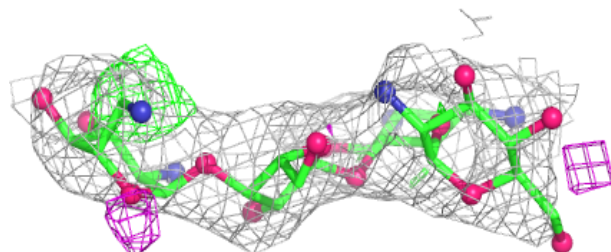
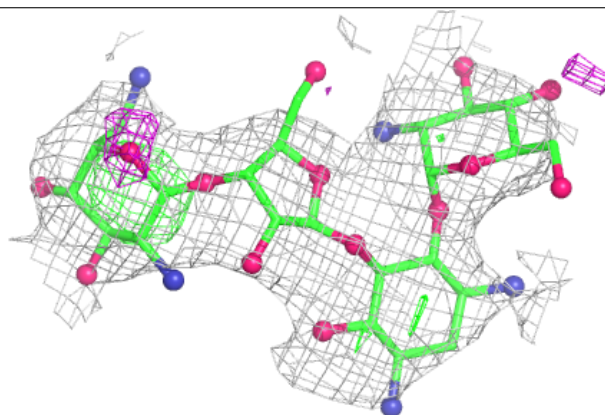
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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | DA    | 9417 | 1/1   | 0.99 | 0.16 | 20,20,20,20                 | 0     |
| 57  | MG   | BA    | 3098 | 1/1   | 0.99 | 0.22 | 36,36,36,36                 | 0     |
| 57  | MG   | DB    | 203  | 1/1   | 0.99 | 0.48 | 1,1,1,1                     | 1     |
| 57  | MG   | CA    | 1603 | 1/1   | 0.99 | 0.05 | 0,0,0,0                     | 0     |
| 57  | MG   | AA    | 7025 | 1/1   | 0.99 | 0.09 | 1,1,1,1                     | 0     |
| 57  | MG   | DA    | 9641 | 1/1   | 0.99 | 0.06 | 11,11,11,11                 | 0     |
| 57  | MG   | CV    | 102  | 1/1   | 0.99 | 0.09 | 1,1,1,1                     | 0     |
| 57  | MG   | AA    | 7024 | 1/1   | 0.99 | 0.19 | 27,27,27,27                 | 0     |
| 57  | MG   | BA    | 3157 | 1/1   | 0.99 | 0.06 | 6,6,6,6                     | 0     |
| 57  | MG   | AA    | 7103 | 1/1   | 0.99 | 0.17 | 13,13,13,13                 | 0     |
| 57  | MG   | DA    | 9560 | 1/1   | 0.99 | 0.11 | 4,4,4,4                     | 0     |
| 57  | MG   | DA    | 9532 | 1/1   | 1.00 | 0.19 | 9,9,9,9                     | 0     |
| 57  | MG   | AA    | 7007 | 1/1   | 1.00 | 0.06 | 1,1,1,1                     | 0     |

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

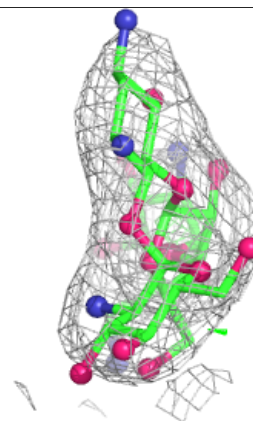
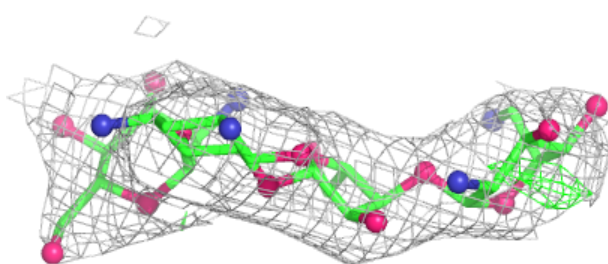
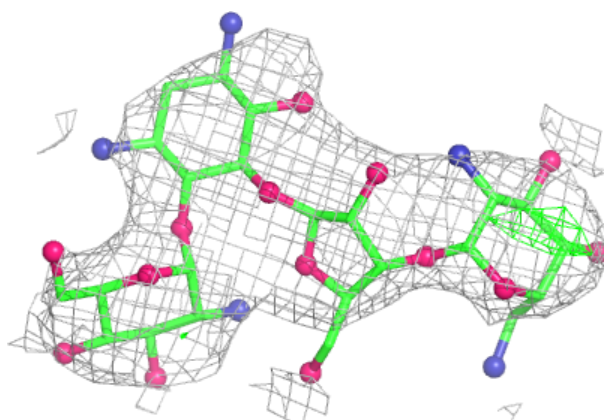
**Electron density around PAR CA 1741:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around PAR AA 7111:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.