



## Full wwPDB EM Validation Report ⓘ

Jun 18, 2026 – 02:02 am BST

PDB ID : 8PKL / pdb\_00008pkl  
EMDB ID : EMD-17743  
Title : Escherichia coli paused disome complex (leading 70S non-rotated closed PRE state)  
Authors : Fluegel, T.; Schacherl, M.  
Deposited on : 2023-06-26  
Resolution : 3.09 Å(reported)  
Based on initial model : 7N1P

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

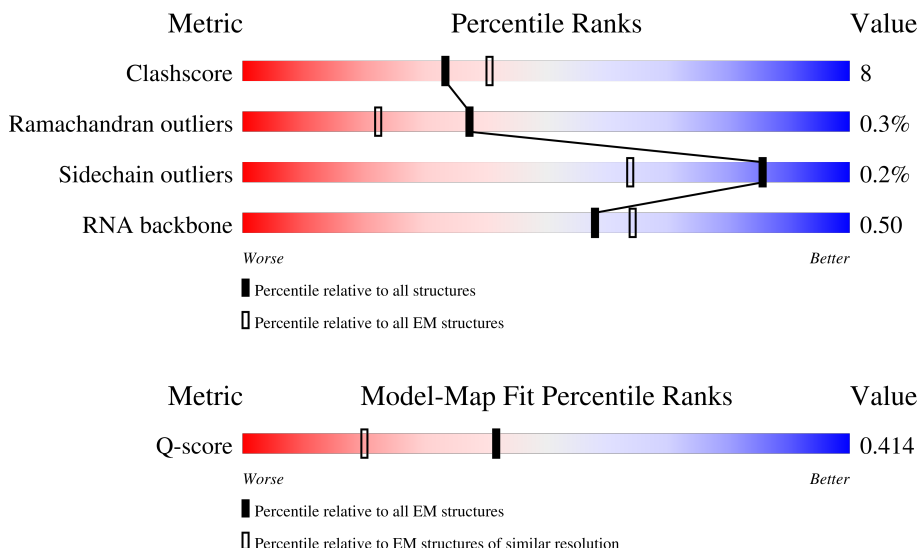
EMDB validation analysis : 0.0.1.dev132  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

# 1 Overall quality at a glance

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

The reported resolution of this entry is 3.09 Å.

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



| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| RNA backbone          | 8273                        | 3508                        | -                                                        |
| Q-score               | -                           | 25397                       | 14003 ( 2.59 - 3.59 )                                    |

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

| Mol | Chain | Length | Quality of chain                                                      |
|-----|-------|--------|-----------------------------------------------------------------------|
| 1   | 0     | 38     | <div> <div>5%</div> <div>63%</div> <div>37%</div> </div>              |
| 2   | 1     | 78     | <div> <div>8%</div> <div>82%</div> <div>17%</div> <div>.</div> </div> |
| 3   | 2     | 63     | <div> <div>19%</div> <div>87%</div> <div>13%</div> </div>             |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 4   | 3     | 59     |                  |
| 5   | 4     | 70     |                  |
| 6   | 5     | 57     |                  |
| 7   | 6     | 65     |                  |
| 8   | 7     | 2921   |                  |
| 9   | 8     | 120    |                  |
| 10  | A     | 1535   |                  |
| 11  | B     | 241    |                  |
| 12  | C     | 233    |                  |
| 13  | D     | 206    |                  |
| 14  | E     | 167    |                  |
| 15  | F     | 135    |                  |
| 16  | G     | 179    |                  |
| 17  | H     | 130    |                  |
| 18  | I     | 130    |                  |
| 19  | J     | 103    |                  |
| 20  | K     | 129    |                  |
| 21  | L     | 124    |                  |
| 22  | M     | 118    |                  |
| 23  | N     | 101    |                  |
| 24  | O     | 89     |                  |
| 25  | P     | 82     |                  |
| 26  | Q     | 84     |                  |
| 27  | R     | 75     |                  |
| 28  | S     | 92     |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 29  | T     | 87     |                  |
| 30  | U     | 71     |                  |
| 31  | V     | 24     |                  |
| 32  | W     | 76     |                  |
| 33  | X     | 77     |                  |
| 34  | Y     | 76     |                  |
| 35  | a     | 234    |                  |
| 36  | b     | 273    |                  |
| 37  | c     | 209    |                  |
| 38  | d     | 201    |                  |
| 39  | e     | 179    |                  |
| 40  | f     | 177    |                  |
| 41  | g     | 55     |                  |
| 42  | h     | 136    |                  |
| 43  | i     | 149    |                  |
| 44  | j     | 165    |                  |
| 45  | k     | 142    |                  |
| 46  | l     | 46     |                  |
| 47  | m     | 142    |                  |
| 48  | n     | 123    |                  |
| 49  | o     | 144    |                  |
| 50  | p     | 36     |                  |
| 51  | q     | 127    |                  |
| 52  | r     | 117    |                  |
| 53  | s     | 115    |                  |

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| Mol | Chain | Length | Quality of chain  |
|-----|-------|--------|-------------------|
| 54  | t     | 118    | <br>19% 80% 19%   |
| 55  | u     | 103    | <br>19% 85% 15%   |
| 56  | v     | 110    | <br>7% 76% 24%    |
| 57  | w     | 100    | <br>6% 78% 15% 7% |
| 58  | x     | 104    | <br>14% 89% 9%    |
| 59  | y     | 94     | <br>17% 82% 18%   |
| 60  | z     | 85     | <br>7% 79% 20%    |

## 2 Entry composition

There are 66 unique types of molecules in this entry. The entry contains 151734 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 50S ribosomal protein L36.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 1   | 0     | 38       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 302   | 185 | 65 | 48 | 4 |         |       |

- Molecule 2 is a protein called 50S ribosomal protein L28.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 2   | 1     | 77       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 625   | 388 | 129 | 106 | 2 |         |       |

- Molecule 3 is a protein called 50S ribosomal protein L29.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 3   | 2     | 63       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 509   | 313 | 99 | 95 | 2 |         |       |

- Molecule 4 is a protein called 50S ribosomal protein L30.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 4   | 3     | 58       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 449   | 281 | 87 | 79 | 2 |         |       |

- Molecule 5 is a protein called Large ribosomal subunit protein bL31A.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 5   | 4     | 68       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 533   | 330 | 101 | 96 | 6 |         |       |

- Molecule 6 is a protein called 50S ribosomal protein L32.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 6   | 5     | 56       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 444   | 269 | 94 | 80 | 1 |         |       |

- Molecule 7 is a protein called 50S ribosomal protein L35.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 7   | 6     | 64       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 504   | 323 | 105 | 74 | 2 |         |       |

- Molecule 8 is a RNA chain called 23S ribosomal RNA.

| Mol | Chain | Residues | Atoms |       |       |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|-------|
| 8   | 7     | 2904     | Total | C     | N     | O     | P    | 0       | 0     |
|     |       |          | 62355 | 27824 | 11468 | 20159 | 2904 |         |       |

- Molecule 9 is a RNA chain called 5S ribosomal RNA.

| Mol | Chain | Residues | Atoms |      |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|-------|
| 9   | 8     | 120      | Total | C    | N   | O   | P   | 0       | 0     |
|     |       |          | 2572  | 1145 | 471 | 836 | 120 |         |       |

- Molecule 10 is a RNA chain called 16S ribosomal RNA.

| Mol | Chain | Residues | Atoms |       |      |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|-------|
| 10  | A     | 1535     | Total | C     | N    | O     | P    | 0       | 0     |
|     |       |          | 32950 | 14703 | 6044 | 10668 | 1535 |         |       |

- Molecule 11 is a protein called Small ribosomal subunit protein uS2.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 11  | B     | 227      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1776  | 1123 | 318 | 327 | 8 |         |       |

- Molecule 12 is a protein called Small ribosomal subunit protein uS3.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 12  | C     | 212      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1658  | 1049 | 311 | 294 | 4 |         |       |

- Molecule 13 is a protein called Small ribosomal subunit protein uS4.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 13  | D     | 205      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1643  | 1026 | 315 | 298 | 4 |         |       |

- Molecule 14 is a protein called Small ribosomal subunit protein uS5.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 14  | E     | 158      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1166  | 725 | 220 | 215 | 6 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 15  | F     | 106      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 862   | 545 | 156 | 154 | 7 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 16  | G     | 153      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1203  | 750 | 231 | 218 | 4 |         |       |

- Molecule 17 is a protein called Small ribosomal subunit protein uS8.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 17  | H     | 129      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 979   | 616 | 173 | 184 | 6 |         |       |

- Molecule 18 is a protein called Small ribosomal subunit protein uS9.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 18  | I     | 127      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1022  | 634 | 206 | 179 | 3 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 19  | J     | 100      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 803   | 502 | 154 | 146 | 1 |         |       |

- Molecule 20 is a protein called Small ribosomal subunit protein uS11.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 20  | K     | 118      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 884   | 545 | 175 | 161 | 3 |         |       |

- Molecule 21 is a protein called Small ribosomal subunit protein uS12.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 21  | L     | 123      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 955   | 590 | 196 | 165 | 4 |         |       |

- Molecule 22 is a protein called Small ribosomal subunit protein uS13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 22  | M     | 117      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 910   | 564 | 183 | 160 | 3 |         |       |

- Molecule 23 is a protein called Small ribosomal subunit protein uS14.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 23  | N     | 100      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 805   | 499 | 164 | 139 | 3 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 24  | O     | 88       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 714   | 439 | 144 | 130 | 1 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 25  | P     | 82       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 649   | 406 | 128 | 114 | 1 |         |       |

- Molecule 26 is a protein called Small ribosomal subunit protein uS17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 26  | Q     | 80       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 648   | 411 | 121 | 113 | 3 |         |       |

- Molecule 27 is a protein called Small ribosomal subunit protein bS18.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 27  | R     | 66       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 544   | 345 | 102 | 96 | 1 |         |       |

- Molecule 28 is a protein called Small ribosomal subunit protein uS19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 28  | S     | 83       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 663   | 424 | 126 | 111 | 2 |         |       |

- Molecule 29 is a protein called Small ribosomal subunit protein bS20.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 29  | T     | 86       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 670   | 414 | 138 | 115 | 3 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 30  | U     | 70       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 584   | 363 | 122 | 98 | 1 |         |       |

- Molecule 31 is a RNA chain called mRNA.

| Mol | Chain | Residues | Atoms |     |    |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|----|---------|-------|
| 31  | V     | 24       | Total | C   | N  | O   | P  | 0       | 0     |
|     |       |          | 516   | 231 | 99 | 162 | 24 |         |       |

- Molecule 32 is a RNA chain called tRNA-Trp (P-site).

| Mol | Chain | Residues | Atoms |     |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---|---------|-------|
| 32  | W     | 76       | Total | C   | N   | O   | P  | S | 0       | 0     |
|     |       |          | 1630  | 730 | 286 | 536 | 76 | 2 |         |       |

- Molecule 33 is a RNA chain called tRNA-Arg (E-site).

| Mol | Chain | Residues | Atoms |     |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---|---------|-------|
| 33  | X     | 77       | Total | C   | N   | O   | P  | S | 0       | 0     |
|     |       |          | 1654  | 740 | 297 | 538 | 77 | 2 |         |       |

- Molecule 34 is a RNA chain called tRNA-Ala (A-site).

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 34  | Y     | 76       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 1628  | 726 | 293 | 533 | 76 |         |       |

- Molecule 35 is a protein called Large ribosomal subunit protein uL1.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 35  | a     | 134      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1026  | 645 | 186 | 193 | 2 |         |       |

- Molecule 36 is a protein called 50S ribosomal protein L2.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 36  | b     | 271      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2082  | 1288 | 423 | 364 | 7 |         |       |

- Molecule 37 is a protein called 50S ribosomal protein L3.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 37  | c     | 209      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1565  | 979 | 288 | 294 | 4 |         |       |

- Molecule 38 is a protein called 50S ribosomal protein L4.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 38  | d     | 201      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1552  | 974 | 283 | 290 | 5 |         |       |

- Molecule 39 is a protein called 50S ribosomal protein L5.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 39  | e     | 178      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1420  | 905 | 251 | 258 | 6 |         |       |

- Molecule 40 is a protein called 50S ribosomal protein L6.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 40  | f     | 176      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1323  | 832 | 243 | 246 | 2 |         |       |

- Molecule 41 is a protein called 50S ribosomal protein L33.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 41  | g     | 52       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 427   | 275 | 78 | 74 |         |       |

- Molecule 42 is a protein called 50S ribosomal protein L16.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 42  | h     | 136      | Total | C   | N   | O   | S | 1       | 0     |
|     |       |          | 1085  | 692 | 209 | 178 | 6 |         |       |

- Molecule 43 is a protein called 50S ribosomal protein L9.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 43  | i     | 149      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1111  | 699 | 197 | 214 | 1 |         |       |

- Molecule 44 is a protein called Large ribosomal subunit protein uL10.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 44  | j     | 135      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1023  | 648 | 179 | 192 | 4 |         |       |

- Molecule 45 is a protein called 50S ribosomal protein L11.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 45  | k     | 134      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 979   | 619 | 169 | 185 | 6 |         |       |

- Molecule 46 is a protein called 50S ribosomal protein L34.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 46  | l     | 46       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 377   | 228 | 90 | 57 | 2 |         |       |

- Molecule 47 is a protein called 50S ribosomal protein L13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 47  | m     | 142      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1129  | 714 | 212 | 199 | 4 |         |       |

- Molecule 48 is a protein called 50S ribosomal protein L14.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 48  | n     | 123      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 946   | 593 | 181 | 166 | 6 |         |       |

- Molecule 49 is a protein called 50S ribosomal protein L15.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 49  | o     | 144      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1053  | 654 | 207 | 190 | 2 |         |       |

- Molecule 50 is a protein called Nascent peptide.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 50  | p     | 36       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 206   | 125 | 44 | 37 |         |       |

- Molecule 51 is a protein called 50S ribosomal protein L17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 51  | q     | 120      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 960   | 593 | 196 | 166 | 5 |         |       |

- Molecule 52 is a protein called 50S ribosomal protein L18.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 52  | r     | 116      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 891   | 552 | 178 | 161 |         |       |

- Molecule 53 is a protein called 50S ribosomal protein L19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 53  | s     | 114      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 917   | 574 | 179 | 163 | 1 |         |       |

- Molecule 54 is a protein called 50S ribosomal protein L20.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 54  | t     | 117      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 947   | 604 | 192 | 151 |         |       |

- Molecule 55 is a protein called 50S ribosomal protein L21.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 55  | u     | 103      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 816   | 516 | 153 | 145 | 2 |         |       |

- Molecule 56 is a protein called 50S ribosomal protein L22.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 56  | v     | 110      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 857   | 532 | 166 | 156 | 3 |         |       |

- Molecule 57 is a protein called 50S ribosomal protein L23.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 57  | w     | 93       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 738   | 466 | 139 | 131 | 2 |         |       |

- Molecule 58 is a protein called 50S ribosomal protein L24.

| Mol | Chain | Residues | Atoms |     |     |     |  | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|-------|
| 58  | x     | 102      | Total | C   | N   | O   |  | 0       | 0     |
|     |       |          | 779   | 492 | 146 | 141 |  |         |       |

- Molecule 59 is a protein called 50S ribosomal protein L25.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 59  | y     | 94       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 753   | 479 | 137 | 134 | 3 |         |       |

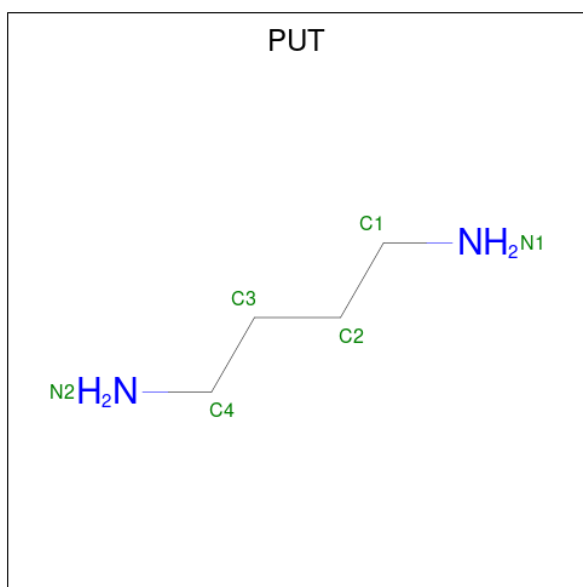
- Molecule 60 is a protein called 50S ribosomal protein L27.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 60  | z     | 84       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 634   | 391 | 129 | 113 | 1 |         |       |

- Molecule 61 is ZINC ION (CCD ID: ZN) (formula: Zn).

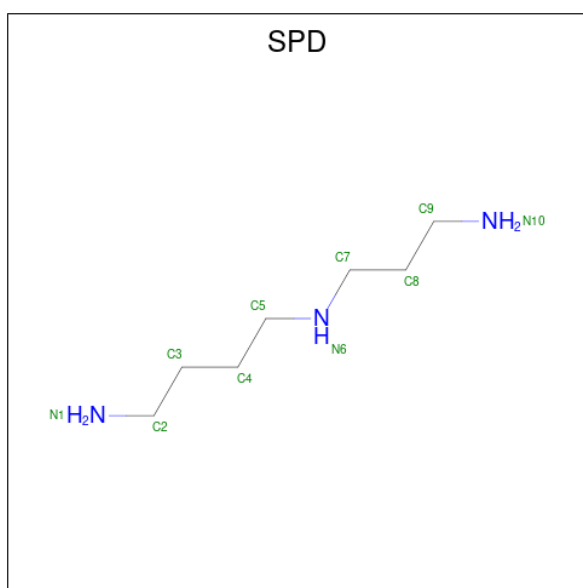
| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 61  | 0     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 61  | 4     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 62 is 1,4-DIAMINOBTUTANE (CCD ID: PUT) (formula: C<sub>4</sub>H<sub>12</sub>N<sub>2</sub>).



| Mol | Chain | Residues | Atoms |   |   | AltConf |
|-----|-------|----------|-------|---|---|---------|
| 62  | 7     | 1        | Total | C | N | 0       |
|     |       |          | 6     | 4 | 2 |         |
| 62  | 7     | 1        | Total | C | N | 0       |
|     |       |          | 6     | 4 | 2 |         |

- Molecule 63 is SPERMIDINE (CCD ID: SPD) (formula: C<sub>7</sub>H<sub>19</sub>N<sub>3</sub>).

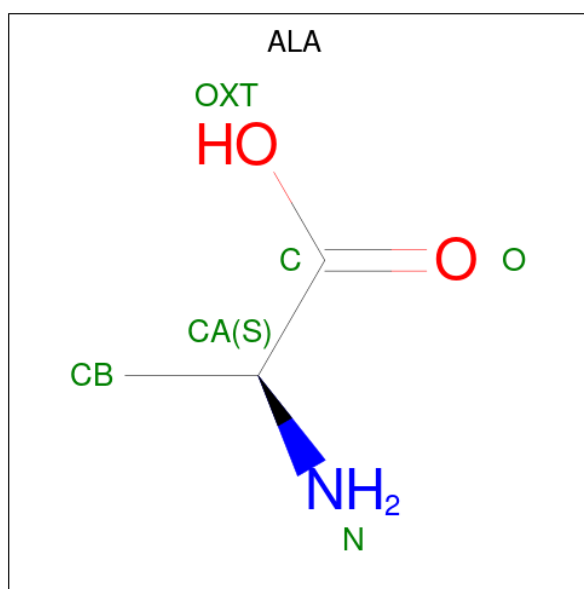


| Mol | Chain | Residues | Atoms |   |   | AltConf |
|-----|-------|----------|-------|---|---|---------|
| 63  | 7     | 1        | Total | C | N | 0       |
|     |       |          | 10    | 7 | 3 |         |

- Molecule 64 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |     | AltConf |
|-----|-------|----------|-------|-----|---------|
| 64  | 7     | 257      | Total | Mg  | 0       |
|     |       |          | 257   | 257 |         |
| 64  | A     | 23       | Total | Mg  | 0       |
|     |       |          | 23    | 23  |         |
| 64  | I     | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |
| 64  | V     | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |
| 64  | X     | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |
| 64  | Y     | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |
| 64  | b     | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |
| 64  | q     | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |
| 64  | r     | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |

- Molecule 65 is ALANINE (CCD ID: ALA) (formula:  $C_3H_7NO_2$ ).



| Mol | Chain | Residues | Atoms |   |   |   | AltConf |
|-----|-------|----------|-------|---|---|---|---------|
| 65  | Y     | 1        | Total | C | N | O | 0       |
|     |       |          | 5     | 3 | 1 | 1 |         |

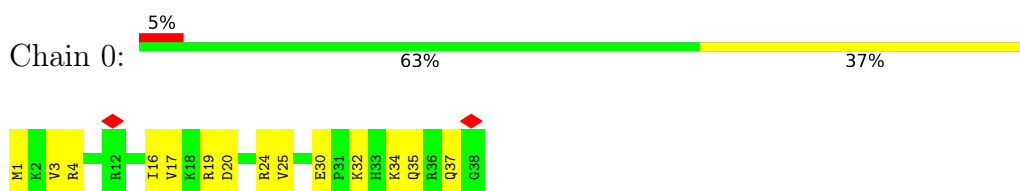
- Molecule 66 is water.

| Mol | Chain | Residues | Atoms       |         | AltConf |
|-----|-------|----------|-------------|---------|---------|
| 66  | 7     | 12       | Total<br>12 | O<br>12 | 0       |
| 66  | x     | 1        | Total<br>1  | O<br>1  | 0       |

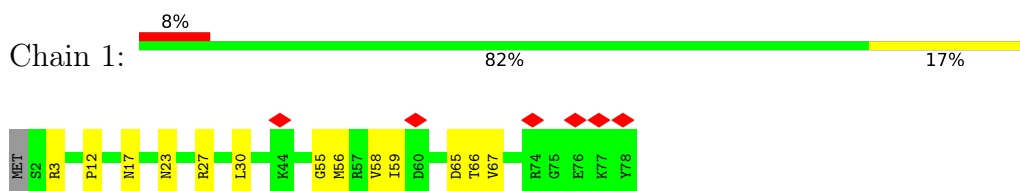
### 3 Residue-property plots [i](#)

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

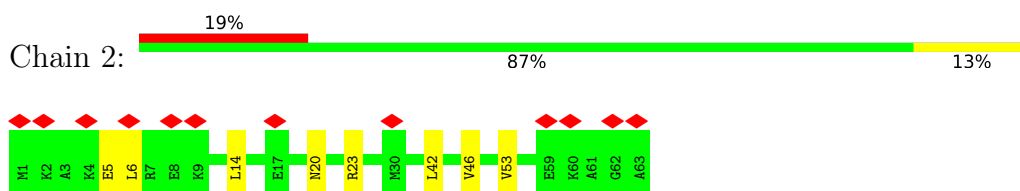
- Molecule 1: 50S ribosomal protein L36



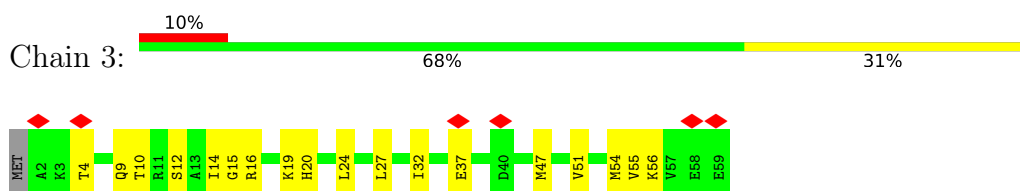
- Molecule 2: 50S ribosomal protein L28



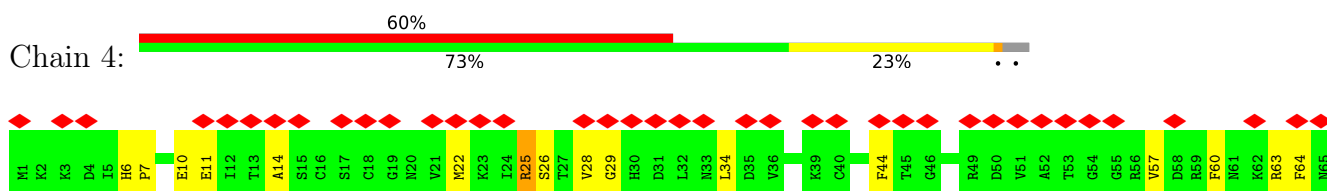
- Molecule 3: 50S ribosomal protein L29



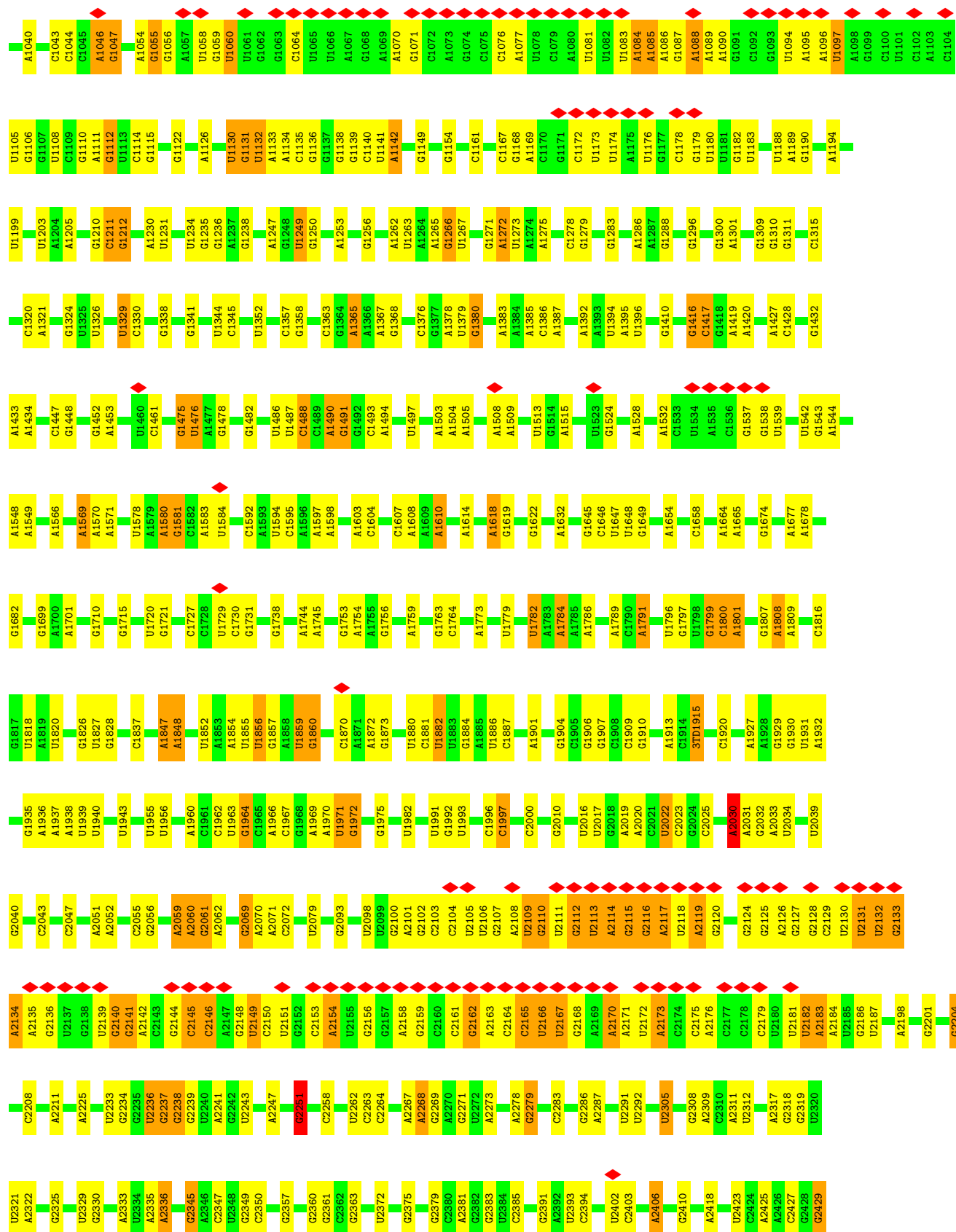
- Molecule 4: 50S ribosomal protein L30

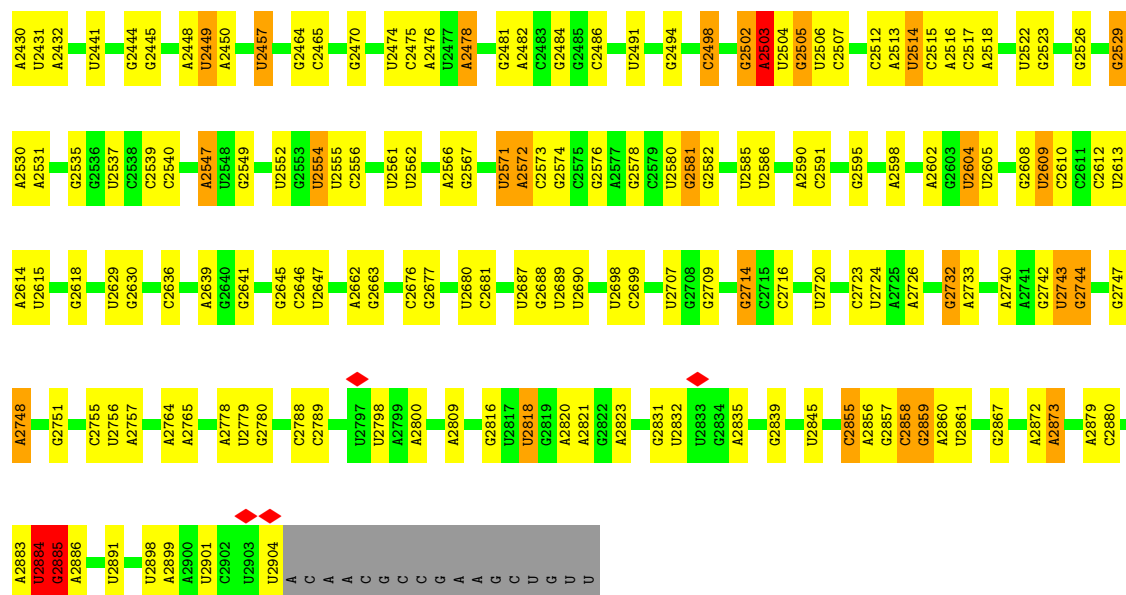


- Molecule 5: Large ribosomal subunit protein bL31A

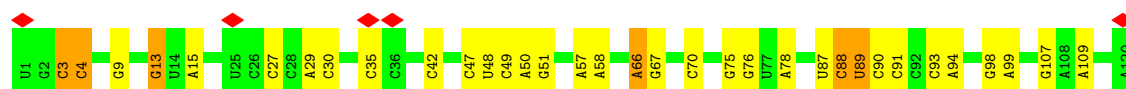




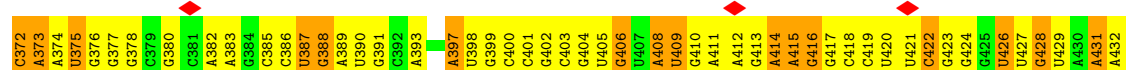
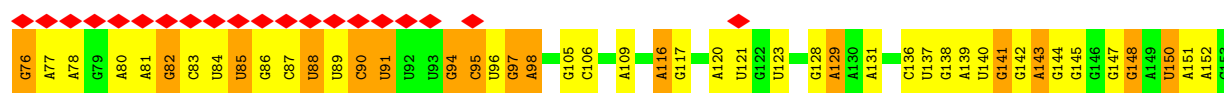
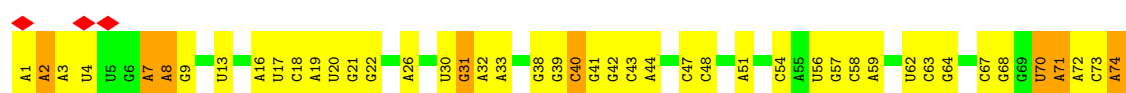


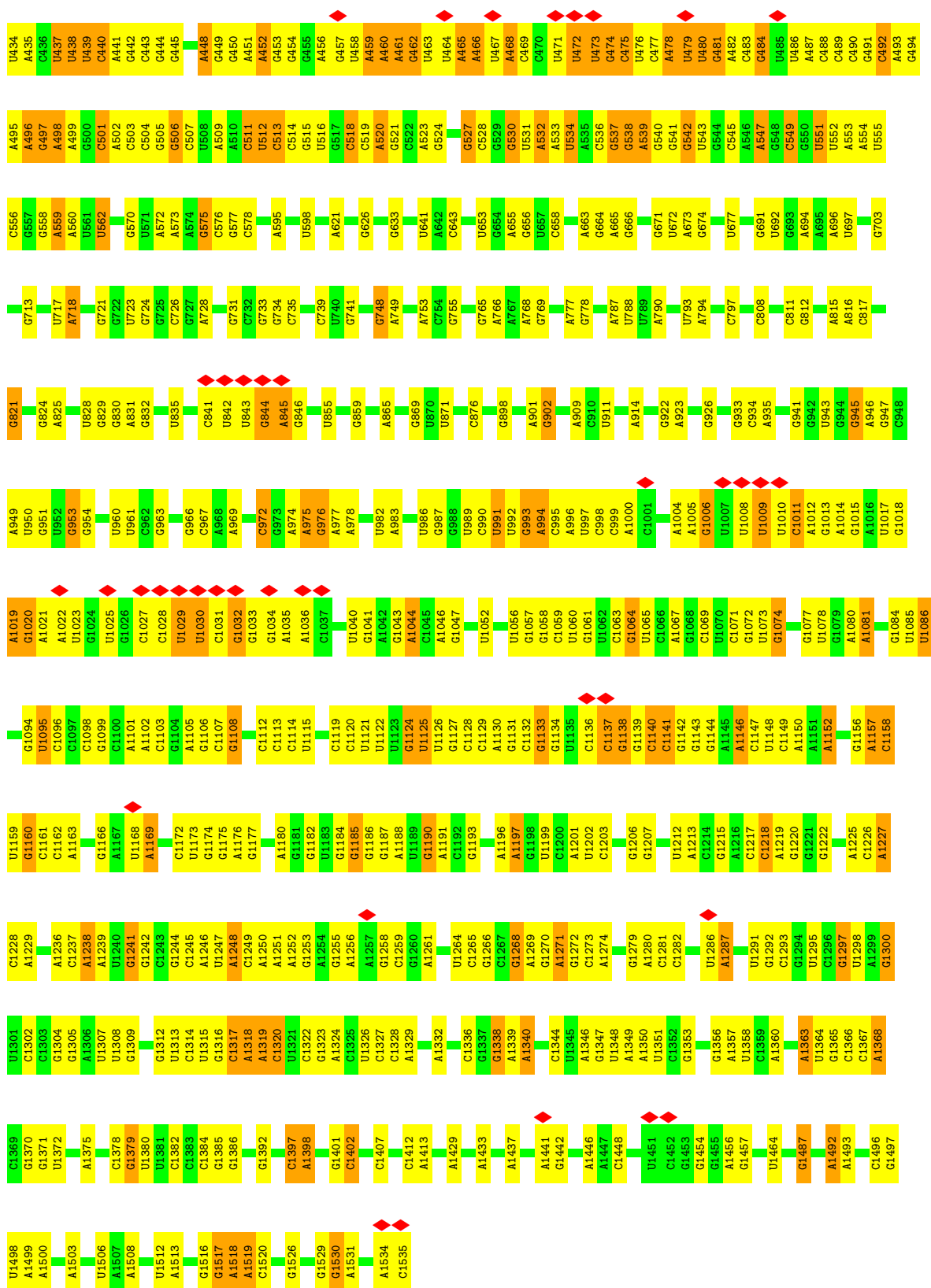


### • Molecule 9: 5S ribosomal RNA



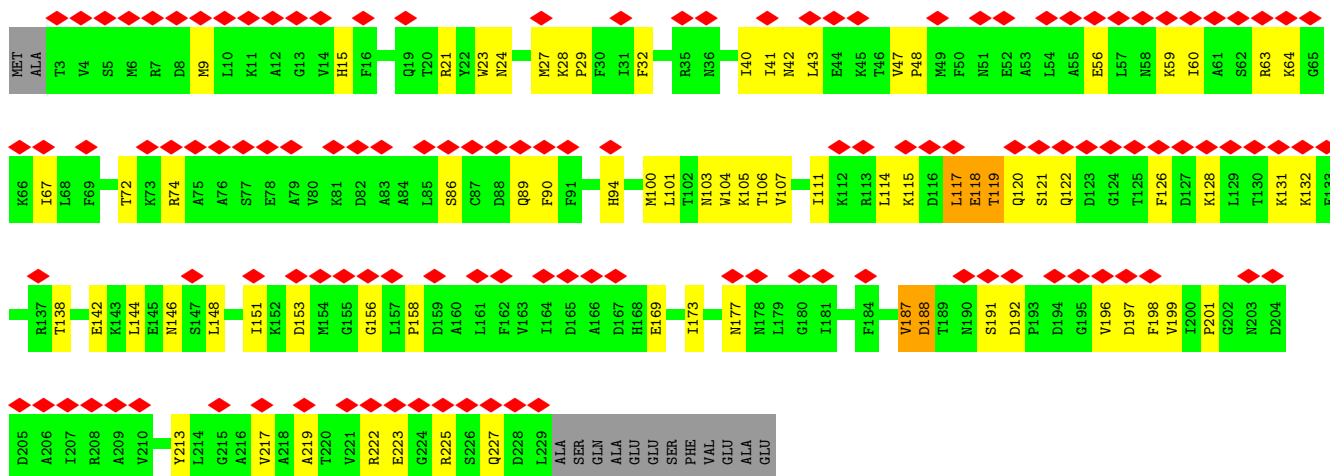
### • Molecule 10: 16S ribosomal RNA



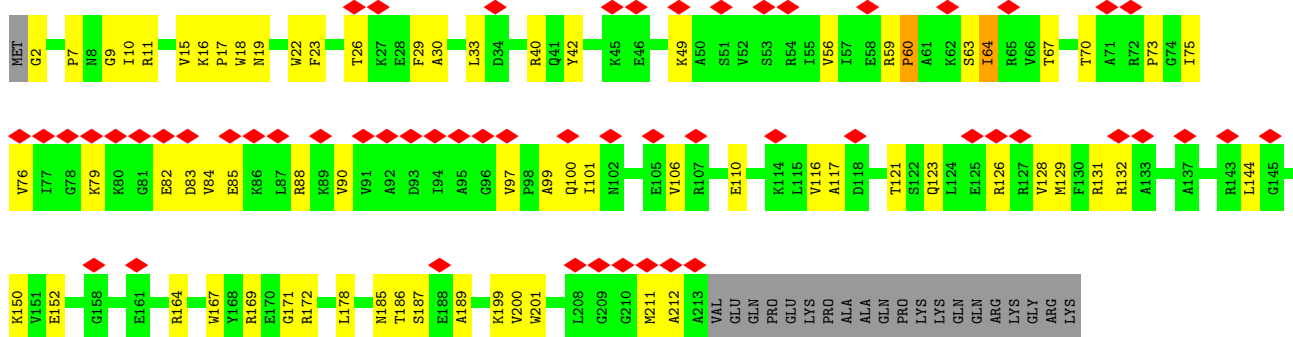


• Molecule 11: Small ribosomal subunit protein uS2

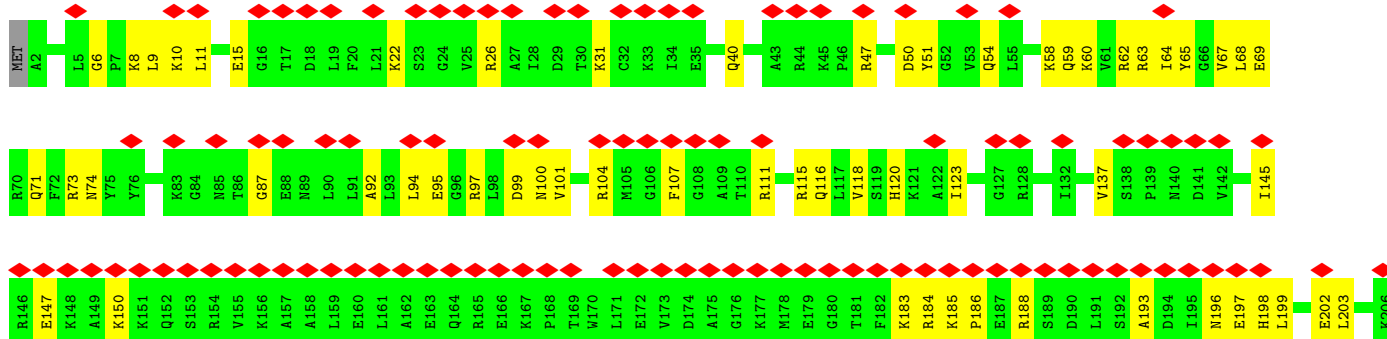




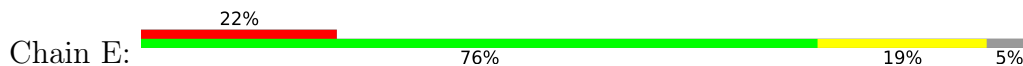
• Molecule 12: Small ribosomal subunit protein uS3

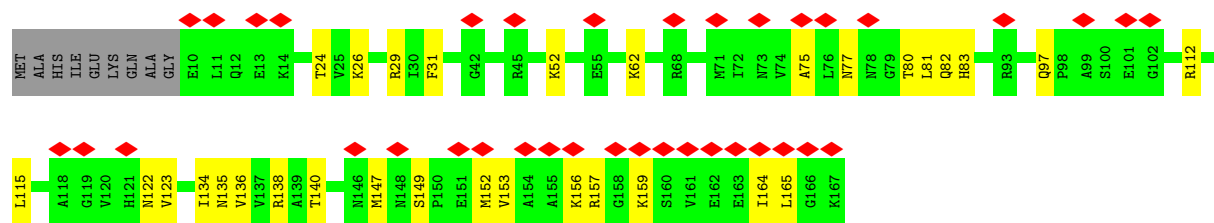


• Molecule 13: Small ribosomal subunit protein uS4

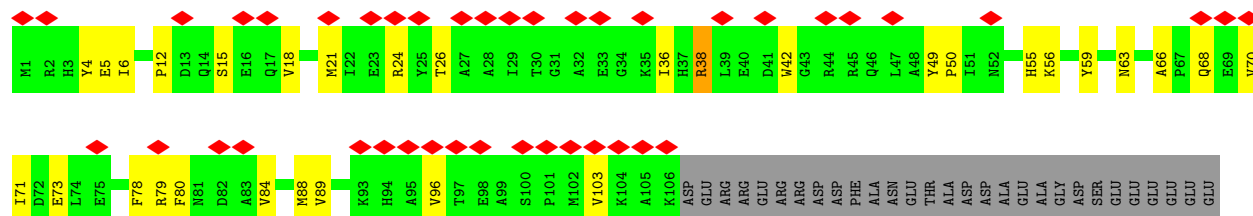


• Molecule 14: Small ribosomal subunit protein uS5

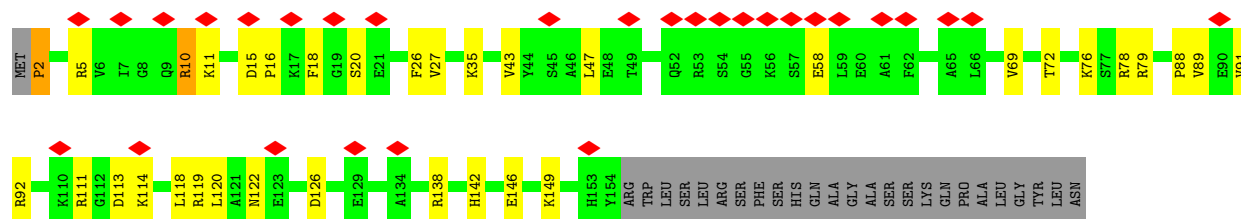




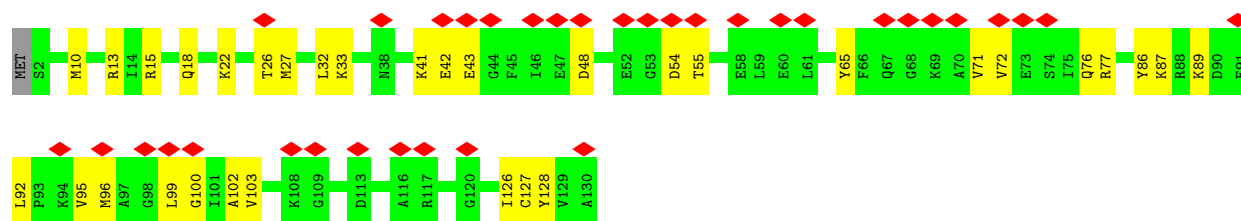
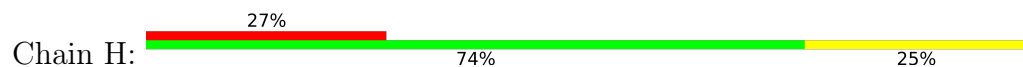
• Molecule 15: 30S ribosomal protein S6



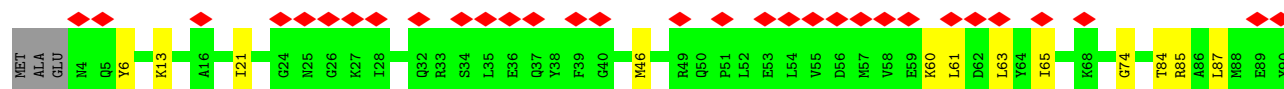
• Molecule 16: 30S ribosomal protein S7

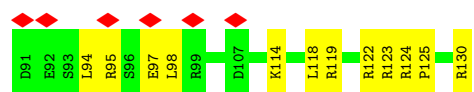


• Molecule 17: Small ribosomal subunit protein uS8

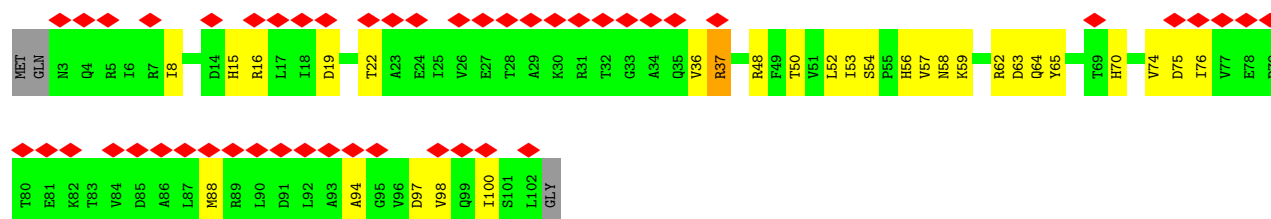


• Molecule 18: Small ribosomal subunit protein uS9

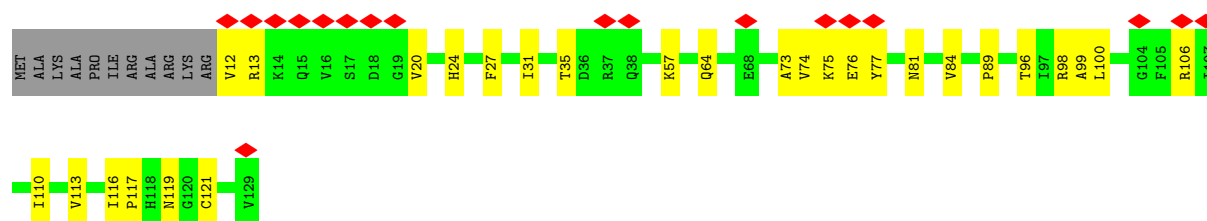




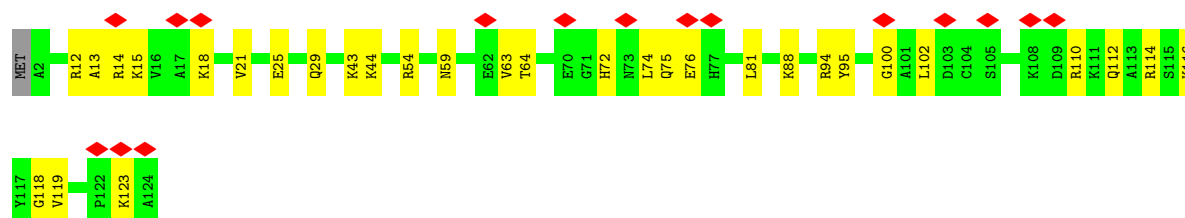
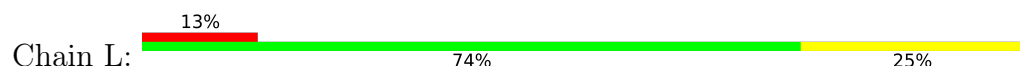
- Molecule 19: 30S ribosomal protein S10



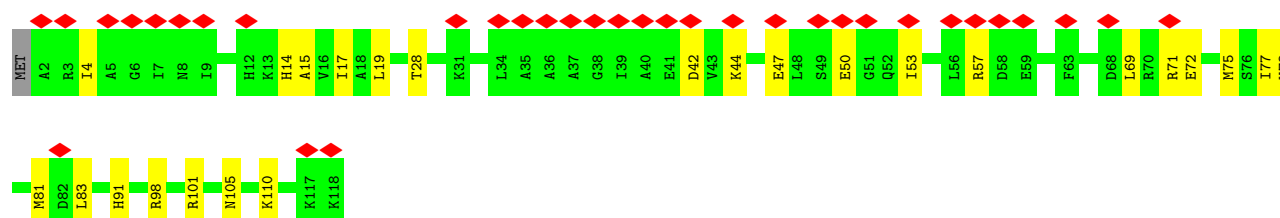
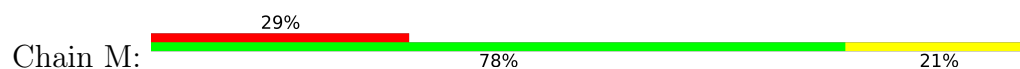
- Molecule 20: Small ribosomal subunit protein uS11



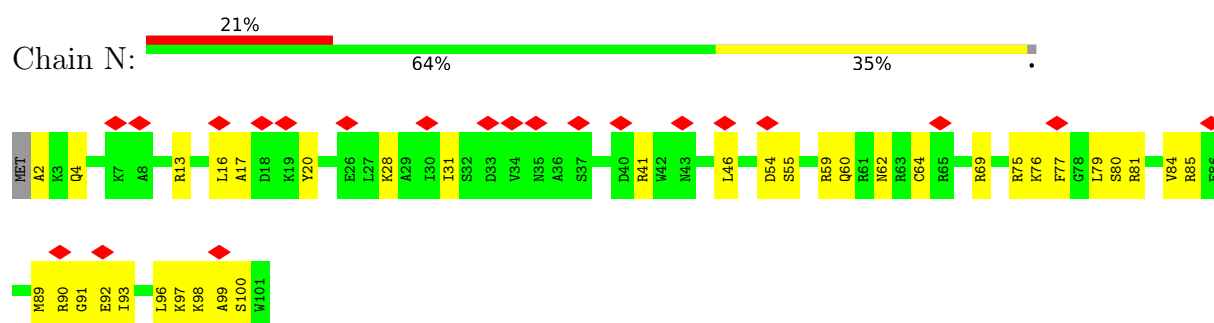
- Molecule 21: Small ribosomal subunit protein uS12



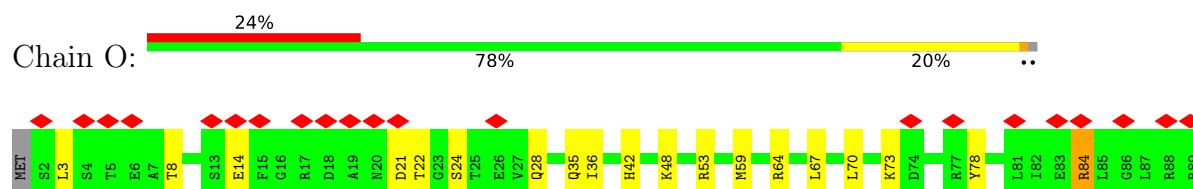
- Molecule 22: Small ribosomal subunit protein uS13



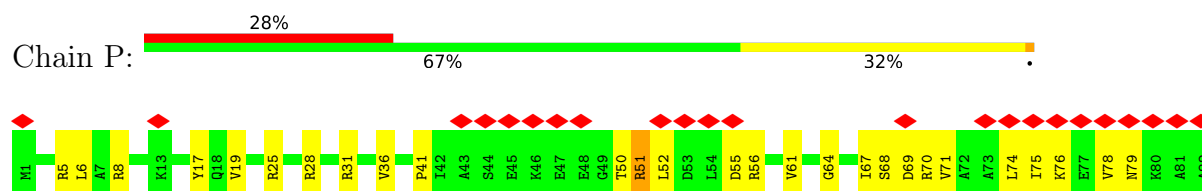
- Molecule 23: Small ribosomal subunit protein uS14



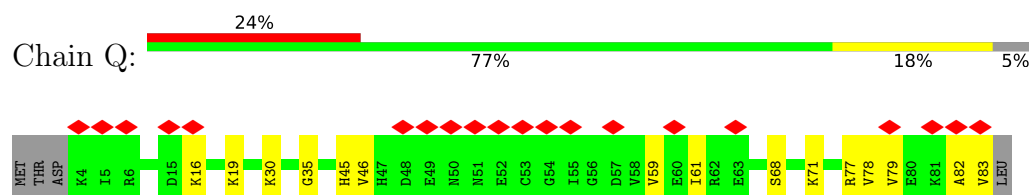
- Molecule 24: 30S ribosomal protein S15



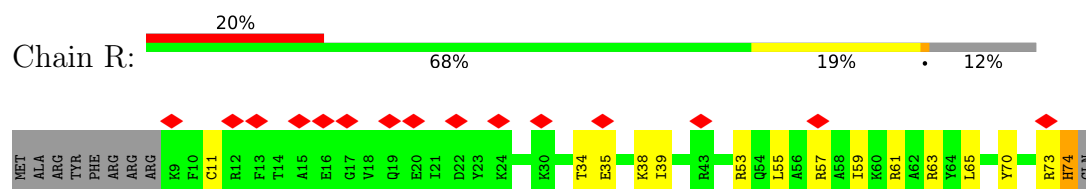
- Molecule 25: 30S ribosomal protein S16



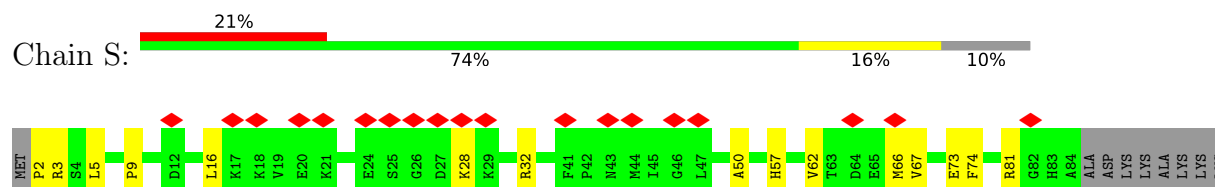
- Molecule 26: Small ribosomal subunit protein uS17



- Molecule 27: Small ribosomal subunit protein bS18

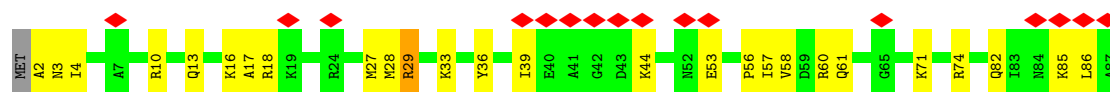


- Molecule 28: Small ribosomal subunit protein uS19

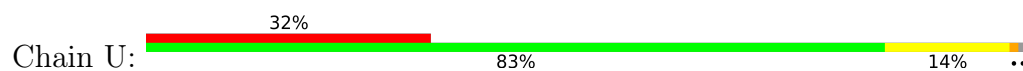


- Molecule 29: Small ribosomal subunit protein bS20

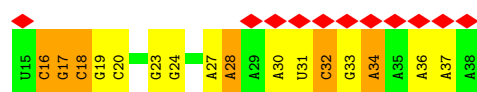




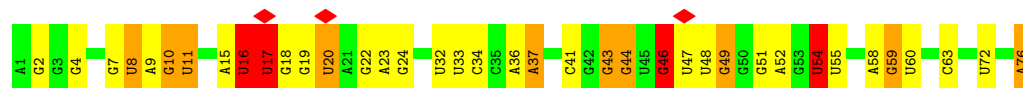
- Molecule 30: 30S ribosomal protein S21



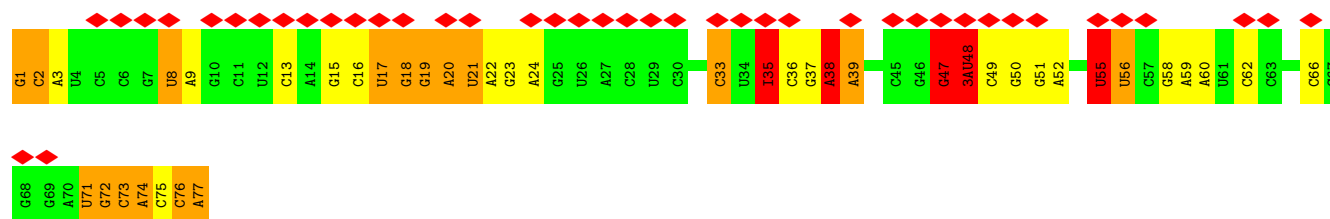
- Molecule 31: mRNA



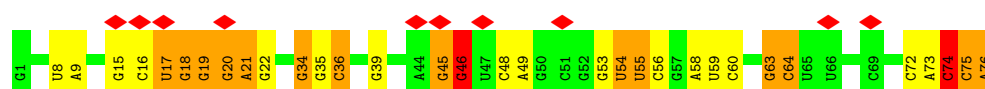
- Molecule 32: tRNA-Trp (P-site)



- Molecule 33: tRNA-Arg (E-site)

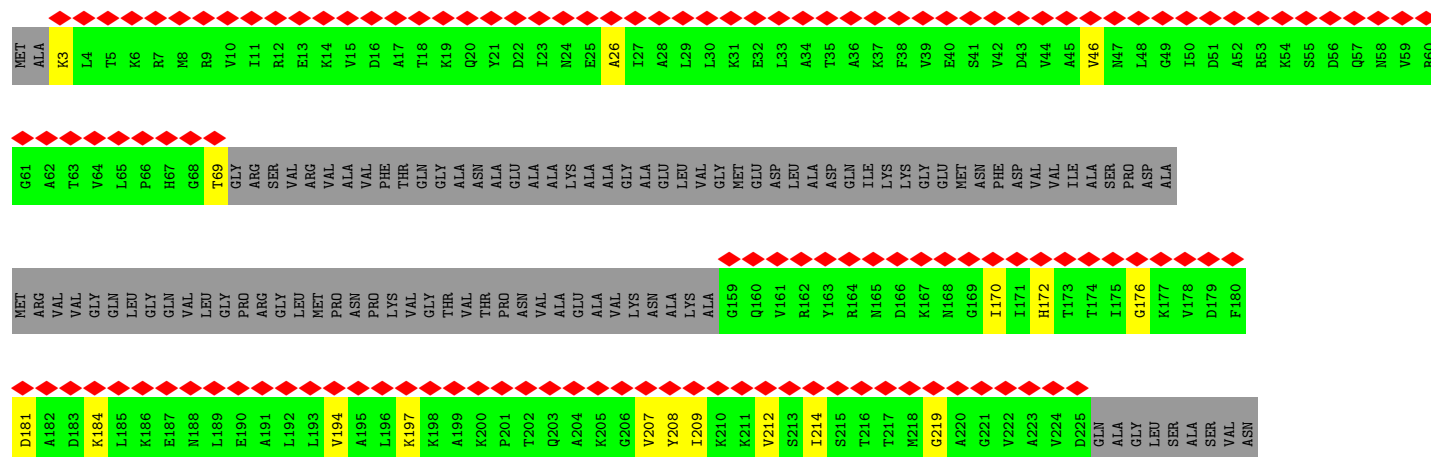


- Molecule 34: tRNA-Ala (A-site)



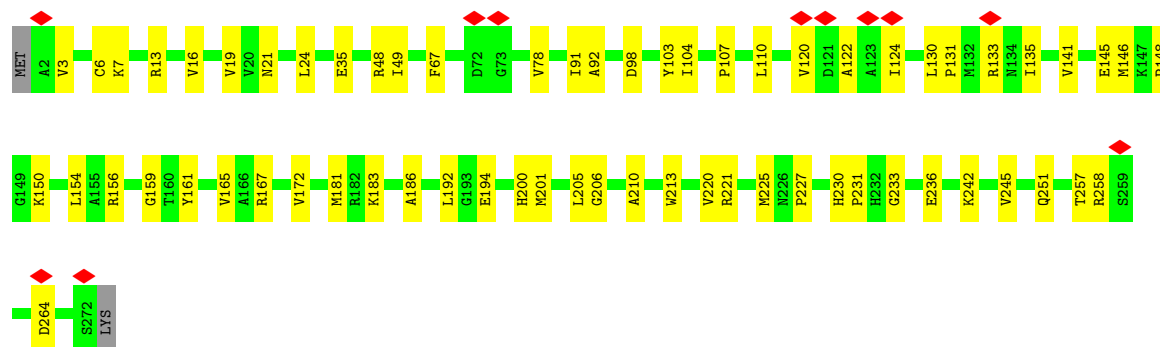
- Molecule 35: Large ribosomal subunit protein uL1





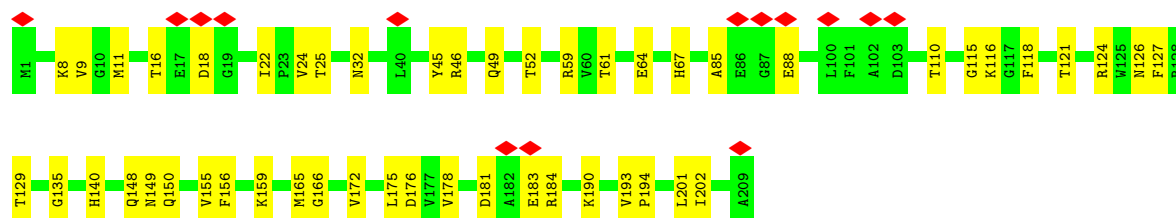
• Molecule 36: 50S ribosomal protein L2

Chain b: 76% 23%



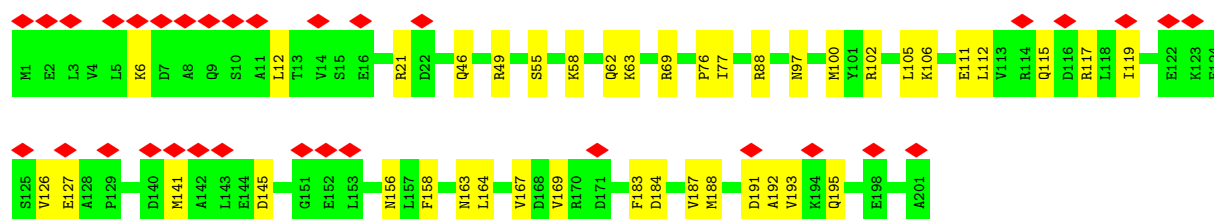
• Molecule 37: 50S ribosomal protein L3

Chain c: 7% 76% 24%

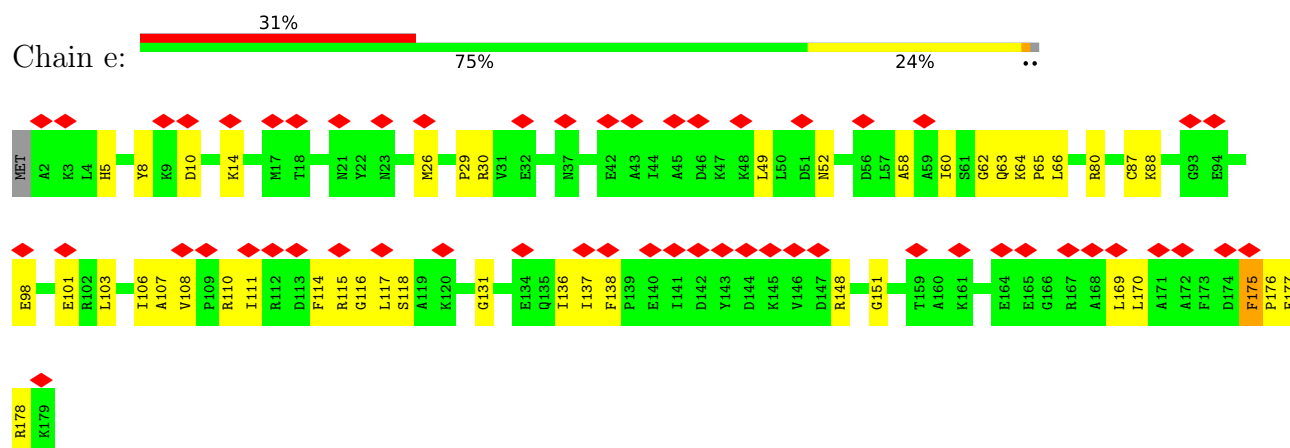


• Molecule 38: 50S ribosomal protein L4

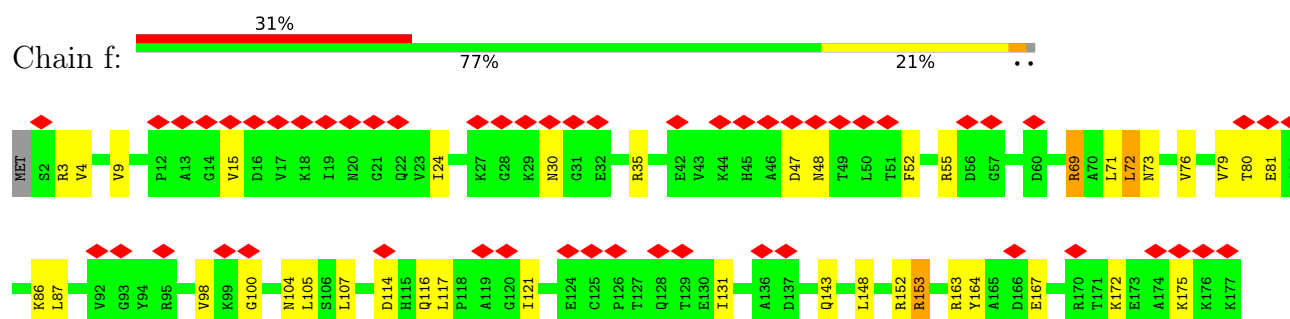
Chain d: 16% 80% 20%



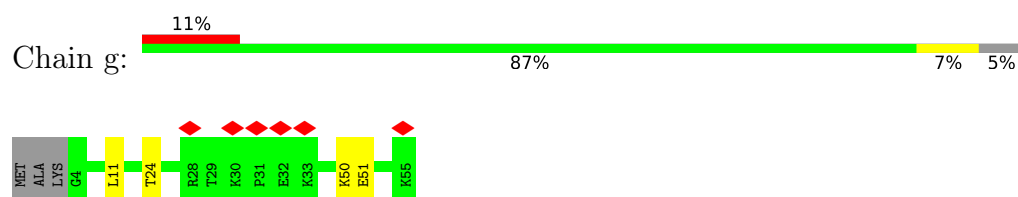
- Molecule 39: 50S ribosomal protein L5



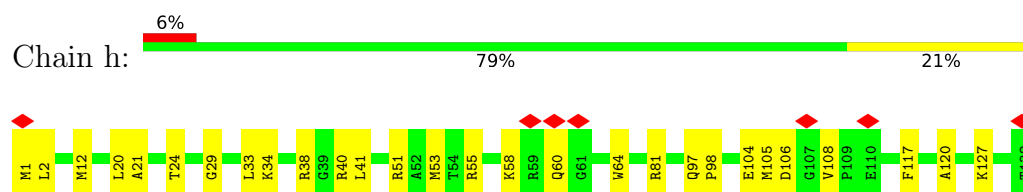
- Molecule 40: 50S ribosomal protein L6



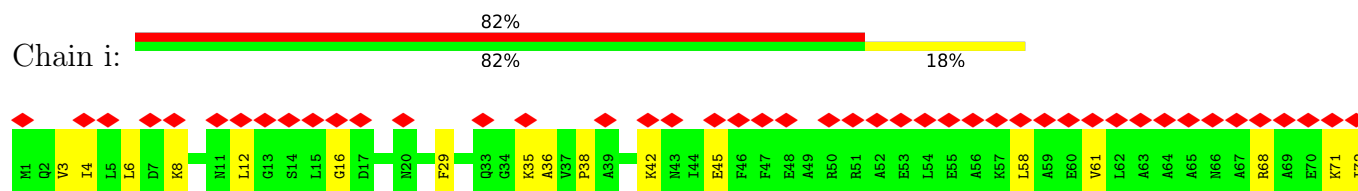
- Molecule 41: 50S ribosomal protein L33



- Molecule 42: 50S ribosomal protein L16

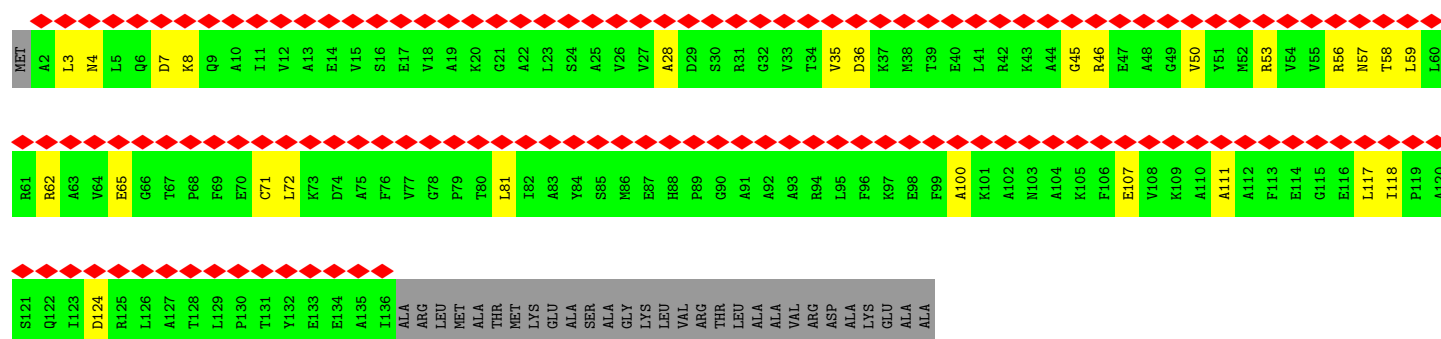
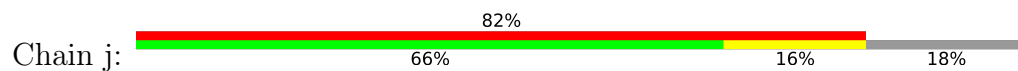


- Molecule 43: 50S ribosomal protein L9

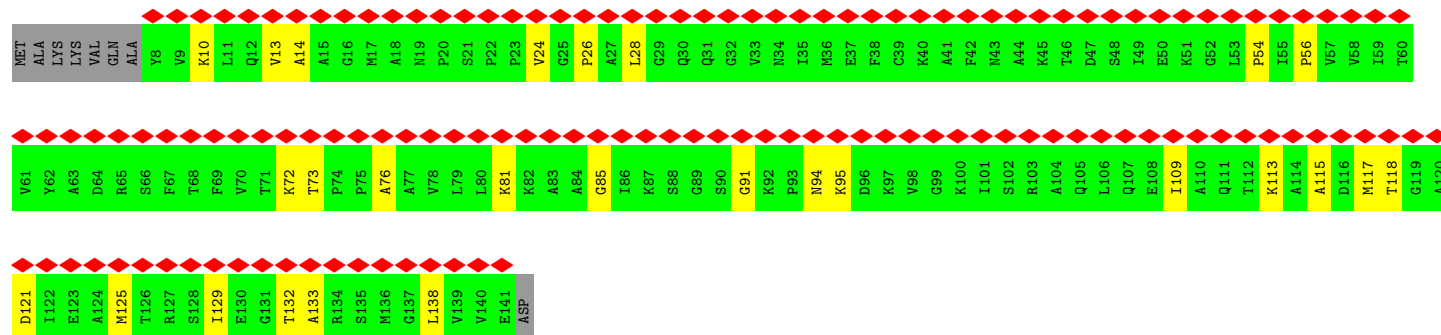
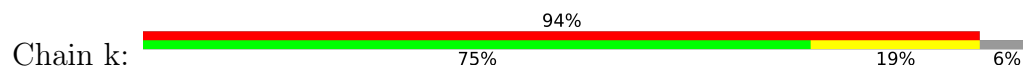




• Molecule 44: Large ribosomal subunit protein uL10



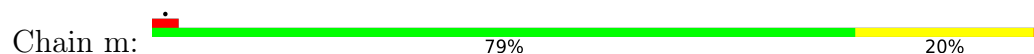
• Molecule 45: 50S ribosomal protein L11

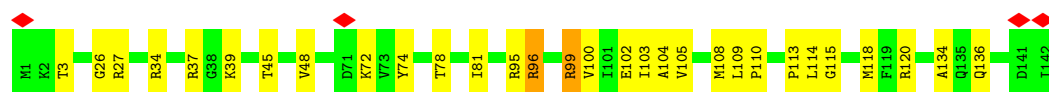


• Molecule 46: 50S ribosomal protein L34

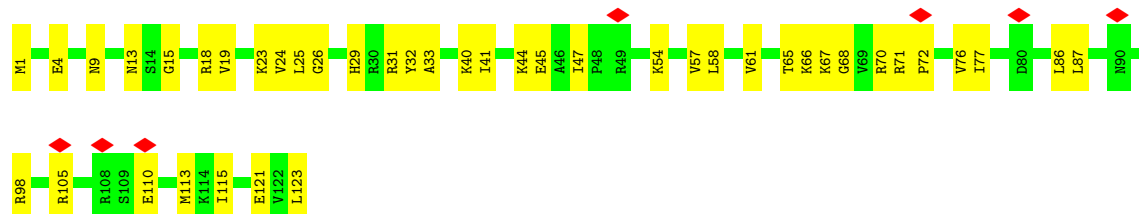


• Molecule 47: 50S ribosomal protein L13

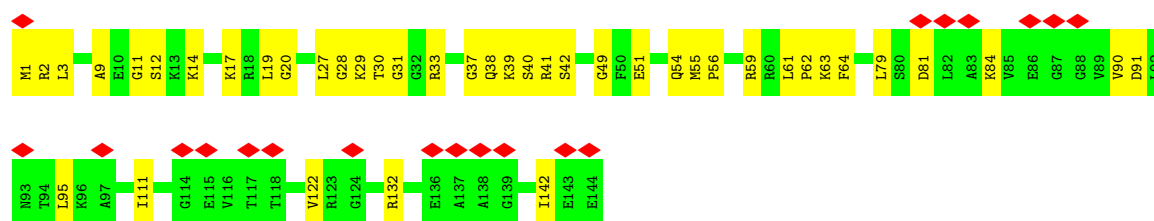




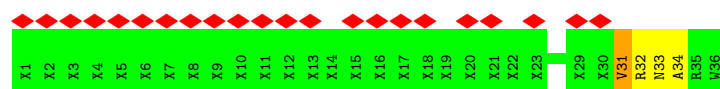
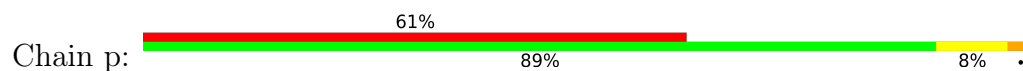
- Molecule 48: 50S ribosomal protein L14



- Molecule 49: 50S ribosomal protein L15



- Molecule 50: Nascent peptide

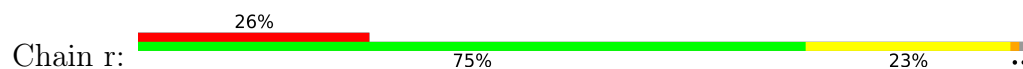


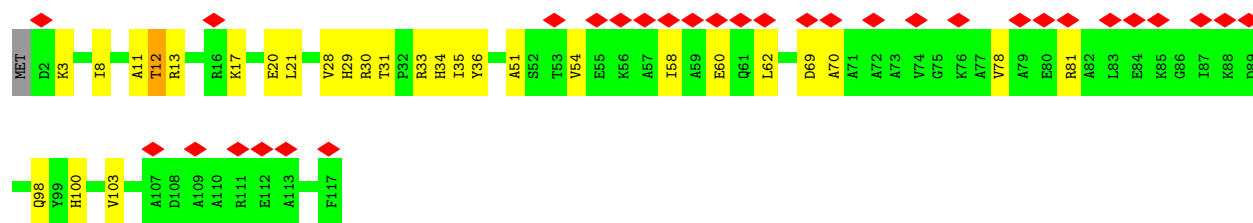
- Molecule 51: 50S ribosomal protein L17



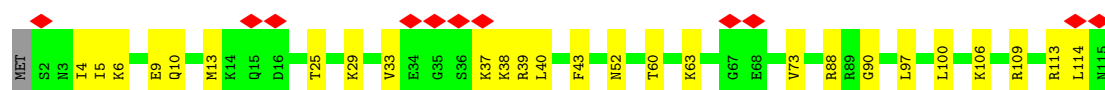
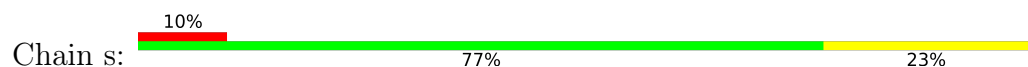
ALA  
ALA  
ALA  
GLU

- Molecule 52: 50S ribosomal protein L18

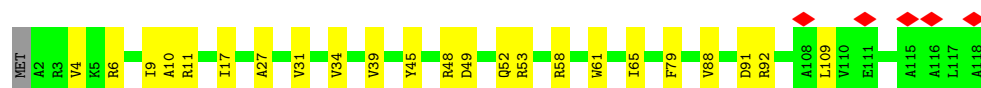




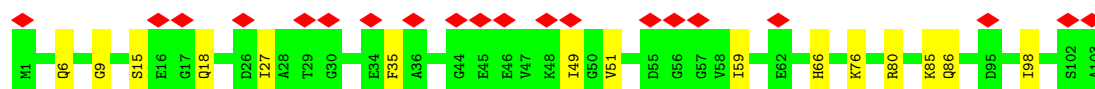
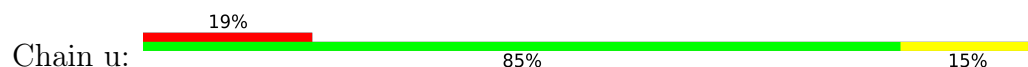
- Molecule 53: 50S ribosomal protein L19



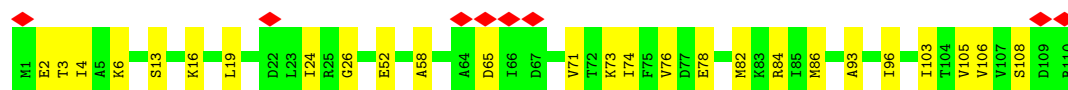
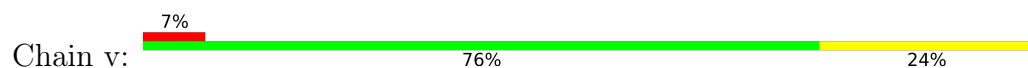
- Molecule 54: 50S ribosomal protein L20



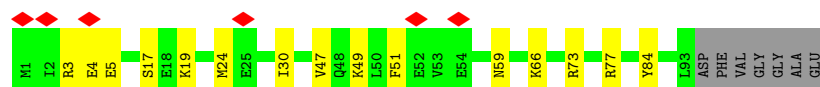
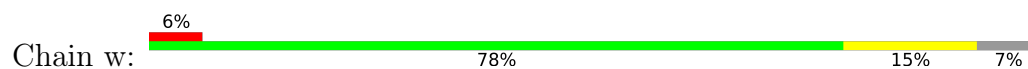
- Molecule 55: 50S ribosomal protein L21



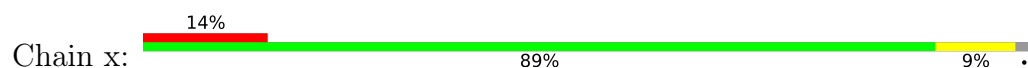
- Molecule 56: 50S ribosomal protein L22

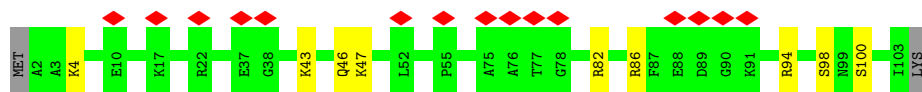


- Molecule 57: 50S ribosomal protein L23

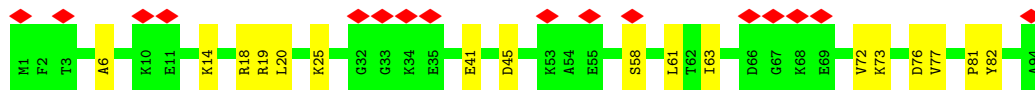
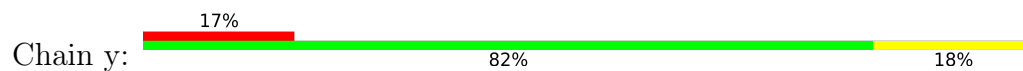


- Molecule 58: 50S ribosomal protein L24

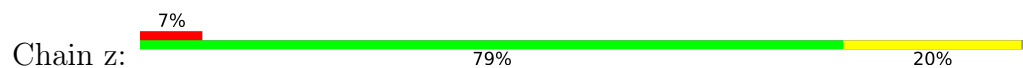




- Molecule 59: 50S ribosomal protein L25



- Molecule 60: 50S ribosomal protein L27



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, C1                               | Depositor |
| Number of particles used             | 34905                                   | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | FEI TITAN KRIOS                         | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 45                                      | Depositor |
| Minimum defocus (nm)                 | 500                                     | Depositor |
| Maximum defocus (nm)                 | 2000                                    | Depositor |
| Magnification                        | 81000                                   | Depositor |
| Image detector                       | GATAN K3 BIOQUANTUM (6k x 4k)           | Depositor |
| Maximum map value                    | 26.876                                  | Depositor |
| Minimum map value                    | -7.076                                  | Depositor |
| Average map value                    | 0.000                                   | Depositor |
| Map value standard deviation         | 1.000                                   | Depositor |
| Recommended contour level            | 5.5                                     | Depositor |
| Map size (Å)                         | 744.11993, 744.11993, 744.11993         | wwPDB     |
| Map dimensions                       | 702, 702, 702                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 1.06, 1.06, 1.06                        | Depositor |

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 5MC, PSU, MA6, 3TD, OMC, PUT, 3AU, RSP, 4SU, 2MG, OMU, G7M, 6MZ, SPD, 4OC, MIA, OMG, ZN, MG, 1MG, 5MU, H2U, 2MA, UR3

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

| Mol | Chain | Bond lengths |         | Bond angles |                  |
|-----|-------|--------------|---------|-------------|------------------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5          |
| 1   | 0     | 0.16         | 0/303   | 0.39        | 0/397            |
| 2   | 1     | 0.12         | 0/635   | 0.32        | 0/848            |
| 3   | 2     | 0.10         | 0/510   | 0.31        | 0/677            |
| 4   | 3     | 0.25         | 0/453   | 0.45        | 0/605            |
| 5   | 4     | 0.24         | 0/543   | 0.53        | 0/726            |
| 6   | 5     | 0.12         | 0/450   | 0.30        | 0/599            |
| 7   | 6     | 0.10         | 0/513   | 0.33        | 0/676            |
| 8   | 7     | 0.15         | 0/69306 | 0.29        | 35/108116 (0.0%) |
| 9   | 8     | 0.09         | 0/2876  | 0.21        | 0/4483           |
| 10  | A     | 0.14         | 0/36637 | 0.29        | 0/57149          |
| 11  | B     | 0.13         | 0/1807  | 0.43        | 0/2435           |
| 12  | C     | 0.12         | 0/1685  | 0.36        | 0/2270           |
| 13  | D     | 0.09         | 0/1665  | 0.30        | 0/2227           |
| 14  | E     | 0.12         | 0/1179  | 0.33        | 0/1584           |
| 15  | F     | 0.12         | 0/881   | 0.37        | 0/1189           |
| 16  | G     | 0.11         | 0/1219  | 0.34        | 0/1635           |
| 17  | H     | 0.11         | 0/989   | 0.33        | 0/1326           |
| 18  | I     | 0.10         | 0/1034  | 0.31        | 0/1375           |
| 19  | J     | 0.12         | 0/813   | 0.42        | 0/1100           |
| 20  | K     | 0.12         | 0/900   | 0.34        | 0/1215           |
| 21  | L     | 0.23         | 0/969   | 0.39        | 0/1300           |
| 22  | M     | 0.12         | 0/919   | 0.34        | 0/1226           |
| 23  | N     | 0.11         | 0/817   | 0.38        | 0/1088           |
| 24  | O     | 0.10         | 0/722   | 0.37        | 0/964            |
| 25  | P     | 0.11         | 0/659   | 0.32        | 0/884            |
| 26  | Q     | 0.12         | 0/657   | 0.38        | 0/881            |
| 27  | R     | 0.25         | 0/553   | 0.50        | 0/742            |
| 28  | S     | 0.12         | 0/680   | 0.33        | 0/915            |
| 29  | T     | 0.11         | 0/676   | 0.34        | 0/895            |
| 30  | U     | 0.15         | 0/592   | 0.35        | 0/785            |
| 31  | V     | 0.20         | 0/578   | 0.40        | 0/899            |

| Mol | Chain | Bond lengths |                 | Bond angles |                  |
|-----|-------|--------------|-----------------|-------------|------------------|
|     |       | RMSZ         | # Z  >5         | RMSZ        | # Z  >5          |
| 32  | W     | 0.23         | 0/1604          | 0.37        | 2/2496 (0.1%)    |
| 33  | X     | 0.40         | 2/1628 (0.1%)   | 0.38        | 0/2526           |
| 34  | Y     | 0.23         | 0/1725          | 0.35        | 2/2687 (0.1%)    |
| 35  | a     | 0.17         | 0/1033          | 0.30        | 0/1387           |
| 36  | b     | 0.12         | 0/2121          | 0.35        | 0/2852           |
| 37  | c     | 0.15         | 0/1586          | 0.36        | 0/2134           |
| 38  | d     | 0.10         | 0/1571          | 0.26        | 0/2113           |
| 39  | e     | 0.24         | 0/1444          | 0.44        | 0/1937           |
| 40  | f     | 0.30         | 0/1343          | 0.47        | 0/1816           |
| 41  | g     | 0.09         | 0/434           | 0.33        | 0/576            |
| 42  | h     | 0.11         | 0/1104          | 0.31        | 0/1474           |
| 43  | i     | 0.11         | 0/1122          | 0.38        | 0/1515           |
| 44  | j     | 0.09         | 0/1037          | 0.29        | 0/1400           |
| 45  | k     | 0.12         | 0/993           | 0.40        | 0/1341           |
| 46  | l     | 0.11         | 0/380           | 0.29        | 0/498            |
| 47  | m     | 0.23         | 0/1152          | 0.40        | 0/1551           |
| 48  | n     | 0.15         | 0/955           | 0.38        | 0/1279           |
| 49  | o     | 0.12         | 0/1062          | 0.35        | 0/1413           |
| 50  | p     | 0.94         | 0/57            | 1.20        | 0/76             |
| 51  | q     | 0.23         | 0/973           | 0.42        | 0/1301           |
| 52  | r     | 0.11         | 0/901           | 0.36        | 0/1209           |
| 53  | s     | 0.10         | 0/929           | 0.29        | 0/1242           |
| 54  | t     | 0.11         | 0/960           | 0.27        | 0/1278           |
| 55  | u     | 0.17         | 0/829           | 0.36        | 0/1107           |
| 56  | v     | 0.12         | 0/864           | 0.34        | 0/1156           |
| 57  | w     | 0.32         | 0/744           | 0.48        | 0/994            |
| 58  | x     | 0.10         | 0/787           | 0.35        | 0/1051           |
| 59  | y     | 0.09         | 0/766           | 0.29        | 0/1025           |
| 60  | z     | 0.10         | 0/642           | 0.33        | 0/848            |
| All | All   | 0.16         | 2/162966 (0.0%) | 0.32        | 39/243493 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 5   | 4     | 0                   | 1                   |
| 13  | D     | 0                   | 1                   |
| 16  | G     | 0                   | 1                   |
| 19  | J     | 0                   | 2                   |
| 20  | K     | 0                   | 1                   |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 24  | O     | 0                   | 1                   |
| 25  | P     | 0                   | 1                   |
| 27  | R     | 0                   | 1                   |
| 29  | T     | 0                   | 2                   |
| 30  | U     | 0                   | 1                   |
| 38  | d     | 0                   | 1                   |
| 39  | e     | 0                   | 1                   |
| 40  | f     | 0                   | 1                   |
| 47  | m     | 0                   | 1                   |
| 57  | w     | 0                   | 1                   |
| All | All   | 0                   | 17                  |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 33  | X     | 35  | I    | C5-C6 | 7.32 | 1.54        | 1.39     |
| 33  | X     | 35  | I    | N3-C4 | 7.00 | 1.50        | 1.35     |

All (39) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 8   | 7     | 1860 | G    | P-O3'-C3' | -9.63 | 105.76      | 120.20   |
| 8   | 7     | 1856 | U    | P-O3'-C3' | -9.32 | 106.22      | 120.20   |
| 8   | 7     | 2237 | G    | P-O3'-C3' | -8.97 | 106.75      | 120.20   |
| 8   | 7     | 1859 | U    | P-O3'-C3' | -8.52 | 107.42      | 120.20   |
| 8   | 7     | 2885 | G    | P-O3'-C3' | -8.31 | 107.73      | 120.20   |
| 8   | 7     | 1886 | U    | P-O3'-C3' | -8.21 | 107.88      | 120.20   |
| 8   | 7     | 2858 | C    | P-O3'-C3' | -8.03 | 108.16      | 120.20   |
| 8   | 7     | 983  | A    | P-O3'-C3' | -7.54 | 108.90      | 120.20   |
| 8   | 7     | 1854 | A    | P-O3'-C3' | -7.38 | 109.13      | 120.20   |
| 8   | 7     | 1309 | G    | P-O3'-C3' | -7.32 | 109.22      | 120.20   |
| 8   | 7     | 2236 | U    | P-O3'-C3' | -7.19 | 109.42      | 120.20   |
| 8   | 7     | 946  | C    | P-O3'-C3' | -7.14 | 109.49      | 120.20   |
| 8   | 7     | 743  | A    | P-O3'-C3' | -6.89 | 109.87      | 120.20   |
| 8   | 7     | 2855 | C    | P-O3'-C3' | -6.86 | 109.91      | 120.20   |
| 8   | 7     | 1887 | C    | P-O3'-C3' | -6.83 | 109.95      | 120.20   |
| 8   | 7     | 1658 | C    | P-O3'-C3' | -6.72 | 110.11      | 120.20   |
| 8   | 7     | 984  | A    | P-O3'-C3' | -6.70 | 110.15      | 120.20   |
| 8   | 7     | 820  | A    | P-O3'-C3' | -6.61 | 110.29      | 120.20   |
| 8   | 7     | 1310 | G    | P-O3'-C3' | -6.58 | 110.33      | 120.20   |
| 8   | 7     | 1855 | U    | P-O3'-C3' | -6.37 | 110.65      | 120.20   |
| 8   | 7     | 2884 | U    | P-O3'-C3' | -6.35 | 110.68      | 120.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 8   | 7     | 2317 | A    | P-O3'-C3'   | -6.21 | 110.88      | 120.20   |
| 8   | 7     | 1884 | G    | P-O3'-C3'   | -6.09 | 111.06      | 120.20   |
| 8   | 7     | 2318 | G    | P-O3'-C3'   | -5.99 | 111.21      | 120.20   |
| 8   | 7     | 1904 | G    | P-O3'-C3'   | -5.97 | 111.25      | 120.20   |
| 8   | 7     | 970  | U    | P-O3'-C3'   | -5.96 | 111.25      | 120.20   |
| 8   | 7     | 819  | A    | P-O3'-C3'   | -5.95 | 111.28      | 120.20   |
| 8   | 7     | 961  | C    | P-O3'-C3'   | -5.88 | 111.38      | 120.20   |
| 8   | 7     | 1882 | U    | P-O3'-C3'   | -5.70 | 111.66      | 120.20   |
| 34  | Y     | 74   | C    | P-O3'-C3'   | -5.69 | 111.66      | 120.20   |
| 8   | 7     | 2857 | G    | P-O3'-C3'   | -5.61 | 111.78      | 120.20   |
| 8   | 7     | 2859 | G    | P-O3'-C3'   | -5.49 | 111.97      | 120.20   |
| 32  | W     | 76   | A    | C4'-C3'-O3' | 5.45  | 117.58      | 109.40   |
| 8   | 7     | 947  | A    | P-O3'-C3'   | -5.27 | 112.30      | 120.20   |
| 8   | 7     | 971  | G    | P-O3'-C3'   | -5.24 | 112.33      | 120.20   |
| 34  | Y     | 75   | C    | P-O3'-C3'   | -5.13 | 112.51      | 120.20   |
| 8   | 7     | 1311 | G    | P-O3'-C3'   | -5.04 | 112.64      | 120.20   |
| 32  | W     | 76   | A    | C3'-C2'-O2' | -5.04 | 107.05      | 114.60   |
| 8   | 7     | 1856 | U    | O3'-P-O5'   | 5.03  | 111.54      | 104.00   |

There are no chirality outliers.

All (17) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 5   | 4     | 25  | ARG  | Sidechain |
| 13  | D     | 104 | ARG  | Sidechain |
| 16  | G     | 78  | ARG  | Sidechain |
| 19  | J     | 37  | ARG  | Sidechain |
| 19  | J     | 48  | ARG  | Sidechain |
| 20  | K     | 98  | ARG  | Sidechain |
| 24  | O     | 84  | ARG  | Sidechain |
| 25  | P     | 51  | ARG  | Sidechain |
| 27  | R     | 73  | ARG  | Sidechain |
| 29  | T     | 29  | ARG  | Sidechain |
| 29  | T     | 60  | ARG  | Sidechain |
| 30  | U     | 47  | ARG  | Sidechain |
| 38  | d     | 69  | ARG  | Sidechain |
| 39  | e     | 80  | ARG  | Sidechain |
| 40  | f     | 153 | ARG  | Sidechain |
| 47  | m     | 96  | ARG  | Sidechain |
| 57  | w     | 73  | ARG  | Sidechain |

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | 0     | 302   | 0        | 340      | 12      | 0            |
| 2   | 1     | 625   | 0        | 652      | 11      | 0            |
| 3   | 2     | 509   | 0        | 543      | 4       | 0            |
| 4   | 3     | 449   | 0        | 488      | 18      | 0            |
| 5   | 4     | 533   | 0        | 530      | 16      | 0            |
| 6   | 5     | 444   | 0        | 458      | 15      | 0            |
| 7   | 6     | 504   | 0        | 572      | 12      | 0            |
| 8   | 7     | 62355 | 0        | 31381    | 498     | 0            |
| 9   | 8     | 2572  | 0        | 1302     | 22      | 0            |
| 10  | A     | 32950 | 0        | 16602    | 537     | 0            |
| 11  | B     | 1776  | 0        | 1802     | 57      | 0            |
| 12  | C     | 1658  | 0        | 1732     | 63      | 0            |
| 13  | D     | 1643  | 0        | 1707     | 42      | 0            |
| 14  | E     | 1166  | 0        | 1212     | 29      | 0            |
| 15  | F     | 862   | 0        | 864      | 24      | 0            |
| 16  | G     | 1203  | 0        | 1254     | 25      | 0            |
| 17  | H     | 979   | 0        | 1031     | 28      | 0            |
| 18  | I     | 1022  | 0        | 1069     | 17      | 0            |
| 19  | J     | 803   | 0        | 842      | 25      | 0            |
| 20  | K     | 884   | 0        | 896      | 18      | 0            |
| 21  | L     | 955   | 0        | 1016     | 27      | 0            |
| 22  | M     | 910   | 0        | 978      | 22      | 0            |
| 23  | N     | 805   | 0        | 844      | 34      | 0            |
| 24  | O     | 714   | 0        | 734      | 13      | 0            |
| 25  | P     | 649   | 0        | 666      | 21      | 0            |
| 26  | Q     | 648   | 0        | 691      | 11      | 0            |
| 27  | R     | 544   | 0        | 565      | 14      | 0            |
| 28  | S     | 663   | 0        | 688      | 14      | 0            |
| 29  | T     | 670   | 0        | 719      | 22      | 0            |
| 30  | U     | 584   | 0        | 618      | 7       | 0            |
| 31  | V     | 516   | 0        | 262      | 11      | 0            |
| 32  | W     | 1630  | 0        | 839      | 20      | 0            |
| 33  | X     | 1654  | 0        | 848      | 29      | 0            |
| 34  | Y     | 1628  | 0        | 828      | 20      | 0            |
| 35  | a     | 1026  | 0        | 1092     | 10      | 0            |
| 36  | b     | 2082  | 0        | 2154     | 54      | 0            |
| 37  | c     | 1565  | 0        | 1616     | 42      | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 38  | d     | 1552   | 0        | 1619     | 32      | 0            |
| 39  | e     | 1420   | 0        | 1457     | 37      | 0            |
| 40  | f     | 1323   | 0        | 1371     | 29      | 0            |
| 41  | g     | 427    | 0        | 464      | 3       | 0            |
| 42  | h     | 1085   | 0        | 1169     | 21      | 0            |
| 43  | i     | 1111   | 0        | 1148     | 16      | 0            |
| 44  | j     | 1023   | 0        | 1050     | 19      | 0            |
| 45  | k     | 979    | 0        | 1028     | 23      | 0            |
| 46  | l     | 377    | 0        | 418      | 16      | 0            |
| 47  | m     | 1129   | 0        | 1162     | 31      | 0            |
| 48  | n     | 946    | 0        | 1023     | 33      | 0            |
| 49  | o     | 1053   | 0        | 1129     | 37      | 0            |
| 50  | p     | 206    | 0        | 95       | 4       | 0            |
| 51  | q     | 960    | 0        | 1000     | 22      | 0            |
| 52  | r     | 891    | 0        | 923      | 22      | 0            |
| 53  | s     | 917    | 0        | 962      | 20      | 0            |
| 54  | t     | 947    | 0        | 1019     | 21      | 0            |
| 55  | u     | 816    | 0        | 839      | 10      | 0            |
| 56  | v     | 857    | 0        | 922      | 19      | 0            |
| 57  | w     | 738    | 0        | 807      | 8       | 0            |
| 58  | x     | 779    | 0        | 831      | 6       | 0            |
| 59  | y     | 753    | 0        | 780      | 14      | 0            |
| 60  | z     | 634    | 0        | 653      | 15      | 0            |
| 61  | 0     | 1      | 0        | 0        | 0       | 0            |
| 61  | 4     | 1      | 0        | 0        | 0       | 0            |
| 62  | 7     | 12     | 0        | 24       | 0       | 0            |
| 63  | 7     | 10     | 0        | 19       | 2       | 0            |
| 64  | 7     | 257    | 0        | 0        | 0       | 0            |
| 64  | A     | 23     | 0        | 0        | 0       | 0            |
| 64  | I     | 1      | 0        | 0        | 0       | 0            |
| 64  | V     | 1      | 0        | 0        | 0       | 0            |
| 64  | X     | 1      | 0        | 0        | 0       | 0            |
| 64  | Y     | 1      | 0        | 0        | 0       | 0            |
| 64  | b     | 1      | 0        | 0        | 0       | 0            |
| 64  | q     | 1      | 0        | 0        | 0       | 0            |
| 64  | r     | 1      | 0        | 0        | 0       | 0            |
| 65  | Y     | 5      | 0        | 4        | 0       | 0            |
| 66  | 7     | 12     | 0        | 0        | 1       | 0            |
| 66  | x     | 1      | 0        | 0        | 0       | 0            |
| All | All   | 151734 | 0        | 102351   | 1911    | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (1911) 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) |
|------------------|-------------------|--------------------------|-------------------|
| 32:W:54:5MU:C4   | 32:W:54:5MU:C5    | 1.79                     | 1.70              |
| 33:X:55:5MU:C4   | 33:X:55:5MU:C5    | 1.80                     | 1.65              |
| 31:V:19:G:H1     | 33:X:36:C:H42     | 1.17                     | 0.92              |
| 10:A:664:G:H22   | 10:A:741:G:H1     | 1.24                     | 0.85              |
| 8:7:1278:C:H4'   | 51:q:34:ILE:HD11  | 1.58                     | 0.85              |
| 10:A:672:U:H5'   | 15:F:79:ARG:HH22  | 1.43                     | 0.82              |
| 10:A:74:A:H61    | 10:A:96:U:H3      | 1.25                     | 0.81              |
| 23:N:93:ILE:HG21 | 23:N:96:LEU:HD12  | 1.61                     | 0.81              |
| 10:A:459:A:H61   | 10:A:473:U:H3     | 1.29                     | 0.80              |
| 38:d:184:ASP:HA  | 49:o:2:ARG:HH12   | 1.45                     | 0.79              |
| 8:7:1800:C:HO2'  | 8:7:1818:U:H3     | 1.26                     | 0.79              |
| 12:C:79:LYS:HA   | 12:C:83:ASP:HB2   | 1.64                     | 0.79              |
| 10:A:375:U:H4'   | 25:P:6:LEU:HD11   | 1.65                     | 0.79              |
| 12:C:22:TRP:HB3  | 12:C:59:ARG:H     | 1.48                     | 0.78              |
| 10:A:1081:A:N7   | 14:E:52:LYS:NZ    | 2.33                     | 0.77              |
| 23:N:54:ASP:HA   | 23:N:59:ARG:HG2   | 1.66                     | 0.77              |
| 10:A:427:U:H3'   | 10:A:428:G:H5''   | 1.66                     | 0.76              |
| 8:7:1478:G:H1    | 8:7:1513:U:H3     | 1.32                     | 0.76              |
| 10:A:537:G:H5''  | 21:L:110:ARG:HH12 | 1.51                     | 0.76              |
| 10:A:1009:U:H3   | 10:A:1020:G:H1    | 1.33                     | 0.75              |
| 53:s:60:THR:HG22 | 53:s:73:VAL:HG12  | 1.68                     | 0.75              |
| 10:A:459:A:N6    | 10:A:474:G:N3     | 2.34                     | 0.75              |
| 10:A:949:A:N7    | 22:M:105:ASN:ND2  | 2.35                     | 0.75              |
| 10:A:1382:C:H4'  | 16:G:79:ARG:HH21  | 1.51                     | 0.75              |
| 13:D:62:ARG:HH21 | 13:D:68:LEU:HA    | 1.50                     | 0.74              |
| 5:4:6:HIS:HE1    | 39:e:63:GLN:HA    | 1.52                     | 0.74              |
| 14:E:157:ARG:NH1 | 17:H:99:LEU:O     | 2.21                     | 0.74              |
| 12:C:10:ILE:HG23 | 12:C:11:ARG:HD3   | 1.68                     | 0.74              |
| 10:A:532:A:N6    | 10:A:1206:G:O2'   | 2.21                     | 0.74              |
| 38:d:97:ASN:HB2  | 38:d:100:MET:HG2  | 1.68                     | 0.74              |
| 10:A:380:G:N2    | 10:A:383:A:OP2    | 2.21                     | 0.73              |
| 8:7:2681:C:H4'   | 37:c:11:MET:HE1   | 1.68                     | 0.73              |
| 11:B:219:ALA:HA  | 11:B:222:ARG:HE   | 1.53                     | 0.73              |
| 10:A:1030:U:O2   | 10:A:1032:G:N2    | 2.18                     | 0.73              |
| 10:A:75:G:H1     | 10:A:95:C:H42     | 1.37                     | 0.73              |
| 13:D:54:GLN:HA   | 13:D:199:LEU:HD21 | 1.71                     | 0.72              |
| 8:7:1779:U:OP2   | 8:7:1784:A:N6     | 2.23                     | 0.72              |
| 39:e:65:PRO:HB2  | 39:e:87:CYS:HB3   | 1.71                     | 0.72              |
| 46:l:18:PHE:HB2  | 46:l:43:THR:HG21  | 1.70                     | 0.72              |
| 8:7:600:G:H1'    | 38:d:100:MET:HE1  | 1.72                     | 0.72              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 13:D:15:GLU:OE2   | 13:D:63:ARG:NH2   | 2.22                     | 0.72              |
| 8:7:2816:G:O3'    | 51:q:99:LYS:NZ    | 2.23                     | 0.72              |
| 48:n:1:MET:HB2    | 48:n:32:TYR:HB3   | 1.71                     | 0.71              |
| 15:F:42:TRP:HD1   | 15:F:59:TYR:HB3   | 1.53                     | 0.71              |
| 8:7:1936:A:H2     | 8:7:1943:U:H3     | 1.35                     | 0.71              |
| 8:7:1211:C:H4'    | 8:7:1212:G:OP2    | 1.89                     | 0.71              |
| 19:J:53:ILE:HD13  | 19:J:63:ASP:HB2   | 1.73                     | 0.71              |
| 10:A:501:C:OP1    | 21:L:114:ARG:NH2  | 2.23                     | 0.71              |
| 11:B:187:VAL:HG21 | 11:B:199:VAL:HG23 | 1.72                     | 0.71              |
| 8:7:1203:U:H4'    | 49:o:3:LEU:HD21   | 1.72                     | 0.71              |
| 10:A:397:A:N7     | 10:A:547:A:O2'    | 2.23                     | 0.71              |
| 37:c:156:PHE:HD2  | 47:m:81:ILE:HG13  | 1.54                     | 0.71              |
| 8:7:896:A:N6      | 34:Y:19:G:O2'     | 2.23                     | 0.70              |
| 10:A:83:C:H2'     | 10:A:84:U:H3'     | 1.73                     | 0.70              |
| 1:0:4:ARG:HE      | 1:0:35:GLN:HG2    | 1.54                     | 0.70              |
| 17:H:13:ARG:NH1   | 17:H:26:THR:O     | 2.24                     | 0.70              |
| 38:d:119:ILE:HB   | 38:d:187:VAL:HG22 | 1.72                     | 0.70              |
| 10:A:501:C:H5'    | 10:A:501:C:H6     | 1.55                     | 0.70              |
| 36:b:3:VAL:HG12   | 36:b:19:VAL:HG12  | 1.74                     | 0.70              |
| 8:7:2263:C:N4     | 60:z:15:ASP:OD1   | 2.24                     | 0.70              |
| 8:7:2264:C:N4     | 60:z:15:ASP:OD2   | 2.25                     | 0.70              |
| 8:7:1665:A:H5''   | 48:n:66:LYS:HE3   | 1.74                     | 0.70              |
| 10:A:963:G:H21    | 19:J:57:VAL:HG11  | 1.56                     | 0.70              |
| 36:b:21:ASN:HB3   | 36:b:24:LEU:HD23  | 1.73                     | 0.69              |
| 11:B:114:LEU:HD13 | 11:B:148:LEU:HD22 | 1.73                     | 0.69              |
| 32:W:11:U:H3      | 32:W:24:G:H1      | 1.39                     | 0.69              |
| 27:R:38:LYS:NZ    | 30:U:26:ALA:O     | 2.26                     | 0.69              |
| 10:A:202:G:H1     | 10:A:215:C:H42    | 1.40                     | 0.69              |
| 21:L:72:HIS:HB2   | 21:L:74:LEU:HD23  | 1.74                     | 0.69              |
| 40:f:104:ASN:ND2  | 40:f:114:ASP:OD1  | 2.25                     | 0.69              |
| 8:7:960:A:H2'     | 8:7:962:G:H5''    | 1.75                     | 0.68              |
| 10:A:1142:G:H3'   | 10:A:1143:G:H8    | 1.58                     | 0.68              |
| 14:E:157:ARG:HH21 | 17:H:43:GLU:HB3   | 1.57                     | 0.68              |
| 48:n:1:MET:HG2    | 48:n:67:LYS:HE2   | 1.74                     | 0.68              |
| 48:n:70:ARG:HG2   | 48:n:76:VAL:HG12  | 1.75                     | 0.68              |
| 8:7:2639:A:H4'    | 47:m:96:ARG:NH2   | 2.09                     | 0.68              |
| 10:A:1368:A:H5''  | 18:I:114:LYS:HB3  | 1.74                     | 0.68              |
| 39:e:10:ASP:O     | 39:e:14:LYS:NZ    | 2.25                     | 0.68              |
| 10:A:502:A:H61    | 10:A:543:U:H3     | 1.38                     | 0.68              |
| 8:7:2554:U:H3     | 34:Y:74:C:H42     | 1.42                     | 0.68              |
| 19:J:65:TYR:HB3   | 23:N:96:LEU:HD22  | 1.76                     | 0.67              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:A:562:U:O2'    | 21:L:14:ARG:NH2   | 2.27                     | 0.67              |
| 10:A:1316:G:N1    | 10:A:1319:A:OP2   | 2.28                     | 0.67              |
| 10:A:1073:U:OP2   | 14:E:62:LYS:NZ    | 2.26                     | 0.67              |
| 10:A:1496:C:O2    | 10:A:1517:G:N2    | 2.18                     | 0.67              |
| 10:A:454:G:H1     | 10:A:478:A:H2     | 1.40                     | 0.67              |
| 57:w:24:MET:HE1   | 57:w:30:ILE:HG22  | 1.77                     | 0.67              |
| 8:7:1537:G:OP2    | 8:7:1537:G:N2     | 2.27                     | 0.67              |
| 10:A:1059:C:O3'   | 23:N:85:ARG:NH1   | 2.25                     | 0.67              |
| 22:M:75:MET:HA    | 22:M:78:LYS:HE3   | 1.77                     | 0.67              |
| 8:7:2561:U:O2     | 48:n:23:LYS:NZ    | 2.28                     | 0.66              |
| 10:A:483:C:H2'    | 10:A:484:G:C8     | 2.29                     | 0.66              |
| 43:i:72:ILE:HB    | 43:i:108:VAL:HG11 | 1.76                     | 0.66              |
| 5:4:14:ALA:HB3    | 5:4:22:MET:HB2    | 1.77                     | 0.66              |
| 8:7:2:G:H1        | 8:7:2901:U:H3     | 1.41                     | 0.66              |
| 8:7:1044:C:O2'    | 8:7:1111:A:N1     | 2.29                     | 0.66              |
| 9:8:93:C:OP2      | 59:y:18:ARG:NH1   | 2.29                     | 0.66              |
| 43:i:6:LEU:HD23   | 43:i:36:ALA:HA    | 1.78                     | 0.66              |
| 8:7:858:G:N2      | 8:7:2269:G:OP2    | 2.27                     | 0.66              |
| 8:7:2330:G:O3'    | 60:z:44:LYS:NZ    | 2.24                     | 0.66              |
| 8:7:2530:A:N7     | 40:f:172:LYS:NZ   | 2.44                     | 0.66              |
| 8:7:2818:U:OP2    | 51:q:42:LYS:NZ    | 2.29                     | 0.66              |
| 5:4:34:LEU:HD22   | 39:e:106:ILE:HD12 | 1.77                     | 0.66              |
| 12:C:150:LYS:HG3  | 12:C:169:ARG:HB3  | 1.78                     | 0.65              |
| 37:c:8:LYS:HB2    | 37:c:201:LEU:HD11 | 1.77                     | 0.65              |
| 37:c:172:VAL:HG12 | 37:c:175:LEU:HD21 | 1.77                     | 0.65              |
| 7:6:13:ARG:NH2    | 8:7:250:G:OP2     | 2.29                     | 0.65              |
| 8:7:475:C:H4'     | 8:7:510:C:H5'     | 1.78                     | 0.65              |
| 17:H:96:MET:HB3   | 17:H:100:GLY:H    | 1.61                     | 0.65              |
| 27:R:70:TYR:HB2   | 27:R:74:HIS:CE1   | 2.31                     | 0.65              |
| 10:A:1320:C:H1'   | 28:S:73:GLU:HG3   | 1.78                     | 0.65              |
| 27:R:70:TYR:HB2   | 27:R:74:HIS:HE1   | 1.60                     | 0.65              |
| 8:7:1112:G:O2'    | 40:f:3:ARG:NH2    | 2.29                     | 0.65              |
| 16:G:113:ASP:HB2  | 16:G:119:ARG:HG3  | 1.78                     | 0.65              |
| 8:7:571:U:H3'     | 55:u:80:ARG:HH12  | 1.62                     | 0.65              |
| 10:A:501:C:H1'    | 10:A:549:C:H1'    | 1.78                     | 0.65              |
| 40:f:24:ILE:HG21  | 40:f:72:LEU:HD11  | 1.78                     | 0.65              |
| 14:E:159:LYS:NZ   | 17:H:42:GLU:O     | 2.27                     | 0.65              |
| 8:7:2470:G:O6     | 8:7:2481:G:N2     | 2.30                     | 0.65              |
| 19:J:54:SER:HB3   | 19:J:58:ASN:HB3   | 1.78                     | 0.65              |
| 37:c:88:GLU:OE1   | 37:c:88:GLU:N     | 2.30                     | 0.65              |
| 45:k:14:ALA:H     | 45:k:54:PRO:HA    | 1.61                     | 0.65              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 13:D:65:TYR:O    | 13:D:97:ARG:NH1   | 2.27                     | 0.64              |
| 8:7:1856:U:H2'   | 8:7:1857:G:H5'    | 1.79                     | 0.64              |
| 10:A:671:G:O2'   | 15:F:79:ARG:NH2   | 2.30                     | 0.64              |
| 10:A:1160:G:OP1  | 11:B:132:LYS:NZ   | 2.27                     | 0.64              |
| 45:k:72:LYS:HG3  | 45:k:73:THR:H     | 1.61                     | 0.64              |
| 13:D:97:ARG:NH2  | 13:D:99:ASP:OD2   | 2.30                     | 0.64              |
| 53:s:97:LEU:HB3  | 53:s:100:LEU:HD23 | 1.80                     | 0.64              |
| 10:A:408:A:H61   | 10:A:434:U:H3     | 1.45                     | 0.64              |
| 23:N:16:LEU:HD23 | 23:N:54:ASP:HB2   | 1.78                     | 0.64              |
| 8:7:1278:C:H5'   | 51:q:24:MET:HE1   | 1.79                     | 0.64              |
| 10:A:203:G:H1    | 10:A:214:C:H42    | 1.44                     | 0.64              |
| 8:7:1427:A:N6    | 8:7:1571:A:OP2    | 2.22                     | 0.64              |
| 8:7:2052:A:O2'   | 37:c:148:GLN:O    | 2.12                     | 0.64              |
| 23:N:46:LEU:HD21 | 28:S:16:LEU:HD23  | 1.80                     | 0.64              |
| 12:C:15:VAL:HG23 | 12:C:16:LYS:H     | 1.63                     | 0.63              |
| 36:b:107:PRO:HD2 | 36:b:110:LEU:HD22 | 1.79                     | 0.63              |
| 49:o:19:LEU:HB2  | 49:o:31:GLY:HA2   | 1.79                     | 0.63              |
| 52:r:31:THR:HG22 | 52:r:33:ARG:H     | 1.64                     | 0.63              |
| 10:A:898:G:N2    | 10:A:901:A:OP2    | 2.28                     | 0.63              |
| 58:x:46:GLN:NE2  | 58:x:47:LYS:O     | 2.32                     | 0.63              |
| 5:4:10:GLU:N     | 5:4:26:SER:O      | 2.32                     | 0.63              |
| 8:7:411:G:OP2    | 8:7:2406:A:O2'    | 2.16                     | 0.63              |
| 10:A:477:C:H3'   | 10:A:478:A:H8     | 1.64                     | 0.63              |
| 38:d:46:GLN:O    | 38:d:88:ARG:NH2   | 2.32                     | 0.63              |
| 39:e:110:ARG:NH2 | 39:e:136:ILE:O    | 2.31                     | 0.63              |
| 9:8:3:C:O2'      | 9:8:4:C:OP1       | 2.12                     | 0.63              |
| 56:v:73:LYS:HB2  | 56:v:106:VAL:HB   | 1.81                     | 0.63              |
| 11:B:9:MET:HB2   | 11:B:43:LEU:HD21  | 1.79                     | 0.63              |
| 8:7:671:C:N4     | 49:o:40:SER:O     | 2.22                     | 0.63              |
| 8:7:2470:G:OP1   | 42:h:55:ARG:NH2   | 2.32                     | 0.63              |
| 10:A:476:U:H2'   | 10:A:477:C:C6     | 2.34                     | 0.63              |
| 10:A:545:C:OP1   | 13:D:58:LYS:NZ    | 2.32                     | 0.63              |
| 33:X:23:G:H2'    | 33:X:24:A:H8      | 1.63                     | 0.63              |
| 54:t:49:ASP:HA   | 54:t:52:GLN:HB2   | 1.81                     | 0.63              |
| 10:A:501:C:O2    | 10:A:549:C:O2'    | 2.16                     | 0.62              |
| 10:A:1437:A:OP1  | 29:T:29:ARG:NH1   | 2.30                     | 0.62              |
| 1:0:3:VAL:HG21   | 8:7:2539:C:H5'    | 1.81                     | 0.62              |
| 7:6:13:ARG:HG2   | 49:o:63:LYS:HA    | 1.80                     | 0.62              |
| 10:A:753:A:OP1   | 24:O:73:LYS:NZ    | 2.32                     | 0.62              |
| 20:K:27:PHE:HE1  | 20:K:89:PRO:HG2   | 1.64                     | 0.62              |
| 39:e:26:MET:O    | 39:e:30:ARG:NH2   | 2.29                     | 0.62              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 8:7:1826:G:O2'   | 8:7:1971:U:OP2    | 2.17                     | 0.62              |
| 10:A:570:G:O6    | 10:A:865:A:N6     | 2.32                     | 0.62              |
| 33:X:74:A:H5''   | 33:X:75:C:H5      | 1.64                     | 0.62              |
| 48:n:4:GLU:HG2   | 48:n:23:LYS:HA    | 1.82                     | 0.62              |
| 60:z:21:LEU:HD21 | 60:z:41:ARG:HG2   | 1.79                     | 0.62              |
| 19:J:53:ILE:HD11 | 23:N:85:ARG:HD2   | 1.81                     | 0.62              |
| 14:E:75:ALA:O    | 14:E:82:GLN:NE2   | 2.26                     | 0.62              |
| 44:j:100:ALA:HB1 | 44:j:107:GLU:HA   | 1.82                     | 0.62              |
| 8:7:2529:G:H4'   | 40:f:175:LYS:HE2  | 1.81                     | 0.62              |
| 10:A:769:G:H4'   | 10:A:1513:A:H4'   | 1.81                     | 0.62              |
| 23:N:64:CYS:HB2  | 23:N:80:SER:HB3   | 1.81                     | 0.62              |
| 36:b:130:LEU:HB2 | 36:b:135:ILE:HD11 | 1.82                     | 0.62              |
| 8:7:2279:G:N7    | 60:z:14:ARG:NH2   | 2.47                     | 0.62              |
| 10:A:87:C:H2'    | 10:A:88:U:H4'     | 1.81                     | 0.62              |
| 8:7:2831:G:N7    | 37:c:59:ARG:NH2   | 2.48                     | 0.61              |
| 8:7:45:G:H5'     | 8:7:46:G:H5'      | 1.81                     | 0.61              |
| 8:7:574:A:N6     | 8:7:2034:U:OP1    | 2.33                     | 0.61              |
| 8:7:1416:G:O2'   | 8:7:1417:C:OP2    | 2.15                     | 0.61              |
| 8:7:1475:G:O2'   | 8:7:1476:U:O5'    | 2.17                     | 0.61              |
| 10:A:33:A:O2'    | 21:L:29:GLN:NE2   | 2.33                     | 0.61              |
| 10:A:70:U:H3     | 10:A:98:A:H61     | 1.47                     | 0.61              |
| 8:7:1194:A:OP2   | 49:o:14:LYS:NZ    | 2.31                     | 0.61              |
| 8:7:2134:A:H1'   | 8:7:2159:G:H1'    | 1.82                     | 0.61              |
| 12:C:40:ARG:NH1  | 23:N:92:GLU:OE1   | 2.33                     | 0.61              |
| 34:Y:34:G:H2'    | 34:Y:35:G:C8      | 2.36                     | 0.61              |
| 6:5:43:ILE:HG22  | 6:5:49:TYR:HB2    | 1.83                     | 0.61              |
| 8:7:1580:A:O2'   | 8:7:1581:G:OP1    | 2.17                     | 0.61              |
| 8:7:686:U:O4     | 46:l:12:ARG:NH1   | 2.29                     | 0.61              |
| 10:A:677:U:H3    | 10:A:713:G:H22    | 1.46                     | 0.61              |
| 11:B:94:HIS:ND1  | 11:B:146:ASN:O    | 2.34                     | 0.61              |
| 8:7:2108:A:H2    | 8:7:2181:U:H3     | 1.48                     | 0.61              |
| 59:y:20:LEU:HG   | 59:y:25:LYS:HB2   | 1.83                     | 0.61              |
| 10:A:553:A:H5''  | 21:L:21:VAL:HG21  | 1.83                     | 0.61              |
| 26:Q:68:SER:HB3  | 26:Q:71:LYS:HB2   | 1.82                     | 0.61              |
| 40:f:163:ARG:NH2 | 40:f:167:GLU:O    | 2.33                     | 0.61              |
| 8:7:1859:U:H2'   | 8:7:1860:G:C8     | 2.36                     | 0.61              |
| 10:A:503:C:OP1   | 21:L:116:LYS:NZ   | 2.32                     | 0.61              |
| 15:F:88:MET:HE1  | 27:R:61:ARG:HB3   | 1.83                     | 0.61              |
| 8:7:1607:C:N4    | 8:7:1622:G:OP2    | 2.27                     | 0.61              |
| 10:A:902:G:H4'   | 10:A:902:G:OP1    | 2.00                     | 0.61              |
| 10:A:1084:G:O2'  | 10:A:1103:C:N4    | 2.32                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 10:A:1356:G:H2'  | 10:A:1357:A:C8   | 2.36                     | 0.61              |
| 55:u:35:PHE:HB2  | 55:u:59:ILE:HB   | 1.81                     | 0.61              |
| 13:D:100:ASN:OD1 | 13:D:111:ARG:NH1 | 2.34                     | 0.60              |
| 29:T:28:MET:HG2  | 29:T:58:VAL:HG12 | 1.82                     | 0.60              |
| 34:Y:20:G:N2     | 34:Y:59:U:OP1    | 2.34                     | 0.60              |
| 8:7:566:U:H5''   | 49:o:29:LYS:HE3  | 1.82                     | 0.60              |
| 12:C:18:TRP:HZ3  | 23:N:97:LYS:HE3  | 1.66                     | 0.60              |
| 47:m:72:LYS:HE3  | 47:m:74:TYR:HE1  | 1.65                     | 0.60              |
| 51:q:29:VAL:HG21 | 51:q:75:ILE:HG23 | 1.84                     | 0.60              |
| 16:G:113:ASP:OD2 | 16:G:122:ASN:ND2 | 2.34                     | 0.60              |
| 8:7:825:A:O2'    | 49:o:54:GLN:OE1  | 2.17                     | 0.60              |
| 18:I:130:ARG:NH2 | 32:W:33:U:OP2    | 2.32                     | 0.60              |
| 26:Q:77:ARG:HH12 | 26:Q:79:VAL:HG22 | 1.67                     | 0.60              |
| 40:f:107:LEU:O   | 40:f:152:ARG:NH2 | 2.34                     | 0.60              |
| 8:7:675:A:OP1    | 38:d:58:LYS:NZ   | 2.34                     | 0.60              |
| 12:C:88:ARG:HH12 | 12:C:100:GLN:HG3 | 1.65                     | 0.60              |
| 10:A:626:G:O3'   | 25:P:51:ARG:NH2  | 2.34                     | 0.60              |
| 10:A:1115:U:H3   | 10:A:1185:G:H1   | 1.49                     | 0.60              |
| 8:7:468:G:OP2    | 46:l:37:LYS:NZ   | 2.35                     | 0.60              |
| 8:7:1664:A:H61   | 8:7:1996:C:H42   | 1.50                     | 0.60              |
| 38:d:117:ARG:NH2 | 38:d:183:PHE:O   | 2.34                     | 0.60              |
| 12:C:33:LEU:HD22 | 23:N:93:ILE:HD13 | 1.83                     | 0.60              |
| 8:7:2788:C:O2'   | 8:7:2809:A:N3    | 2.35                     | 0.60              |
| 10:A:390:U:H4'   | 25:P:28:ARG:HH21 | 1.66                     | 0.60              |
| 51:q:53:THR:HA   | 51:q:56:LYS:HE3  | 1.83                     | 0.60              |
| 10:A:195:A:H2'   | 10:A:196:A:C8    | 2.37                     | 0.59              |
| 10:A:363:A:H1'   | 21:L:29:GLN:HE21 | 1.67                     | 0.59              |
| 39:e:60:ILE:HD13 | 39:e:138:PHE:HD2 | 1.66                     | 0.59              |
| 46:l:22:MET:HG3  | 46:l:28:ARG:HG2  | 1.85                     | 0.59              |
| 12:C:212:ALA:H   | 19:J:16:ARG:HH12 | 1.50                     | 0.59              |
| 10:A:1:A:OP1     | 10:A:3:A:N6      | 2.35                     | 0.59              |
| 10:A:297:G:N2    | 10:A:300:A:OP2   | 2.35                     | 0.59              |
| 8:7:476:G:H22    | 8:7:479:A:H5''   | 1.68                     | 0.59              |
| 10:A:438:U:H4'   | 10:A:439:U:O5'   | 2.02                     | 0.59              |
| 13:D:6:GLY:O     | 13:D:8:LYS:NZ    | 2.33                     | 0.59              |
| 8:7:2522:U:O2'   | 8:7:2647:U:OP1   | 2.18                     | 0.59              |
| 10:A:975:A:N1    | 10:A:1366:C:O2'  | 2.34                     | 0.59              |
| 45:k:10:LYS:HD3  | 45:k:56:PRO:HB3  | 1.83                     | 0.59              |
| 59:y:76:ASP:OD1  | 59:y:77:VAL:N    | 2.35                     | 0.59              |
| 8:7:858:G:O2'    | 8:7:859:G:O4'    | 2.15                     | 0.59              |
| 8:7:1138:G:H2'   | 8:7:1139:G:O4'   | 2.03                     | 0.59              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 28:S:50:ALA:HB1  | 28:S:57:HIS:HB3   | 1.84                     | 0.59              |
| 43:i:58:LEU:O    | 43:i:61:VAL:HG12  | 2.03                     | 0.59              |
| 54:t:88:VAL:HG22 | 55:u:51:VAL:HG12  | 1.85                     | 0.59              |
| 8:7:2859:G:H2'   | 8:7:2860:A:C8     | 2.37                     | 0.59              |
| 10:A:835:U:OP1   | 27:R:53:ARG:NH1   | 2.35                     | 0.59              |
| 11:B:117:LEU:O   | 11:B:121:SER:N    | 2.34                     | 0.59              |
| 12:C:85:GLU:HA   | 12:C:88:ARG:HD3   | 1.85                     | 0.59              |
| 22:M:81:MET:HE2  | 22:M:91:HIS:HB3   | 1.85                     | 0.59              |
| 30:U:13:ASP:OD1  | 30:U:14:VAL:N     | 2.35                     | 0.59              |
| 32:W:54:5MU:C4   | 32:W:54:5MU:C6    | 2.58                     | 0.59              |
| 10:A:532:A:H2    | 10:A:1206:G:H21   | 1.50                     | 0.59              |
| 8:7:2512:C:H5''  | 37:c:127:PHE:CD1  | 2.38                     | 0.59              |
| 10:A:7:A:N6      | 14:E:97:GLN:OE1   | 2.36                     | 0.59              |
| 10:A:999:C:H2'   | 10:A:1000:A:H8    | 1.68                     | 0.59              |
| 8:7:1249:U:H4'   | 54:t:4:VAL:HG21   | 1.85                     | 0.58              |
| 10:A:1011:C:H2'  | 10:A:1012:A:C8    | 2.37                     | 0.58              |
| 10:A:1255:G:O2'  | 10:A:1258:G:N3    | 2.35                     | 0.58              |
| 13:D:185:LYS:HG3 | 13:D:186:PRO:HD2  | 1.85                     | 0.58              |
| 16:G:111:ARG:HB3 | 16:G:119:ARG:HG2  | 1.84                     | 0.58              |
| 2:1:23:ASN:OD1   | 8:7:2079:U:O2'    | 2.21                     | 0.58              |
| 8:7:1040:A:H61   | 8:7:1115:G:H1     | 1.51                     | 0.58              |
| 8:7:1791:A:H5''  | 36:b:205:LEU:HD11 | 1.85                     | 0.58              |
| 8:7:2141:G:H2'   | 8:7:2142:A:C8     | 2.38                     | 0.58              |
| 8:7:2393:U:H5''  | 49:o:62:PRO:HB3   | 1.86                     | 0.58              |
| 10:A:454:G:N2    | 10:A:479:U:O4'    | 2.36                     | 0.58              |
| 48:n:24:VAL:HG23 | 48:n:33:ALA:HB2   | 1.85                     | 0.58              |
| 8:7:463:G:N2     | 8:7:466:A:OP2     | 2.27                     | 0.58              |
| 8:7:2571:U:O2    | 37:c:148:GLN:NE2  | 2.36                     | 0.58              |
| 53:s:6:LYS:O     | 53:s:10:GLN:NE2   | 2.35                     | 0.58              |
| 8:7:858:G:OP2    | 60:z:78:LYS:NZ    | 2.36                     | 0.58              |
| 8:7:1278:C:H2'   | 8:7:1279:G:C8     | 2.39                     | 0.58              |
| 10:A:74:A:H3'    | 10:A:75:G:H8      | 1.67                     | 0.58              |
| 20:K:24:HIS:HB3  | 20:K:31:ILE:HB    | 1.85                     | 0.58              |
| 33:X:35:I:H3'    | 33:X:36:C:C6      | 2.38                     | 0.58              |
| 8:7:1820:U:H1'   | 36:b:200:HIS:HD2  | 1.68                     | 0.58              |
| 37:c:115:GLY:HA2 | 37:c:166:GLY:HA3  | 1.85                     | 0.58              |
| 52:r:20:GLU:HG2  | 52:r:21:LEU:HD12  | 1.85                     | 0.58              |
| 54:t:91:ASP:OD1  | 54:t:92:ARG:N     | 2.36                     | 0.58              |
| 1:0:34:LYS:NZ    | 8:7:2743:U:OP1    | 2.37                     | 0.58              |
| 8:7:2127:G:H2'   | 8:7:2128:G:O4'    | 2.04                     | 0.58              |
| 9:8:30:C:H1'     | 9:8:57:A:H61      | 1.68                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:A:416:G:H1     | 10:A:427:U:H3     | 1.50                     | 0.58              |
| 13:D:95:GLU:O     | 13:D:100:ASN:ND2  | 2.36                     | 0.58              |
| 53:s:25:THR:HB    | 53:s:88:ARG:HB3   | 1.86                     | 0.58              |
| 8:7:2676:C:OP2    | 48:n:31:ARG:NH2   | 2.35                     | 0.58              |
| 10:A:855:U:OP2    | 10:A:871:U:N3     | 2.30                     | 0.58              |
| 10:A:1106:G:O2'   | 12:C:169:ARG:NH1  | 2.36                     | 0.58              |
| 51:q:95:THR:HB    | 51:q:113:ILE:HD11 | 1.84                     | 0.58              |
| 8:7:1030:C:OP2    | 42:h:127:LYS:NZ   | 2.36                     | 0.58              |
| 10:A:191:G:H3'    | 10:A:192:A:H8     | 1.69                     | 0.58              |
| 8:7:1791:A:N6     | 8:7:1828:G:O2'    | 2.33                     | 0.58              |
| 10:A:56:U:H2'     | 10:A:57:G:C8      | 2.39                     | 0.58              |
| 25:P:55:ASP:OD1   | 25:P:56:ARG:N     | 2.36                     | 0.58              |
| 8:7:1537:G:H3'    | 8:7:1538:G:O4'    | 2.04                     | 0.58              |
| 10:A:352:C:O2     | 10:A:355:C:N4     | 2.37                     | 0.58              |
| 10:A:811:C:O2'    | 10:A:901:A:N1     | 2.37                     | 0.58              |
| 10:A:1309:G:N7    | 22:M:98:ARG:NH2   | 2.52                     | 0.58              |
| 11:B:64:LYS:HE2   | 11:B:225:ARG:HG3  | 1.85                     | 0.58              |
| 14:E:115:LEU:HD13 | 14:E:123:VAL:HG11 | 1.84                     | 0.58              |
| 10:A:180:U:O2     | 10:A:196:A:N6     | 2.36                     | 0.57              |
| 42:h:64:TRP:HB2   | 42:h:104:GLU:HB2  | 1.85                     | 0.57              |
| 8:7:776:G:O2'     | 8:7:2241:A:OP1    | 2.22                     | 0.57              |
| 8:7:455:C:H3'     | 8:7:456:C:H5''    | 1.86                     | 0.57              |
| 8:7:1654:A:O2'    | 37:c:118:PHE:O    | 2.20                     | 0.57              |
| 37:c:121:THR:HB   | 37:c:127:PHE:HD2  | 1.68                     | 0.57              |
| 8:7:584:C:P       | 54:t:6:ARG:HH21   | 2.27                     | 0.57              |
| 10:A:1015:G:N2    | 10:A:1218:C:O2    | 2.36                     | 0.57              |
| 8:7:2114:A:H62    | 8:7:2115:G:H21    | 1.51                     | 0.57              |
| 10:A:212:G:H2'    | 10:A:213:G:C8     | 2.39                     | 0.57              |
| 10:A:375:U:H3     | 10:A:389:A:H61    | 1.52                     | 0.57              |
| 10:A:1261:A:N6    | 10:A:1274:A:O2'   | 2.38                     | 0.57              |
| 10:A:1073:U:O2    | 11:B:103:ASN:ND2  | 2.37                     | 0.57              |
| 10:A:1372:U:OP1   | 18:I:74:GLY:N     | 2.30                     | 0.57              |
| 53:s:29:LYS:HE2   | 53:s:40:LEU:HB3   | 1.87                     | 0.57              |
| 6:5:16:ARG:HH12   | 8:7:1265:A:H3'    | 1.69                     | 0.57              |
| 8:7:833:A:OP1     | 49:o:39:LYS:NZ    | 2.33                     | 0.57              |
| 45:k:72:LYS:HE2   | 45:k:115:ALA:HB3  | 1.87                     | 0.57              |
| 8:7:1131:G:N2     | 8:7:1132:U:O4     | 2.36                     | 0.57              |
| 8:7:1528:A:N6     | 8:7:1543:G:O2'    | 2.38                     | 0.57              |
| 10:A:376:G:H2'    | 10:A:377:G:H8     | 1.70                     | 0.57              |
| 49:o:90:VAL:HG13  | 49:o:95:LEU:HD21  | 1.85                     | 0.57              |
| 8:7:1682:G:OP2    | 8:7:1699:G:N2     | 2.36                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:A:1040:U:H2'   | 10:A:1041:G:H8    | 1.69                     | 0.57              |
| 11:B:111:ILE:HG22 | 11:B:115:LYS:HE3  | 1.85                     | 0.57              |
| 20:K:20:VAL:HG13  | 20:K:35:THR:HG23  | 1.87                     | 0.57              |
| 44:j:71:CYS:HB2   | 44:j:117:LEU:HB3  | 1.87                     | 0.57              |
| 9:8:98:G:H1       | 59:y:14:LYS:HB2   | 1.70                     | 0.57              |
| 10:A:40:C:H2'     | 10:A:41:G:C8      | 2.39                     | 0.57              |
| 10:A:269:C:H2'    | 10:A:270:A:H8     | 1.68                     | 0.57              |
| 10:A:1010:U:H3    | 10:A:1019:A:H61   | 1.51                     | 0.57              |
| 42:h:24:THR:O     | 42:h:34:LYS:NZ    | 2.35                     | 0.57              |
| 48:n:19:VAL:HG21  | 48:n:41:ILE:HD12  | 1.87                     | 0.57              |
| 8:7:2444:G:OP1    | 38:d:62:GLN:NE2   | 2.38                     | 0.56              |
| 38:d:145:ASP:HB3  | 38:d:184:ASP:HB2  | 1.87                     | 0.56              |
| 39:e:117:LEU:HD13 | 39:e:176:PRO:HB2  | 1.86                     | 0.56              |
| 46:l:24:THR:HG23  | 46:l:27:GLY:H     | 1.69                     | 0.56              |
| 10:A:1236:A:H4'   | 10:A:1304:G:H4'   | 1.87                     | 0.56              |
| 11:B:67:ILE:HG12  | 11:B:89:GLN:HE21  | 1.69                     | 0.56              |
| 11:B:72:THR:OG1   | 11:B:169:GLU:OE2  | 2.22                     | 0.56              |
| 12:C:152:GLU:HG3  | 12:C:199:LYS:HB2  | 1.85                     | 0.56              |
| 3:2:20:ASN:OD1    | 3:2:23:ARG:NH2    | 2.31                     | 0.56              |
| 8:7:684:G:OP1     | 46:l:21:ARG:NH1   | 2.35                     | 0.56              |
| 8:7:2595:G:N2     | 8:7:2598:A:OP2    | 2.29                     | 0.56              |
| 10:A:154:U:H2'    | 10:A:155:A:C8     | 2.40                     | 0.56              |
| 10:A:269:C:H2'    | 10:A:270:A:C8     | 2.40                     | 0.56              |
| 10:A:358:U:H2'    | 10:A:359:G:C8     | 2.40                     | 0.56              |
| 10:A:1069:C:H42   | 10:A:1106:G:H1    | 1.52                     | 0.56              |
| 10:A:1397:C:OP2   | 14:E:29:ARG:NH2   | 2.38                     | 0.56              |
| 11:B:24:ASN:HD21  | 11:B:192:ASP:HB3  | 1.71                     | 0.56              |
| 21:L:114:ARG:HG2  | 21:L:119:VAL:HB   | 1.86                     | 0.56              |
| 23:N:31:ILE:O     | 23:N:41:ARG:NH1   | 2.37                     | 0.56              |
| 36:b:231:PRO:O    | 36:b:242:LYS:NZ   | 2.22                     | 0.56              |
| 10:A:1380:U:O2    | 10:A:1382:C:N4    | 2.38                     | 0.56              |
| 10:A:1497:G:H1'   | 10:A:1518:MA6:H2  | 1.87                     | 0.56              |
| 16:G:2:PRO:HD2    | 16:G:5:ARG:HE     | 1.70                     | 0.56              |
| 8:7:813:U:O3'     | 55:u:86:GLN:NE2   | 2.39                     | 0.56              |
| 8:7:2554:U:H2'    | 8:7:2555:U:C6     | 2.40                     | 0.56              |
| 14:E:156:LYS:NZ   | 17:H:71:VAL:O     | 2.26                     | 0.56              |
| 8:7:1378:A:O2'    | 8:7:1380:G:OP2    | 2.24                     | 0.56              |
| 10:A:358:U:H2'    | 10:A:359:G:H8     | 1.70                     | 0.56              |
| 13:D:118:VAL:HG22 | 13:D:123:ILE:HG13 | 1.88                     | 0.56              |
| 13:D:196:ASN:HB2  | 13:D:198:HIS:CE1  | 2.41                     | 0.56              |
| 15:F:49:TYR:OH    | 27:R:63:ARG:O     | 2.21                     | 0.56              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:0:16:ILE:HG22  | 1:0:25:VAL:HG22   | 1.88                     | 0.56              |
| 8:7:487:C:O2'    | 56:v:52:GLU:OE1   | 2.23                     | 0.56              |
| 8:7:2688:G:N1    | 8:7:2720:U:OP2    | 2.28                     | 0.56              |
| 10:A:1071:C:H2'  | 10:A:1072:G:H8    | 1.71                     | 0.56              |
| 10:A:1199:U:H4'  | 19:J:56:HIS:CD2   | 2.40                     | 0.56              |
| 24:O:70:LEU:HD22 | 24:O:78:TYR:HB2   | 1.88                     | 0.56              |
| 32:W:9:A:H5'     | 32:W:46:G7M:H8    | 1.88                     | 0.56              |
| 55:u:76:LYS:HB2  | 55:u:85:LYS:HB2   | 1.88                     | 0.56              |
| 8:7:1190:G:OP1   | 49:o:30:THR:OG1   | 2.18                     | 0.56              |
| 8:7:1288:G:OP2   | 8:7:1288:G:N2     | 2.30                     | 0.56              |
| 9:8:75:G:H2'     | 9:8:76:G:H8       | 1.70                     | 0.56              |
| 10:A:1162:C:H2'  | 10:A:1163:A:C8    | 2.41                     | 0.56              |
| 12:C:9:GLY:HA3   | 23:N:89:MET:SD    | 2.46                     | 0.56              |
| 42:h:20:LEU:HD13 | 59:y:81:PRO:HG3   | 1.87                     | 0.56              |
| 2:1:3:ARG:NH1    | 8:7:1365:A:OP1    | 2.34                     | 0.56              |
| 8:7:65:U:O2'     | 8:7:456:C:N3      | 2.38                     | 0.56              |
| 8:7:499:U:H5''   | 58:x:43:LYS:HD2   | 1.87                     | 0.56              |
| 8:7:1130:U:O2'   | 8:7:1131:G:OP1    | 2.22                     | 0.56              |
| 10:A:414:A:H3'   | 10:A:415:A:H8     | 1.71                     | 0.56              |
| 10:A:1308:U:H2'  | 10:A:1309:G:H8    | 1.69                     | 0.56              |
| 12:C:110:GLU:HB2 | 12:C:144:LEU:HD12 | 1.88                     | 0.56              |
| 40:f:86:LYS:NZ   | 40:f:87:LEU:O     | 2.39                     | 0.56              |
| 51:q:29:VAL:HG11 | 51:q:79:LEU:HD21  | 1.88                     | 0.56              |
| 10:A:67:C:O2'    | 10:A:171:A:N3     | 2.34                     | 0.56              |
| 10:A:418:C:H2'   | 10:A:419:C:C6     | 2.41                     | 0.56              |
| 10:A:1302:C:C6   | 22:M:17:ILE:HG13  | 2.40                     | 0.56              |
| 20:K:73:ALA:O    | 20:K:77:TYR:N     | 2.30                     | 0.56              |
| 46:l:41:ARG:NH2  | 46:l:45:SER:O     | 2.38                     | 0.56              |
| 8:7:754:U:O2'    | 8:7:1272:A:N1     | 2.39                     | 0.55              |
| 8:7:1341:G:O6    | 57:w:19:LYS:NZ    | 2.39                     | 0.55              |
| 8:7:2512:C:H2'   | 8:7:2513:A:O4'    | 2.06                     | 0.55              |
| 10:A:33:A:H1'    | 21:L:29:GLN:HE22  | 1.71                     | 0.55              |
| 10:A:58:C:O2'    | 10:A:388:G:N7     | 2.39                     | 0.55              |
| 42:h:58:LYS:O    | 42:h:60:GLN:NE2   | 2.39                     | 0.55              |
| 2:1:58:VAL:HG12  | 8:7:372:G:H2'     | 1.88                     | 0.55              |
| 10:A:150:U:H2'   | 10:A:151:A:H8     | 1.71                     | 0.55              |
| 10:A:766:A:OP2   | 10:A:812:G:N2     | 2.39                     | 0.55              |
| 12:C:73:PRO:O    | 12:C:76:VAL:HG22  | 2.06                     | 0.55              |
| 20:K:84:VAL:HB   | 20:K:110:ILE:HG22 | 1.89                     | 0.55              |
| 8:7:858:G:N3     | 8:7:2268:A:H2'    | 2.21                     | 0.55              |
| 8:7:1094:U:H1'   | 8:7:1097:U:H5     | 1.70                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:7:2618:G:H21    | 37:c:155:VAL:HG21 | 1.70                     | 0.55              |
| 39:e:116:GLY:C    | 39:e:178:ARG:HB3  | 2.32                     | 0.55              |
| 51:q:97:ILE:HG13  | 51:q:113:ILE:HD13 | 1.88                     | 0.55              |
| 60:z:75:LYS:HB2   | 60:z:77:ARG:HG3   | 1.87                     | 0.55              |
| 8:7:684:G:P       | 46:l:21:ARG:HH12  | 2.30                     | 0.55              |
| 8:7:1006:C:O3'    | 47:m:37:ARG:NH2   | 2.40                     | 0.55              |
| 10:A:922:G:H1'    | 14:E:24:THR:HG23  | 1.89                     | 0.55              |
| 10:A:1040:U:H2'   | 10:A:1041:G:C8    | 2.42                     | 0.55              |
| 54:t:45:TYR:HD1   | 54:t:48:ARG:HH12  | 1.54                     | 0.55              |
| 8:7:1594:U:H2'    | 8:7:1595:C:C6     | 2.42                     | 0.55              |
| 8:7:1789:A:OP2    | 36:b:221:ARG:NH1  | 2.39                     | 0.55              |
| 44:j:56:ARG:HG3   | 44:j:58:THR:H     | 1.72                     | 0.55              |
| 1:0:1:MET:N       | 8:7:2526:G:N3     | 2.55                     | 0.55              |
| 8:7:494:G:H4'     | 56:v:6:LYS:HB2    | 1.88                     | 0.55              |
| 8:7:2562:U:H1'    | 48:n:23:LYS:HZ1   | 1.71                     | 0.55              |
| 9:8:75:G:H2'      | 9:8:76:G:C8       | 2.42                     | 0.55              |
| 10:A:428:G:H5'    | 13:D:10:LYS:HE3   | 1.89                     | 0.55              |
| 23:N:17:ALA:HA    | 23:N:55:SER:HA    | 1.88                     | 0.55              |
| 45:k:94:ASN:OD1   | 45:k:95:LYS:HD3   | 2.06                     | 0.55              |
| 10:A:483:C:O2'    | 10:A:484:G:OP1    | 2.21                     | 0.55              |
| 10:A:1060:U:H2'   | 10:A:1061:G:H8    | 1.71                     | 0.55              |
| 38:d:158:PHE:HA   | 38:d:169:VAL:HG11 | 1.87                     | 0.55              |
| 42:h:1:MET:HG2    | 42:h:2:LEU:H      | 1.71                     | 0.55              |
| 55:u:15:SER:N     | 55:u:18:GLN:OE1   | 2.38                     | 0.55              |
| 8:7:1800:C:H3'    | 36:b:146:MET:HE1  | 1.88                     | 0.55              |
| 8:7:2748:A:H5'    | 40:f:4:VAL:HG21   | 1.89                     | 0.55              |
| 10:A:530:G:N3     | 34:Y:35:G:O2'     | 2.38                     | 0.55              |
| 13:D:47:ARG:HH22  | 31:V:34:A:H62     | 1.55                     | 0.55              |
| 48:n:15:GLY:O     | 48:n:47:ILE:HD12  | 2.07                     | 0.55              |
| 8:7:503:A:H5''    | 8:7:504:A:H3'     | 1.88                     | 0.55              |
| 8:7:2166:U:H2'    | 8:7:2167:U:H5'    | 1.89                     | 0.55              |
| 9:8:48:U:P        | 52:r:30:ARG:HH12  | 2.30                     | 0.55              |
| 10:A:694:A:N1     | 10:A:787:A:O2'    | 2.39                     | 0.55              |
| 15:F:59:TYR:OH    | 27:R:65:LEU:O     | 2.19                     | 0.55              |
| 20:K:81:ASN:HA    | 20:K:106:ARG:HB2  | 1.87                     | 0.55              |
| 8:7:829:A:N7      | 8:7:2247:A:O2'    | 2.39                     | 0.55              |
| 10:A:43:C:H2'     | 10:A:44:A:C8      | 2.41                     | 0.55              |
| 11:B:101:LEU:HD11 | 11:B:158:PRO:HD2  | 1.88                     | 0.55              |
| 48:n:1:MET:HG3    | 48:n:1:MET:O      | 2.07                     | 0.55              |
| 49:o:19:LEU:HD13  | 49:o:31:GLY:HA3   | 1.89                     | 0.55              |
| 8:7:1028:A:N3     | 8:7:2486:C:O2'    | 2.34                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:7:2070:A:H2'    | 8:7:2071:A:O4'    | 2.07                     | 0.54              |
| 10:A:147:G:H2'    | 10:A:148:G:C8     | 2.42                     | 0.54              |
| 10:A:1241:G:OP1   | 16:G:35:LYS:NZ    | 2.36                     | 0.54              |
| 10:A:1402:4OC:O5' | 10:A:1402:4OC:H6  | 2.07                     | 0.54              |
| 36:b:205:LEU:HD13 | 36:b:210:ALA:HB3  | 1.89                     | 0.54              |
| 37:c:110:THR:HB   | 37:c:202:ILE:HB   | 1.88                     | 0.54              |
| 8:7:2335:A:OP1    | 52:r:13:ARG:NE    | 2.38                     | 0.54              |
| 11:B:32:PHE:HB2   | 11:B:42:ASN:HB2   | 1.88                     | 0.54              |
| 8:7:987:C:O2'     | 8:7:1000:A:N3     | 2.40                     | 0.54              |
| 11:B:104:TRP:HA   | 11:B:107:VAL:HG22 | 1.88                     | 0.54              |
| 32:W:43:G:H2'     | 32:W:44:G:C8      | 2.43                     | 0.54              |
| 33:X:23:G:H2'     | 33:X:24:A:C8      | 2.41                     | 0.54              |
| 36:b:16:VAL:HG12  | 36:b:206:GLY:HA3  | 1.89                     | 0.54              |
| 8:7:788:A:OP1     | 8:7:791:C:N4      | 2.35                     | 0.54              |
| 13:D:73:ARG:NH2   | 13:D:74:ASN:OD1   | 2.34                     | 0.54              |
| 8:7:324:A:OP2     | 8:7:1205:A:N6     | 2.41                     | 0.54              |
| 8:7:617:G:OP1     | 38:d:102:ARG:NH1  | 2.40                     | 0.54              |
| 8:7:1167:C:H2'    | 8:7:1168:G:C8     | 2.43                     | 0.54              |
| 10:A:951:G:OP2    | 22:M:101:ARG:NH2  | 2.39                     | 0.54              |
| 10:A:1175:G:H2'   | 10:A:1176:A:C8    | 2.42                     | 0.54              |
| 8:7:1043:C:H5''   | 44:j:3:LEU:HD13   | 1.89                     | 0.54              |
| 8:7:1363:C:O2'    | 8:7:1809:A:N3     | 2.37                     | 0.54              |
| 10:A:345:C:OP1    | 53:s:37:LYS:NZ    | 2.40                     | 0.54              |
| 10:A:486:U:H2'    | 10:A:487:A:H8     | 1.73                     | 0.54              |
| 10:A:542:G:OP1    | 13:D:10:LYS:NZ    | 2.40                     | 0.54              |
| 10:A:1137:C:O2    | 10:A:1138:G:N2    | 2.41                     | 0.54              |
| 45:k:133:ALA:HB1  | 45:k:138:LEU:HB2  | 1.88                     | 0.54              |
| 53:s:106:LYS:HD3  | 53:s:109:ARG:HD3  | 1.90                     | 0.54              |
| 6:5:13:ARG:O      | 6:5:17:ARG:HG3    | 2.08                     | 0.54              |
| 10:A:876:C:P      | 17:H:15:ARG:HH12  | 2.31                     | 0.54              |
| 10:A:1218:C:H2'   | 10:A:1219:A:C8    | 2.42                     | 0.54              |
| 10:A:1247:U:H2'   | 10:A:1248:A:H5''  | 1.89                     | 0.54              |
| 11:B:101:LEU:HD13 | 11:B:104:TRP:HE1  | 1.73                     | 0.54              |
| 12:C:150:LYS:O    | 12:C:201:TRP:N    | 2.40                     | 0.54              |
| 36:b:245:VAL:HG12 | 36:b:251:GLN:HA   | 1.90                     | 0.54              |
| 53:s:6:LYS:HG2    | 53:s:10:GLN:HE22  | 1.71                     | 0.54              |
| 8:7:517:C:O2'     | 56:v:78:GLU:OE2   | 2.18                     | 0.54              |
| 8:7:715:A:H61     | 24:O:53:ARG:NH2   | 2.06                     | 0.54              |
| 10:A:362:G:N2     | 10:A:365:U:OP2    | 2.41                     | 0.54              |
| 10:A:808:C:OP2    | 24:O:48:LYS:NZ    | 2.25                     | 0.54              |
| 10:A:1380:U:H1'   | 10:A:1382:C:H41   | 1.73                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:F:38:ARG:NH1   | 15:F:96:VAL:O     | 2.41                     | 0.54              |
| 25:P:50:THR:HG21  | 25:P:74:LEU:HD12  | 1.90                     | 0.54              |
| 44:j:124:ASP:N    | 44:j:124:ASP:OD1  | 2.41                     | 0.54              |
| 10:A:183:C:O2'    | 10:A:184:G:H5'    | 2.08                     | 0.53              |
| 10:A:545:C:O2'    | 10:A:549:C:H5'    | 2.08                     | 0.53              |
| 32:W:16:H2U:H3'   | 32:W:16:H2U:H61   | 1.90                     | 0.53              |
| 49:o:17:LYS:HD2   | 49:o:27:LEU:HD21  | 1.89                     | 0.53              |
| 8:7:514:A:N3      | 8:7:581:C:O2'     | 2.37                     | 0.53              |
| 8:7:2572:A:H2'    | 37:c:149:ASN:HD21 | 1.73                     | 0.53              |
| 10:A:575:G:O2'    | 10:A:821:G:H5'    | 2.08                     | 0.53              |
| 32:W:16:H2U:C4    | 32:W:59:G:H22     | 2.22                     | 0.53              |
| 47:m:114:LEU:HB3  | 47:m:118:MET:HE2  | 1.90                     | 0.53              |
| 8:7:453:A:N3      | 8:7:457:A:O2'     | 2.41                     | 0.53              |
| 8:7:534:U:O2'     | 54:t:49:ASP:OD2   | 2.10                     | 0.53              |
| 8:7:1447:C:O2'    | 8:7:1544:A:N3     | 2.37                     | 0.53              |
| 8:7:1797:G:HO2'   | 36:b:257:THR:HG1  | 1.54                     | 0.53              |
| 10:A:437:U:O2'    | 13:D:120:HIS:ND1  | 2.38                     | 0.53              |
| 11:B:101:LEU:O    | 11:B:104:TRP:HD1  | 1.92                     | 0.53              |
| 8:7:779:U:OP1     | 36:b:49:ILE:HD12  | 2.08                     | 0.53              |
| 8:7:1105:U:H2'    | 8:7:1106:G:C8     | 2.44                     | 0.53              |
| 8:7:1800:C:O2'    | 8:7:1818:U:N3     | 2.28                     | 0.53              |
| 8:7:2540:C:O2'    | 8:7:2740:A:N3     | 2.39                     | 0.53              |
| 10:A:1077:G:N2    | 10:A:1080:A:OP2   | 2.33                     | 0.53              |
| 11:B:86:SER:OG    | 11:B:222:ARG:NH1  | 2.41                     | 0.53              |
| 15:F:42:TRP:CD1   | 15:F:59:TYR:HB3   | 2.40                     | 0.53              |
| 27:R:39:ILE:H     | 27:R:39:ILE:HD12  | 1.74                     | 0.53              |
| 36:b:236:GLU:OE1  | 36:b:236:GLU:N    | 2.34                     | 0.53              |
| 37:c:46:ARG:NH1   | 37:c:85:ALA:O     | 2.41                     | 0.53              |
| 47:m:72:LYS:HE3   | 47:m:74:TYR:CE1   | 2.44                     | 0.53              |
| 5:4:63:ARG:HB3    | 28:S:5:LEU:HD11   | 1.90                     | 0.53              |
| 8:7:964:C:O2'     | 8:7:2273:A:N3     | 2.35                     | 0.53              |
| 10:A:142:G:H3'    | 10:A:143:A:H8     | 1.74                     | 0.53              |
| 29:T:44:LYS:HG2   | 29:T:86:LEU:HD22  | 1.89                     | 0.53              |
| 39:e:98:GLU:O     | 39:e:101:GLU:HG2  | 2.08                     | 0.53              |
| 8:7:1859:U:H2'    | 8:7:1860:G:H8     | 1.74                     | 0.53              |
| 10:A:1121:U:H3    | 10:A:1152:A:H61   | 1.57                     | 0.53              |
| 11:B:199:VAL:HG22 | 11:B:201:PRO:HD3  | 1.88                     | 0.53              |
| 8:7:706:A:OP1     | 36:b:7:LYS:NZ     | 2.41                     | 0.53              |
| 10:A:376:G:H2'    | 10:A:377:G:C8     | 2.43                     | 0.53              |
| 10:A:389:A:H3'    | 10:A:390:U:H6     | 1.73                     | 0.53              |
| 10:A:1072:G:N2    | 11:B:106:THR:OG1  | 2.42                     | 0.53              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 23:N:60:GLN:OE1  | 23:N:60:GLN:N     | 2.41                     | 0.53              |
| 2:1:55:GLY:O     | 2:1:59:ILE:HG12   | 2.08                     | 0.53              |
| 4:3:14:ILE:HD13  | 8:7:988:A:C5      | 2.43                     | 0.53              |
| 9:8:94:A:OP1     | 59:y:19:ARG:NE    | 2.31                     | 0.53              |
| 10:A:545:C:H5'   | 13:D:69:GLU:HB2   | 1.91                     | 0.53              |
| 10:A:1218:C:H2'  | 10:A:1219:A:H8    | 1.73                     | 0.53              |
| 33:X:36:C:H2'    | 33:X:37:G:C8      | 2.44                     | 0.53              |
| 5:4:64:PHE:HB3   | 28:S:9:PRO:HD3    | 1.89                     | 0.53              |
| 8:7:2680:U:H5'   | 37:c:194:PRO:HA   | 1.90                     | 0.53              |
| 10:A:1268:G:N3   | 10:A:1326:U:O2'   | 2.42                     | 0.53              |
| 25:P:6:LEU:HD13  | 25:P:17:TYR:CD1   | 2.44                     | 0.53              |
| 32:W:16:H2U:P    | 32:W:16:H2U:H62   | 2.49                     | 0.53              |
| 49:o:49:GLY:O    | 49:o:56:PRO:HB3   | 2.09                     | 0.53              |
| 8:7:630:G:N2     | 8:7:633:A:OP2     | 2.34                     | 0.53              |
| 10:A:160:A:H2'   | 10:A:161:A:O4'    | 2.09                     | 0.53              |
| 10:A:1161:C:H42  | 10:A:1175:G:H1    | 1.54                     | 0.53              |
| 10:A:1297:G:H21  | 16:G:114:LYS:HB3  | 1.73                     | 0.53              |
| 24:O:24:SER:O    | 24:O:28:GLN:HG2   | 2.09                     | 0.53              |
| 4:3:54:MET:HG3   | 4:3:55:VAL:HG13   | 1.90                     | 0.52              |
| 8:7:1028:A:OP2   | 8:7:1126:A:N6     | 2.33                     | 0.52              |
| 8:7:2162:G:H3'   | 8:7:2163:A:H8     | 1.73                     | 0.52              |
| 10:A:382:A:H2'   | 10:A:383:A:C8     | 2.44                     | 0.52              |
| 10:A:401:C:O2'   | 10:A:621:A:N3     | 2.37                     | 0.52              |
| 10:A:514:C:H2'   | 10:A:515:G:H8     | 1.74                     | 0.52              |
| 10:A:1030:U:H2'  | 10:A:1032:G:H1    | 1.73                     | 0.52              |
| 19:J:52:LEU:HD11 | 23:N:81:ARG:HD2   | 1.91                     | 0.52              |
| 33:X:19:G:H22    | 33:X:56:PSU:HN3   | 1.57                     | 0.52              |
| 38:d:117:ARG:NE  | 38:d:184:ASP:O    | 2.42                     | 0.52              |
| 50:p:31:VAL:C    | 50:p:33:ASN:H     | 2.17                     | 0.52              |
| 10:A:1029:U:H2'  | 10:A:1030:U:H6    | 1.75                     | 0.52              |
| 10:A:1162:C:H2'  | 10:A:1163:A:H8    | 1.74                     | 0.52              |
| 10:A:1245:C:H2'  | 10:A:1246:A:C8    | 2.44                     | 0.52              |
| 13:D:54:GLN:HB3  | 13:D:203:LEU:HD13 | 1.90                     | 0.52              |
| 13:D:67:VAL:HG21 | 13:D:94:LEU:HD22  | 1.91                     | 0.52              |
| 30:U:31:GLU:OE2  | 30:U:34:ARG:NH2   | 2.42                     | 0.52              |
| 5:4:11:GLU:HA    | 5:4:25:ARG:HA     | 1.91                     | 0.52              |
| 8:7:1604:C:O2'   | 8:7:1610:A:N1     | 2.33                     | 0.52              |
| 8:7:2175:C:H2'   | 8:7:2176:A:H8     | 1.74                     | 0.52              |
| 8:7:2641:G:H5''  | 47:m:78:THR:HB    | 1.91                     | 0.52              |
| 10:A:1121:U:H2'  | 10:A:1122:U:C6    | 2.44                     | 0.52              |
| 10:A:1187:G:N3   | 23:N:100:SER:OG   | 2.35                     | 0.52              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 12:C:75:ILE:HG13 | 12:C:79:LYS:HE3   | 1.91                     | 0.52              |
| 13:D:92:ALA:O    | 13:D:185:LYS:NZ   | 2.37                     | 0.52              |
| 16:G:58:GLU:OE1  | 16:G:58:GLU:N     | 2.34                     | 0.52              |
| 33:X:1:G:O2'     | 33:X:2:C:OP1      | 2.25                     | 0.52              |
| 37:c:116:LYS:HB2 | 37:c:165:MET:HB2  | 1.90                     | 0.52              |
| 1:0:37:GLN:NE2   | 8:7:1031:G:N3     | 2.55                     | 0.52              |
| 8:7:1210:G:H4'   | 8:7:1211:C:H5''   | 1.92                     | 0.52              |
| 8:7:1570:A:H2'   | 8:7:1571:A:C8     | 2.45                     | 0.52              |
| 9:8:78:A:OP2     | 59:y:14:LYS:NZ    | 2.42                     | 0.52              |
| 10:A:406:G:N2    | 13:D:116:GLN:OE1  | 2.38                     | 0.52              |
| 10:A:830:G:O2'   | 11:B:21:ARG:NH1   | 2.43                     | 0.52              |
| 11:B:67:ILE:H    | 11:B:89:GLN:NE2   | 2.07                     | 0.52              |
| 13:D:147:GLU:HA  | 13:D:150:LYS:HG2  | 1.91                     | 0.52              |
| 49:o:20:GLY:HA2  | 49:o:28:GLY:HA2   | 1.90                     | 0.52              |
| 8:7:2131:U:H5'   | 8:7:2133:G:H4'    | 1.91                     | 0.52              |
| 9:8:47:C:O2'     | 52:r:98:GLN:NE2   | 2.43                     | 0.52              |
| 10:A:17:U:H2'    | 10:A:18:C:C6      | 2.45                     | 0.52              |
| 10:A:58:C:H2'    | 10:A:59:A:H8      | 1.73                     | 0.52              |
| 10:A:859:G:OP2   | 10:A:869:G:N1     | 2.27                     | 0.52              |
| 10:A:1326:U:H2'  | 10:A:1327:C:C6    | 2.44                     | 0.52              |
| 32:W:10:G:O2'    | 32:W:11:U:OP1     | 2.25                     | 0.52              |
| 39:e:170:LEU:O   | 39:e:175:PHE:HB2  | 2.09                     | 0.52              |
| 7:6:25:LYS:HE3   | 49:o:64:PHE:HB3   | 1.90                     | 0.52              |
| 8:7:717:C:H3'    | 8:7:718:A:H8      | 1.74                     | 0.52              |
| 8:7:883:G:H1     | 8:7:893:C:H42     | 1.58                     | 0.52              |
| 8:7:958:U:OP1    | 42:h:40:ARG:NH2   | 2.43                     | 0.52              |
| 8:7:2019:A:H4'   | 54:t:34:VAL:HG21  | 1.90                     | 0.52              |
| 12:C:19:ASN:ND2  | 23:N:90:ARG:O     | 2.43                     | 0.52              |
| 8:7:1047:G:HO2'  | 8:7:1110:G:H1     | 1.57                     | 0.52              |
| 8:7:2394:C:H5''  | 49:o:63:LYS:HD3   | 1.91                     | 0.52              |
| 8:7:2506:U:OP2   | 8:7:2576:G:N1     | 2.35                     | 0.52              |
| 10:A:414:A:OP2   | 10:A:428:G:N2     | 2.43                     | 0.52              |
| 10:A:1238:A:H2'  | 10:A:1239:A:H5''  | 1.91                     | 0.52              |
| 34:Y:8:U:O2'     | 34:Y:21:A:N1      | 2.40                     | 0.52              |
| 10:A:181:A:H61   | 10:A:194:C:H3'    | 1.73                     | 0.52              |
| 15:F:68:GLN:H    | 15:F:68:GLN:CD    | 2.17                     | 0.52              |
| 17:H:87:LYS:HG2  | 17:H:92:LEU:HA    | 1.92                     | 0.52              |
| 39:e:29:PRO:HB2  | 39:e:169:LEU:HD22 | 1.91                     | 0.52              |
| 47:m:74:TYR:HE2  | 47:m:100:VAL:HG12 | 1.74                     | 0.52              |
| 1:0:24:ARG:NH2   | 8:7:2742:G:OP2    | 2.43                     | 0.52              |
| 8:7:910:A:H62    | 42:h:12:MET:HA    | 1.75                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:7:2047:C:O2'    | 8:7:2823:A:N1     | 2.42                     | 0.52              |
| 34:Y:53:G:O2'     | 42:h:51:ARG:NH2   | 2.43                     | 0.52              |
| 38:d:49:ARG:HD2   | 38:d:76:PRO:HD3   | 1.92                     | 0.52              |
| 47:m:34:ARG:HG3   | 47:m:39:LYS:HB2   | 1.91                     | 0.52              |
| 53:s:33:VAL:HG22  | 53:s:38:LYS:HG3   | 1.92                     | 0.52              |
| 10:A:474:G:H2'    | 10:A:475:C:C2     | 2.45                     | 0.52              |
| 10:A:909:A:OP2    | 21:L:18:LYS:NZ    | 2.42                     | 0.52              |
| 10:A:978:A:H61    | 10:A:1316:G:H1'   | 1.75                     | 0.52              |
| 40:f:52:PHE:CE1   | 40:f:69:ARG:HA    | 2.45                     | 0.52              |
| 40:f:116:GLN:NE2  | 40:f:117:LEU:O    | 2.43                     | 0.52              |
| 49:o:81:ASP:HA    | 49:o:84:LYS:HD2   | 1.90                     | 0.52              |
| 63:7:3003:SPD:H82 | 56:v:86:MET:HE1   | 1.92                     | 0.51              |
| 10:A:538:G:H5''   | 21:L:112:GLN:HE22 | 1.74                     | 0.51              |
| 16:G:16:PRO:HA    | 18:I:46:MET:HG3   | 1.91                     | 0.51              |
| 17:H:10:MET:HE1   | 17:H:33:LYS:HA    | 1.90                     | 0.51              |
| 37:c:183:GLU:OE2  | 37:c:184:ARG:HG3  | 2.09                     | 0.51              |
| 47:m:96:ARG:HH11  | 47:m:99:ARG:HH11  | 1.56                     | 0.51              |
| 8:7:1801:A:N6     | 8:7:2201:G:O2'    | 2.43                     | 0.51              |
| 8:7:2677:G:P      | 37:c:126:ASN:HD21 | 2.33                     | 0.51              |
| 35:a:69:THR:HA    | 35:a:176:GLY:HA2  | 1.91                     | 0.51              |
| 36:b:165:VAL:HG21 | 36:b:181:MET:HE1  | 1.92                     | 0.51              |
| 48:n:13:ASN:OD1   | 48:n:98:ARG:N     | 2.44                     | 0.51              |
| 8:7:1006:C:H1'    | 47:m:108:MET:SD   | 2.50                     | 0.51              |
| 8:7:1076:C:O2'    | 45:k:95:LYS:NZ    | 2.35                     | 0.51              |
| 12:C:76:VAL:HA    | 12:C:79:LYS:HD2   | 1.92                     | 0.51              |
| 13:D:188:ARG:HH22 | 13:D:193:ALA:HA   | 1.74                     | 0.51              |
| 40:f:164:TYR:HB2  | 40:f:167:GLU:HB2  | 1.91                     | 0.51              |
| 5:4:28:VAL:HG23   | 5:4:29:GLY:H      | 1.75                     | 0.51              |
| 8:7:570:G:H2'     | 8:7:2030:6MZ:C8   | 2.41                     | 0.51              |
| 8:7:2855:C:H2'    | 8:7:2856:A:C8     | 2.45                     | 0.51              |
| 10:A:150:U:H2'    | 10:A:151:A:C8     | 2.45                     | 0.51              |
| 36:b:107:PRO:HG2  | 36:b:110:LEU:HB2  | 1.92                     | 0.51              |
| 44:j:4:ASN:HB3    | 44:j:7:ASP:HB2    | 1.93                     | 0.51              |
| 47:m:114:LEU:O    | 47:m:118:MET:HG3  | 2.11                     | 0.51              |
| 57:w:59:ASN:O     | 57:w:84:TYR:N     | 2.33                     | 0.51              |
| 8:7:910:A:N3      | 8:7:2264:C:O2'    | 2.39                     | 0.51              |
| 8:7:1032:A:H2     | 8:7:1122:G:H22    | 1.59                     | 0.51              |
| 8:7:1230:A:H2'    | 8:7:1231:U:C6     | 2.46                     | 0.51              |
| 8:7:1296:G:OP1    | 8:7:2709:G:O2'    | 2.22                     | 0.51              |
| 10:A:1107:C:H5'   | 12:C:169:ARG:HH12 | 1.76                     | 0.51              |
| 10:A:1250:A:H2'   | 10:A:1251:A:C8    | 2.46                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:A:1314:C:H2'   | 10:A:1315:U:C6    | 2.45                     | 0.51              |
| 17:H:54:ASP:OD1   | 17:H:55:THR:N     | 2.44                     | 0.51              |
| 34:Y:53:G:H3'     | 34:Y:54:5MU:H5'   | 1.93                     | 0.51              |
| 43:i:4:ILE:HD11   | 43:i:16:GLY:HA2   | 1.92                     | 0.51              |
| 10:A:188:C:H3'    | 10:A:189:A:H8     | 1.76                     | 0.51              |
| 10:A:1308:U:H2'   | 10:A:1309:G:C8    | 2.45                     | 0.51              |
| 10:A:1338:G:H21   | 32:W:41:C:H1'     | 1.76                     | 0.51              |
| 10:A:1413:A:H2    | 10:A:1487:G:H22   | 1.57                     | 0.51              |
| 11:B:111:ILE:HG23 | 11:B:148:LEU:HD21 | 1.91                     | 0.51              |
| 11:B:114:LEU:HD12 | 11:B:144:LEU:HB3  | 1.92                     | 0.51              |
| 10:A:598:U:H4'    | 17:H:86:TYR:CD2   | 2.46                     | 0.51              |
| 14:E:149:SER:OG   | 14:E:152:MET:HE3  | 2.11                     | 0.51              |
| 36:b:145:GLU:OE2  | 36:b:150:LYS:N    | 2.44                     | 0.51              |
| 51:q:79:LEU:HA    | 51:q:83:LEU:HB2   | 1.93                     | 0.51              |
| 2:l:65:ASP:OD1    | 2:l:66:THR:N      | 2.43                     | 0.51              |
| 8:7:2061:G:H5'    | 8:7:2503:2MA:C2   | 2.41                     | 0.51              |
| 11:B:59:LYS:HG2   | 11:B:63:ARG:HH12  | 1.75                     | 0.51              |
| 40:f:30:ASN:ND2   | 40:f:79:VAL:O     | 2.35                     | 0.51              |
| 8:7:1105:U:H2'    | 8:7:1106:G:H8     | 1.76                     | 0.51              |
| 9:8:88:C:H4'      | 9:8:89:U:OP1      | 2.10                     | 0.51              |
| 10:A:1185:G:H2'   | 10:A:1186:G:C8    | 2.46                     | 0.51              |
| 10:A:1287:A:H8    | 10:A:1287:A:H5''  | 1.76                     | 0.51              |
| 11:B:117:LEU:O    | 11:B:118:GLU:C    | 2.53                     | 0.51              |
| 12:C:22:TRP:HB2   | 12:C:59:ARG:HB2   | 1.93                     | 0.51              |
| 44:j:72:LEU:HD23  | 44:j:72:LEU:H     | 1.76                     | 0.51              |
| 59:y:20:LEU:HD21  | 59:y:41:GLU:HB2   | 1.93                     | 0.51              |
| 8:7:1808:A:H3'    | 8:7:1809:A:C8     | 2.46                     | 0.51              |
| 8:7:2512:C:O2'    | 37:c:159:LYS:NZ   | 2.44                     | 0.51              |
| 10:A:999:C:H2'    | 10:A:1000:A:C8    | 2.45                     | 0.51              |
| 23:N:4:GLN:OE1    | 23:N:4:GLN:N      | 2.42                     | 0.51              |
| 23:N:20:TYR:HB2   | 23:N:55:SER:HB2   | 1.93                     | 0.51              |
| 26:Q:82:ALA:O     | 26:Q:83:VAL:HG12  | 2.11                     | 0.51              |
| 39:e:118:SER:HB2  | 39:e:178:ARG:HE   | 1.76                     | 0.51              |
| 8:7:1199:U:H1'    | 54:t:4:VAL:HG12   | 1.92                     | 0.50              |
| 14:E:77:ASN:HB2   | 14:E:82:GLN:HG2   | 1.93                     | 0.50              |
| 19:J:64:GLN:O     | 23:N:99:ALA:N     | 2.35                     | 0.50              |
| 29:T:53:GLU:O     | 29:T:56:PRO:HD2   | 2.12                     | 0.50              |
| 48:n:110:GLU:HA   | 48:n:113:MET:HG2  | 1.91                     | 0.50              |
| 8:7:1856:U:C2'    | 8:7:1857:G:H5'    | 2.41                     | 0.50              |
| 8:7:2165:C:H3'    | 8:7:2166:U:H5''   | 1.93                     | 0.50              |
| 10:A:144:G:H2'    | 10:A:145:G:C8     | 2.47                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:A:154:U:H2'    | 10:A:155:A:H8     | 1.77                     | 0.50              |
| 10:A:739:C:O2'    | 24:O:42:HIS:ND1   | 2.43                     | 0.50              |
| 12:C:79:LYS:HB3   | 12:C:84:VAL:HB    | 1.93                     | 0.50              |
| 28:S:81:ARG:HA    | 28:S:81:ARG:HE    | 1.75                     | 0.50              |
| 39:e:117:LEU:O    | 39:e:178:ARG:N    | 2.33                     | 0.50              |
| 8:7:2140:G:H2'    | 8:7:2141:G:O4'    | 2.11                     | 0.50              |
| 10:A:1323:G:H2'   | 10:A:1324:A:C8    | 2.47                     | 0.50              |
| 8:7:465:G:O2'     | 46:l:21:ARG:NH2   | 2.42                     | 0.50              |
| 8:7:888:C:OP2     | 8:7:888:C:H4'     | 2.12                     | 0.50              |
| 10:A:96:U:H2'     | 10:A:97:G:C8      | 2.47                     | 0.50              |
| 10:A:486:U:H2'    | 10:A:487:A:C8     | 2.46                     | 0.50              |
| 24:O:36:ILE:HD11  | 24:O:59:MET:HG3   | 1.94                     | 0.50              |
| 35:a:46:VAL:HG22  | 35:a:212:VAL:HG13 | 1.94                     | 0.50              |
| 5:4:25:ARG:HD3    | 39:e:98:GLU:OE2   | 2.12                     | 0.50              |
| 8:7:2305:U:H5''   | 39:e:131:GLY:HA3  | 1.93                     | 0.50              |
| 16:G:72:THR:HG22  | 16:G:142:HIS:NE2  | 2.26                     | 0.50              |
| 21:L:63:VAL:HG21  | 21:L:95:TYR:HE2   | 1.77                     | 0.50              |
| 50:p:31:VAL:HG12  | 50:p:33:ASN:H     | 1.75                     | 0.50              |
| 10:A:402:G:O5'    | 13:D:71:GLN:NE2   | 2.45                     | 0.50              |
| 10:A:1115:U:O2    | 10:A:1185:G:N2    | 2.40                     | 0.50              |
| 11:B:187:VAL:HG23 | 11:B:201:PRO:HA   | 1.93                     | 0.50              |
| 29:T:82:GLN:HA    | 29:T:85:LYS:HE3   | 1.93                     | 0.50              |
| 44:j:28:ALA:HB3   | 44:j:81:LEU:HD23  | 1.93                     | 0.50              |
| 8:7:807:U:O2'     | 8:7:2060:A:N1     | 2.45                     | 0.50              |
| 10:A:197:A:H4'    | 10:A:198:G:O5'    | 2.12                     | 0.50              |
| 10:A:1245:C:H2'   | 10:A:1246:A:H8    | 1.76                     | 0.50              |
| 20:K:116:ILE:HD11 | 30:U:31:GLU:HG3   | 1.93                     | 0.50              |
| 33:X:35:I:H5''    | 33:X:35:I:C8      | 2.46                     | 0.50              |
| 43:i:71:LYS:HB3   | 43:i:108:VAL:HG22 | 1.94                     | 0.50              |
| 54:t:9:ILE:HG13   | 54:t:10:ALA:H     | 1.76                     | 0.50              |
| 10:A:254:G:H2'    | 10:A:255:G:H8     | 1.77                     | 0.50              |
| 10:A:1371:G:H2'   | 10:A:1372:U:C6    | 2.46                     | 0.50              |
| 29:T:10:ARG:HA    | 29:T:13:GLN:NE2   | 2.27                     | 0.50              |
| 52:r:69:ASP:OD1   | 52:r:70:ALA:N     | 2.44                     | 0.50              |
| 8:7:717:C:H2'     | 8:7:718:A:O4'     | 2.12                     | 0.50              |
| 8:7:2898:U:O2'    | 47:m:136:GLN:NE2  | 2.23                     | 0.50              |
| 10:A:88:U:O2'     | 10:A:89:U:O5'     | 2.28                     | 0.50              |
| 10:A:519:C:H3'    | 10:A:520:A:H8     | 1.76                     | 0.50              |
| 10:A:923:A:OP1    | 14:E:26:LYS:NZ    | 2.34                     | 0.50              |
| 10:A:972:C:OP2    | 19:J:59:LYS:NZ    | 2.43                     | 0.50              |
| 10:A:1344:C:H4'   | 18:I:122:ARG:HB2  | 1.93                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:B:169:GLU:OE1  | 11:B:169:GLU:N    | 2.45                     | 0.50              |
| 28:S:32:ARG:HH21  | 28:S:57:HIS:CE1   | 2.30                     | 0.50              |
| 33:X:38:2MA:H3'   | 33:X:39:A:H8      | 1.77                     | 0.50              |
| 47:m:99:ARG:O     | 47:m:100:VAL:C    | 2.55                     | 0.50              |
| 12:C:82:GLU:HG2   | 12:C:85:GLU:HB3   | 1.94                     | 0.49              |
| 12:C:121:THR:HG22 | 12:C:189:ALA:HB2  | 1.94                     | 0.49              |
| 12:C:131:ARG:HH12 | 31:V:32:C:H5''    | 1.77                     | 0.49              |
| 39:e:103:LEU:O    | 39:e:108:VAL:HG23 | 2.12                     | 0.49              |
| 4:3:15:GLY:O      | 8:7:969:G:H4'     | 2.12                     | 0.49              |
| 8:7:1060:U:OP1    | 45:k:76:ALA:N     | 2.45                     | 0.49              |
| 8:7:2109:U:H2'    | 8:7:2110:G:C8     | 2.47                     | 0.49              |
| 10:A:459:A:H2'    | 10:A:460:A:O4'    | 2.12                     | 0.49              |
| 10:A:1188:A:O3'   | 23:N:98:LYS:HE2   | 2.11                     | 0.49              |
| 10:A:1328:C:OP1   | 22:M:28:THR:HG21  | 2.12                     | 0.49              |
| 29:T:27:MET:HE2   | 29:T:27:MET:HA    | 1.92                     | 0.49              |
| 8:7:998:C:OP1     | 54:t:92:ARG:NH2   | 2.44                     | 0.49              |
| 8:7:2162:G:H2'    | 8:7:2162:G:N3     | 2.27                     | 0.49              |
| 10:A:552:U:H2'    | 10:A:553:A:H8     | 1.77                     | 0.49              |
| 10:A:1142:G:H3'   | 10:A:1143:G:C8    | 2.42                     | 0.49              |
| 12:C:7:PRO:HG3    | 12:C:201:TRP:HE1  | 1.77                     | 0.49              |
| 12:C:70:THR:O     | 12:C:106:VAL:N    | 2.42                     | 0.49              |
| 13:D:50:ASP:OD1   | 13:D:51:TYR:N     | 2.45                     | 0.49              |
| 32:W:37:MIA:N1    | 32:W:37:MIA:H131  | 2.27                     | 0.49              |
| 38:d:126:VAL:HG23 | 38:d:156:ASN:HB3  | 1.94                     | 0.49              |
| 8:7:2258:C:O2'    | 8:7:2427:C:OP2    | 2.23                     | 0.49              |
| 9:8:98:G:N1       | 59:y:14:LYS:HB2   | 2.27                     | 0.49              |
| 10:A:452:A:H61    | 10:A:480:U:H3     | 1.60                     | 0.49              |
| 10:A:595:A:N6     | 10:A:641:U:O2'    | 2.45                     | 0.49              |
| 12:C:56:VAL:HB    | 12:C:67:THR:HB    | 1.94                     | 0.49              |
| 6:5:13:ARG:NH1    | 8:7:1263:U:OP1    | 2.46                     | 0.49              |
| 8:7:1:G:H2'       | 8:7:2:G:H8        | 1.77                     | 0.49              |
| 8:7:2267:A:H5''   | 8:7:2268:A:H5'    | 1.95                     | 0.49              |
| 10:A:173:U:H5''   | 10:A:197:A:O4'    | 2.12                     | 0.49              |
| 10:A:377:G:H2'    | 10:A:378:G:H8     | 1.77                     | 0.49              |
| 10:A:559:A:H4'    | 10:A:560:A:H3'    | 1.93                     | 0.49              |
| 10:A:655:A:H2'    | 10:A:656:G:H8     | 1.78                     | 0.49              |
| 10:A:1412:C:H2'   | 10:A:1413:A:C8    | 2.47                     | 0.49              |
| 13:D:60:LYS:O     | 13:D:64:ILE:HD12  | 2.12                     | 0.49              |
| 14:E:136:VAL:O    | 14:E:140:THR:HG23 | 2.12                     | 0.49              |
| 8:7:1056:G:H4'    | 8:7:1086:A:H8     | 1.77                     | 0.49              |
| 10:A:400:C:H2'    | 10:A:401:C:O4'    | 2.13                     | 0.49              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 10:A:497:G:N2     | 10:A:498:A:N1    | 2.60                     | 0.49              |
| 12:C:164:ARG:HD3  | 31:V:30:A:O2'    | 2.13                     | 0.49              |
| 16:G:76:LYS:HB2   | 16:G:89:VAL:HG11 | 1.95                     | 0.49              |
| 25:P:71:VAL:O     | 25:P:75:ILE:HG13 | 2.12                     | 0.49              |
| 42:h:38:ARG:HB3   | 42:h:98:PRO:HD3  | 1.93                     | 0.49              |
| 8:7:276:U:H2'     | 8:7:277:G:C2     | 2.48                     | 0.49              |
| 8:7:1085:A:H61    | 44:j:35:VAL:HB   | 1.78                     | 0.49              |
| 8:7:1278:C:H2'    | 8:7:1279:G:H8    | 1.76                     | 0.49              |
| 10:A:946:A:H2'    | 10:A:947:G:C8    | 2.47                     | 0.49              |
| 40:f:9:VAL:HG22   | 40:f:69:ARG:HE   | 1.78                     | 0.49              |
| 43:i:130:VAL:HG12 | 43:i:131:SER:H   | 1.76                     | 0.49              |
| 8:7:1490:A:O2'    | 8:7:1491:G:OP1   | 2.25                     | 0.49              |
| 8:7:2514:U:H2'    | 8:7:2515:C:C6    | 2.48                     | 0.49              |
| 10:A:263:A:OP2    | 29:T:74:ARG:NH1  | 2.46                     | 0.49              |
| 10:A:431:A:H2'    | 10:A:432:A:C8    | 2.47                     | 0.49              |
| 10:A:694:A:O2'    | 33:X:39:A:O3'    | 2.31                     | 0.49              |
| 34:Y:63:G:O2'     | 34:Y:64:C:OP1    | 2.28                     | 0.49              |
| 48:n:25:LEU:HD12  | 48:n:26:GLY:H    | 1.78                     | 0.49              |
| 8:7:355:U:H2'     | 8:7:356:G:H8     | 1.78                     | 0.49              |
| 8:7:1315:C:O2'    | 8:7:1392:A:N3    | 2.39                     | 0.49              |
| 10:A:263:A:H2'    | 10:A:264:C:C6    | 2.47                     | 0.49              |
| 10:A:1203:C:OP1   | 23:N:2:ALA:N     | 2.46                     | 0.49              |
| 10:A:1228:C:H2'   | 10:A:1229:A:C8   | 2.47                     | 0.49              |
| 10:A:1251:A:H2'   | 10:A:1252:A:C8   | 2.47                     | 0.49              |
| 11:B:173:ILE:O    | 11:B:177:ASN:ND2 | 2.46                     | 0.49              |
| 15:F:26:THR:HG23  | 15:F:36:ILE:HG13 | 1.94                     | 0.49              |
| 17:H:18:GLN:HE21  | 17:H:72:VAL:H    | 1.59                     | 0.49              |
| 35:a:194:VAL:HA   | 35:a:197:LYS:HD2 | 1.95                     | 0.49              |
| 37:c:129:THR:OG1  | 37:c:140:HIS:O   | 2.31                     | 0.49              |
| 8:7:1915:3TD:H6   | 8:7:1915:3TD:O5' | 2.12                     | 0.49              |
| 8:7:2859:G:O5'    | 8:7:2859:G:H8    | 1.96                     | 0.49              |
| 9:8:42:C:C5       | 39:e:66:LEU:HD22 | 2.48                     | 0.49              |
| 10:A:236:A:H2'    | 10:A:237:G:C8    | 2.48                     | 0.49              |
| 10:A:655:A:H2'    | 10:A:656:G:C8    | 2.48                     | 0.49              |
| 10:A:1149:C:H2'   | 10:A:1150:A:C8   | 2.48                     | 0.49              |
| 16:G:27:VAL:HG12  | 16:G:43:VAL:HG21 | 1.95                     | 0.49              |
| 23:N:13:ARG:NH1   | 23:N:54:ASP:OD2  | 2.46                     | 0.49              |
| 24:O:3:LEU:HB2    | 24:O:35:GLN:OE1  | 2.13                     | 0.49              |
| 51:q:2:ARG:O      | 51:q:3:HIS:C     | 2.56                     | 0.49              |
| 52:r:29:HIS:HB3   | 52:r:36:TYR:HB2  | 1.95                     | 0.49              |
| 8:7:160:A:N3      | 8:7:2208:C:O2'   | 2.40                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:7:1754:A:N1     | 8:7:2716:C:O2'    | 2.40                     | 0.48              |
| 8:7:1837:C:O2'    | 8:7:1927:A:N3     | 2.40                     | 0.48              |
| 17:H:76:GLN:NE2   | 17:H:77:ARG:O     | 2.46                     | 0.48              |
| 20:K:74:VAL:HG23  | 20:K:75:LYS:H     | 1.78                     | 0.48              |
| 8:7:1380:G:N2     | 8:7:1570:A:N1     | 2.59                     | 0.48              |
| 10:A:231:U:H2'    | 10:A:232:G:H8     | 1.78                     | 0.48              |
| 10:A:299:G:H2'    | 10:A:300:A:C8     | 2.48                     | 0.48              |
| 10:A:1124:G:N2    | 10:A:1125:U:O4    | 2.46                     | 0.48              |
| 22:M:83:LEU:HG    | 28:S:74:PHE:HE1   | 1.78                     | 0.48              |
| 26:Q:46:VAL:HG11  | 26:Q:61:ILE:HD12  | 1.95                     | 0.48              |
| 27:R:34:THR:HG22  | 27:R:38:LYS:H     | 1.78                     | 0.48              |
| 33:X:18:G:H1'     | 33:X:62:C:H5'     | 1.96                     | 0.48              |
| 39:e:108:VAL:HG11 | 39:e:176:PRO:HG3  | 1.94                     | 0.48              |
| 48:n:105:ARG:NH2  | 53:s:33:VAL:O     | 2.42                     | 0.48              |
| 54:t:27:ALA:O     | 54:t:31:VAL:HG12  | 2.12                     | 0.48              |
| 3:2:42:LEU:O      | 3:2:46:VAL:HG12   | 2.14                     | 0.48              |
| 8:7:158:U:O2'     | 8:7:159:G:OP1     | 2.29                     | 0.48              |
| 8:7:1141:U:H5''   | 47:m:27:ARG:NH2   | 2.29                     | 0.48              |
| 8:7:2039:U:H2'    | 8:7:2040:G:C8     | 2.48                     | 0.48              |
| 8:7:2581:G:H1     | 8:7:2610:C:HO2'   | 1.61                     | 0.48              |
| 10:A:136:C:O2'    | 25:P:64:GLY:O     | 2.30                     | 0.48              |
| 10:A:360:G:O2'    | 10:A:361:G:H5'    | 2.13                     | 0.48              |
| 10:A:523:A:C2     | 21:L:88:LYS:HB3   | 2.48                     | 0.48              |
| 10:A:993:G:H2'    | 10:A:995:C:H41    | 1.77                     | 0.48              |
| 10:A:1086:U:H3    | 10:A:1099:G:H22   | 1.59                     | 0.48              |
| 10:A:1193:G:O6    | 12:C:2:GLY:N      | 2.46                     | 0.48              |
| 10:A:1328:C:H2'   | 10:A:1329:A:C8    | 2.48                     | 0.48              |
| 11:B:107:VAL:O    | 11:B:111:ILE:HG13 | 2.12                     | 0.48              |
| 11:B:119:THR:OG1  | 11:B:120:GLN:N    | 2.45                     | 0.48              |
| 15:F:66:ALA:HB3   | 15:F:71:ILE:HD11  | 1.95                     | 0.48              |
| 19:J:37:ARG:HB2   | 19:J:75:ASP:HB2   | 1.96                     | 0.48              |
| 22:M:72:GLU:O     | 22:M:75:MET:HG2   | 2.12                     | 0.48              |
| 8:7:1058:U:O2'    | 45:k:117:MET:SD   | 2.69                     | 0.48              |
| 12:C:116:VAL:HG21 | 12:C:200:VAL:HG11 | 1.95                     | 0.48              |
| 48:n:44:LYS:HB2   | 48:n:45:GLU:OE1   | 2.13                     | 0.48              |
| 48:n:115:ILE:H    | 48:n:115:ILE:HD12 | 1.78                     | 0.48              |
| 8:7:571:U:O2      | 8:7:2030:6MZ:O2'  | 2.27                     | 0.48              |
| 10:A:1:A:N3       | 10:A:1:A:H2'      | 2.28                     | 0.48              |
| 10:A:1222:G:OP2   | 10:A:1322:C:N4    | 2.37                     | 0.48              |
| 12:C:19:ASN:HB2   | 23:N:91:GLY:HA3   | 1.96                     | 0.48              |
| 18:I:87:LEU:HB3   | 18:I:94:LEU:HD12  | 1.95                     | 0.48              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 31:V:30:A:N3     | 31:V:30:A:H2'     | 2.29                     | 0.48              |
| 4:3:4:THR:OG1    | 4:3:37:GLU:OE2    | 2.23                     | 0.48              |
| 8:7:192:C:O2'    | 8:7:802:A:N3      | 2.43                     | 0.48              |
| 8:7:372:G:O2'    | 8:7:400:G:O6      | 2.25                     | 0.48              |
| 8:7:782:A:C2     | 36:b:225:MET:HG2  | 2.48                     | 0.48              |
| 8:7:1071:G:N3    | 8:7:1089:A:O2'    | 2.42                     | 0.48              |
| 8:7:1141:U:H4'   | 8:7:1142:A:O4'    | 2.13                     | 0.48              |
| 10:A:200:G:H2'   | 10:A:201:G:H8     | 1.78                     | 0.48              |
| 10:A:1244:G:H2'  | 10:A:1245:C:C6    | 2.49                     | 0.48              |
| 16:G:88:PRO:HG2  | 16:G:149:LYS:HA   | 1.96                     | 0.48              |
| 16:G:146:GLU:HA  | 16:G:149:LYS:HE3  | 1.94                     | 0.48              |
| 39:e:49:LEU:HA   | 39:e:52:ASN:HD21  | 1.79                     | 0.48              |
| 8:7:672:C:H5     | 49:o:42:SER:HB3   | 1.79                     | 0.48              |
| 8:7:2102:G:C2    | 8:7:2103:C:H1'    | 2.49                     | 0.48              |
| 9:8:27:C:OP1     | 52:r:34:HIS:NE2   | 2.36                     | 0.48              |
| 10:A:421:U:C3'   | 10:A:422:C:H5'    | 2.43                     | 0.48              |
| 10:A:459:A:C6    | 10:A:474:G:H1'    | 2.48                     | 0.48              |
| 10:A:1144:G:N2   | 10:A:1146:A:H62   | 2.11                     | 0.48              |
| 11:B:24:ASN:ND2  | 11:B:192:ASP:HB3  | 2.28                     | 0.48              |
| 11:B:114:LEU:O   | 11:B:118:GLU:HG2  | 2.12                     | 0.48              |
| 8:7:1167:C:H2'   | 8:7:1168:G:H8     | 1.78                     | 0.48              |
| 8:7:1329:U:H5''  | 8:7:1330:C:H5     | 1.79                     | 0.48              |
| 10:A:214:C:H2'   | 10:A:215:C:H6     | 1.79                     | 0.48              |
| 10:A:493:A:H2'   | 10:A:494:G:O4'    | 2.14                     | 0.48              |
| 10:A:552:U:H2'   | 10:A:553:A:C8     | 2.48                     | 0.48              |
| 10:A:1292:G:H2'  | 10:A:1293:C:C6    | 2.47                     | 0.48              |
| 36:b:78:VAL:HG21 | 36:b:110:LEU:HD11 | 1.96                     | 0.48              |
| 59:y:45:ASP:N    | 59:y:45:ASP:OD1   | 2.42                     | 0.48              |
| 8:7:558:U:OP1    | 47:m:113:PRO:HD2  | 2.14                     | 0.48              |
| 8:7:2144:G:C2    | 8:7:2146:C:H1'    | 2.49                     | 0.48              |
| 8:7:2251:OMG:OP2 | 42:h:81:ARG:NH1   | 2.47                     | 0.48              |
| 10:A:453:G:H2'   | 10:A:454:G:C8     | 2.49                     | 0.48              |
| 36:b:13:ARG:O    | 36:b:16:VAL:HG22  | 2.14                     | 0.48              |
| 36:b:172:VAL:O   | 36:b:183:LYS:HA   | 2.13                     | 0.48              |
| 38:d:21:ARG:HD3  | 38:d:106:LYS:HB3  | 1.96                     | 0.48              |
| 44:j:46:ARG:NE   | 45:k:121:ASP:OD1  | 2.43                     | 0.48              |
| 6:5:38:HIS:HE1   | 8:7:2884:U:O4     | 1.97                     | 0.48              |
| 8:7:784:G:H5'    | 8:7:785:G:OP1     | 2.14                     | 0.48              |
| 8:7:1130:U:O2'   | 8:7:1131:G:P      | 2.71                     | 0.48              |
| 10:A:21:G:H2'    | 10:A:22:G:C8      | 2.49                     | 0.48              |
| 10:A:109:A:H2'   | 10:A:326:G:H21    | 1.79                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:B:138:THR:O    | 11:B:142:GLU:HG3  | 2.14                     | 0.48              |
| 33:X:20:A:C6      | 33:X:58:G:H1'     | 2.49                     | 0.48              |
| 36:b:91:ILE:HD12  | 36:b:103:TYR:CD1  | 2.49                     | 0.48              |
| 37:c:156:PHE:CD2  | 47:m:81:ILE:HG13  | 2.43                     | 0.48              |
| 49:o:91:ASP:N     | 49:o:91:ASP:OD1   | 2.47                     | 0.48              |
| 8:7:1094:U:O2'    | 8:7:1096:A:N7     | 2.40                     | 0.47              |
| 8:7:2105:U:H2'    | 8:7:2106:U:C6     | 2.49                     | 0.47              |
| 8:7:2839:G:O2'    | 51:q:49:GLU:OE1   | 2.22                     | 0.47              |
| 15:F:80:PHE:CG    | 36:b:124:ILE:HD11 | 2.49                     | 0.47              |
| 36:b:135:ILE:HD12 | 36:b:192:LEU:HD21 | 1.95                     | 0.47              |
| 42:h:29:GLY:HA2   | 42:h:106:ASP:OD2  | 2.14                     | 0.47              |
| 51:q:35:LYS:HG2   | 51:q:112:TYR:CE1  | 2.49                     | 0.47              |
| 53:s:90:GLY:O     | 53:s:113:ARG:NH1  | 2.39                     | 0.47              |
| 8:7:2562:U:H1'    | 48:n:23:LYS:NZ    | 2.29                     | 0.47              |
| 10:A:377:G:H2'    | 10:A:378:G:C8     | 2.49                     | 0.47              |
| 10:A:454:G:N1     | 10:A:478:A:H2     | 2.10                     | 0.47              |
| 13:D:9:LEU:HD21   | 13:D:22:LYS:HG2   | 1.96                     | 0.47              |
| 27:R:35:GLU:H     | 27:R:35:GLU:CD    | 2.22                     | 0.47              |
| 8:7:1417:C:H42    | 8:7:1581:G:H1     | 1.62                     | 0.47              |
| 8:7:2449:H2U:H4'  | 8:7:2450:A:OP1    | 2.15                     | 0.47              |
| 8:7:2646:C:OP2    | 8:7:2732:G:O2'    | 2.28                     | 0.47              |
| 10:A:691:G:O6     | 20:K:57:LYS:NZ    | 2.37                     | 0.47              |
| 10:A:1175:G:H2'   | 10:A:1176:A:H8    | 1.80                     | 0.47              |
| 12:C:29:PHE:CE1   | 12:C:33:LEU:HD21  | 2.49                     | 0.47              |
| 21:L:25:GLU:OE1   | 21:L:59:ASN:ND2   | 2.47                     | 0.47              |
| 21:L:75:GLN:NE2   | 21:L:76:GLU:O     | 2.47                     | 0.47              |
| 27:R:55:LEU:O     | 27:R:59:ILE:HG12  | 2.15                     | 0.47              |
| 32:W:23:A:H2'     | 32:W:24:G:H8      | 1.79                     | 0.47              |
| 38:d:191:ASP:OD1  | 38:d:191:ASP:N    | 2.47                     | 0.47              |
| 10:A:1011:C:H2'   | 10:A:1012:A:H8    | 1.78                     | 0.47              |
| 10:A:1057:G:H2'   | 10:A:1058:G:O4'   | 2.14                     | 0.47              |
| 10:A:1095:U:P     | 10:A:1108:G:H1    | 2.37                     | 0.47              |
| 19:J:8:ILE:HB     | 19:J:74:VAL:HG23  | 1.95                     | 0.47              |
| 21:L:54:ARG:HH11  | 21:L:64:THR:HB    | 1.79                     | 0.47              |
| 35:a:181:ASP:H    | 35:a:184:LYS:HE2  | 1.79                     | 0.47              |
| 37:c:150:GLN:HG2  | 37:c:150:GLN:O    | 2.14                     | 0.47              |
| 8:7:747:5MU:H72   | 8:7:2612:C:H4'    | 1.97                     | 0.47              |
| 8:7:1394:U:H4'    | 8:7:1603:A:H4'    | 1.95                     | 0.47              |
| 8:7:1992:G:N2     | 8:7:1996:C:O2'    | 2.47                     | 0.47              |
| 8:7:2175:C:H2'    | 8:7:2176:A:C8     | 2.49                     | 0.47              |
| 10:A:666:G:H5'    | 10:A:726:C:H1'    | 1.96                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:A:1177:G:OP2   | 18:I:95:ARG:NH2   | 2.47                     | 0.47              |
| 10:A:1242:G:H1    | 10:A:1295:U:H3    | 1.63                     | 0.47              |
| 11:B:24:ASN:ND2   | 11:B:191:SER:O    | 2.33                     | 0.47              |
| 43:i:3:VAL:HG12   | 43:i:38:PRO:HA    | 1.97                     | 0.47              |
| 8:7:1140:C:H5'    | 47:m:26:GLY:HA3   | 1.97                     | 0.47              |
| 8:7:1580:A:HO2'   | 8:7:1581:G:P      | 2.37                     | 0.47              |
| 8:7:2186:G:H2'    | 8:7:2187:U:O4'    | 2.14                     | 0.47              |
| 10:A:206:C:OP2    | 10:A:207:C:N4     | 2.47                     | 0.47              |
| 10:A:1060:U:OP1   | 23:N:85:ARG:NH2   | 2.44                     | 0.47              |
| 10:A:1349:A:H5''  | 18:I:123:ARG:HG2  | 1.97                     | 0.47              |
| 15:F:4:TYR:CD2    | 15:F:71:ILE:HG13  | 2.50                     | 0.47              |
| 17:H:89:LYS:O     | 17:H:92:LEU:HD22  | 2.14                     | 0.47              |
| 36:b:258:ARG:HH12 | 36:b:264:ASP:HB3  | 1.78                     | 0.47              |
| 5:4:63:ARG:NH2    | 10:A:1312:G:OP2   | 2.48                     | 0.47              |
| 8:7:278:A:OP2     | 8:7:361:G:N1      | 2.48                     | 0.47              |
| 8:7:1710:G:H4'    | 8:7:2858:C:O2     | 2.14                     | 0.47              |
| 8:7:1909:C:H2'    | 8:7:1910:G:H8     | 1.80                     | 0.47              |
| 8:7:1931:U:H2'    | 8:7:1932:A:C8     | 2.50                     | 0.47              |
| 8:7:2135:A:C5     | 8:7:2136:G:H1'    | 2.50                     | 0.47              |
| 8:7:2149:U:H2'    | 8:7:2150:C:C6     | 2.49                     | 0.47              |
| 8:7:2780:G:P      | 47:m:120:ARG:HE   | 2.37                     | 0.47              |
| 9:8:29:A:O2'      | 9:8:58:A:N1       | 2.43                     | 0.47              |
| 10:A:203:G:O2'    | 10:A:465:A:N1     | 2.48                     | 0.47              |
| 10:A:205:A:H2'    | 10:A:206:C:O4'    | 2.14                     | 0.47              |
| 10:A:421:U:O2'    | 10:A:422:C:H5'    | 2.15                     | 0.47              |
| 13:D:101:VAL:HG21 | 13:D:137:VAL:HG21 | 1.97                     | 0.47              |
| 24:O:14:GLU:HB2   | 24:O:84:ARG:HH22  | 1.79                     | 0.47              |
| 24:O:21:ASP:OD1   | 24:O:24:SER:HB3   | 2.15                     | 0.47              |
| 31:V:19:G:O5'     | 31:V:19:G:H8      | 1.97                     | 0.47              |
| 33:X:19:G:N2      | 33:X:59:A:OP2     | 2.48                     | 0.47              |
| 40:f:80:THR:OG1   | 40:f:81:GLU:OE1   | 2.29                     | 0.47              |
| 54:t:17:ILE:HG23  | 54:t:39:VAL:HG21  | 1.97                     | 0.47              |
| 8:7:301:G:OP2     | 58:x:82:ARG:NH2   | 2.44                     | 0.47              |
| 8:7:1416:G:HO2'   | 8:7:1417:C:P      | 2.36                     | 0.47              |
| 8:7:2059:A:H2'    | 8:7:2503:2MA:HM22 | 1.97                     | 0.47              |
| 8:7:2144:G:O5'    | 8:7:2144:G:H8     | 1.97                     | 0.47              |
| 10:A:372:C:H4'    | 10:A:373:A:OP1    | 2.14                     | 0.47              |
| 17:H:10:MET:HA    | 17:H:27:MET:HE1   | 1.95                     | 0.47              |
| 17:H:103:VAL:HG12 | 17:H:126:ILE:HD13 | 1.96                     | 0.47              |
| 18:I:63:LEU:HB3   | 18:I:65:ILE:HD11  | 1.96                     | 0.47              |
| 26:Q:59:VAL:HG12  | 26:Q:78:VAL:HG22  | 1.97                     | 0.47              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 48:n:61:VAL:HG12 | 48:n:87:LEU:HD11  | 1.96                     | 0.47              |
| 54:t:65:ILE:HD11 | 54:t:79:PHE:HE2   | 1.80                     | 0.47              |
| 59:y:6:ALA:HB2   | 59:y:63:ILE:HD11  | 1.95                     | 0.47              |
| 5:4:60:PHE:HE1   | 5:4:66:ILE:HG21   | 1.80                     | 0.47              |
| 8:7:83:A:O2'     | 8:7:103:A:N6      | 2.48                     | 0.47              |
| 8:7:2153:C:H2'   | 8:7:2154:A:C8     | 2.49                     | 0.47              |
| 10:A:56:U:H2'    | 10:A:57:G:H8      | 1.79                     | 0.47              |
| 10:A:986:U:H2'   | 10:A:987:G:C8     | 2.50                     | 0.47              |
| 10:A:1166:G:O2'  | 10:A:1169:A:N6    | 2.44                     | 0.47              |
| 19:J:97:ASP:OD1  | 19:J:98:VAL:N     | 2.47                     | 0.47              |
| 49:o:33:ARG:NE   | 49:o:39:LYS:O     | 2.40                     | 0.47              |
| 51:q:102:PHE:HD1 | 51:q:109:PRO:HA   | 1.80                     | 0.47              |
| 55:u:27:ILE:O    | 55:u:66:HIS:NE2   | 2.48                     | 0.47              |
| 1:0:19:ARG:HB3   | 1:0:20:ASP:H      | 1.59                     | 0.47              |
| 2:1:3:ARG:O      | 2:1:12:PRO:HD3    | 2.15                     | 0.47              |
| 8:7:962:G:H5'    | 8:7:962:G:H8      | 1.80                     | 0.47              |
| 10:A:161:A:H2'   | 10:A:162:A:C8     | 2.50                     | 0.47              |
| 10:A:188:C:H3'   | 10:A:189:A:C8     | 2.50                     | 0.47              |
| 10:A:345:C:H5''  | 53:s:39:ARG:HH11  | 1.79                     | 0.47              |
| 13:D:59:GLN:O    | 13:D:63:ARG:NE    | 2.47                     | 0.47              |
| 16:G:72:THR:O    | 16:G:91:VAL:HG22  | 2.15                     | 0.47              |
| 8:7:87:U:H5'     | 8:7:88:G:H5''     | 1.97                     | 0.46              |
| 8:7:1820:U:C2    | 36:b:201:MET:SD   | 3.08                     | 0.46              |
| 10:A:54:C:H2'    | 10:A:352:C:H41    | 1.79                     | 0.46              |
| 10:A:768:A:N3    | 10:A:1512:U:O2'   | 2.45                     | 0.46              |
| 11:B:223:GLU:O   | 11:B:227:GLN:HG2  | 2.15                     | 0.46              |
| 12:C:123:GLN:HB3 | 12:C:128:VAL:HB   | 1.97                     | 0.46              |
| 15:F:56:LYS:HE3  | 15:F:56:LYS:HB3   | 1.80                     | 0.46              |
| 19:J:88:MET:HE1  | 19:J:100:ILE:HD13 | 1.97                     | 0.46              |
| 51:q:87:PHE:HE2  | 51:q:115:LEU:HD23 | 1.80                     | 0.46              |
| 52:r:8:ILE:O     | 52:r:12:THR:OG1   | 2.28                     | 0.46              |
| 8:7:851:C:H2'    | 8:7:852:U:C6      | 2.50                     | 0.46              |
| 10:A:151:A:H2'   | 10:A:152:A:H8     | 1.80                     | 0.46              |
| 10:A:1363:A:O2'  | 10:A:1365:G:N7    | 2.42                     | 0.46              |
| 13:D:99:ASP:OD1  | 13:D:100:ASN:N    | 2.49                     | 0.46              |
| 32:W:10:G:HO2'   | 32:W:11:U:P       | 2.37                     | 0.46              |
| 54:t:49:ASP:O    | 54:t:53:ARG:N     | 2.46                     | 0.46              |
| 8:7:969:G:H2'    | 8:7:970:U:C6      | 2.49                     | 0.46              |
| 8:7:2262:U:OP2   | 60:z:16:SER:OG    | 2.28                     | 0.46              |
| 10:A:537:G:HO2'  | 10:A:538:G:P      | 2.38                     | 0.46              |
| 10:A:1078:U:H4'  | 14:E:138:ARG:NH1  | 2.30                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:A:1312:G:H2'   | 10:A:1313:U:C6    | 2.51                     | 0.46              |
| 20:K:64:GLN:HG3   | 20:K:99:ALA:HB2   | 1.97                     | 0.46              |
| 22:M:44:LYS:HB2   | 22:M:47:GLU:OE1   | 2.14                     | 0.46              |
| 25:P:8:ARG:HG3    | 25:P:17:TYR:CE1   | 2.50                     | 0.46              |
| 27:R:57:ARG:HD3   | 27:R:61:ARG:HH22  | 1.80                     | 0.46              |
| 39:e:64:LYS:HG2   | 39:e:65:PRO:HD2   | 1.97                     | 0.46              |
| 42:h:21:ALA:HB2   | 42:h:97:GLN:HB2   | 1.97                     | 0.46              |
| 42:h:41:LEU:HD23  | 42:h:41:LEU:HA    | 1.73                     | 0.46              |
| 8:7:79:C:O2'      | 8:7:346:A:N3      | 2.39                     | 0.46              |
| 8:7:593:U:H2'     | 8:7:594:U:C6      | 2.51                     | 0.46              |
| 8:7:2554:U:H2'    | 8:7:2555:U:H6     | 1.77                     | 0.46              |
| 10:A:765:G:N1     | 10:A:812:G:O2'    | 2.39                     | 0.46              |
| 16:G:26:PHE:HE2   | 16:G:120:LEU:HD21 | 1.81                     | 0.46              |
| 31:V:16:C:H5''    | 31:V:17:G:C8      | 2.50                     | 0.46              |
| 8:7:1432:G:H2'    | 8:7:1433:A:C8     | 2.51                     | 0.46              |
| 8:7:2531:A:H61    | 8:7:2662:A:H61    | 1.62                     | 0.46              |
| 10:A:335:C:O2'    | 10:A:1433:A:N3    | 2.42                     | 0.46              |
| 10:A:369:G:H2'    | 10:A:370:C:C6     | 2.50                     | 0.46              |
| 10:A:1328:C:H2'   | 10:A:1329:A:H8    | 1.80                     | 0.46              |
| 11:B:60:ILE:O     | 11:B:63:ARG:HG2   | 2.16                     | 0.46              |
| 28:S:28:LYS:HA    | 28:S:28:LYS:HE3   | 1.98                     | 0.46              |
| 32:W:36:A:H2'     | 32:W:37:MIA:O4'   | 2.14                     | 0.46              |
| 55:u:98:ILE:H     | 55:u:98:ILE:HD12  | 1.80                     | 0.46              |
| 8:7:1789:A:OP1    | 36:b:221:ARG:HG3  | 2.16                     | 0.46              |
| 8:7:1847:A:HO2'   | 8:7:1848:A:P      | 2.38                     | 0.46              |
| 8:7:1909:C:H2'    | 8:7:1910:G:C8     | 2.51                     | 0.46              |
| 10:A:80:A:H2'     | 10:A:81:A:O4'     | 2.15                     | 0.46              |
| 10:A:309:A:H2'    | 10:A:310:G:H8     | 1.80                     | 0.46              |
| 10:A:448:A:H3'    | 10:A:449:G:H8     | 1.81                     | 0.46              |
| 10:A:953:G:H2'    | 10:A:954:G:O4'    | 2.15                     | 0.46              |
| 11:B:122:GLN:O    | 11:B:126:PHE:HD1  | 1.98                     | 0.46              |
| 12:C:150:LYS:HB3  | 12:C:201:TRP:HB2  | 1.98                     | 0.46              |
| 14:E:31:PHE:H     | 31:V:30:A:N6      | 2.14                     | 0.46              |
| 36:b:120:VAL:HG12 | 36:b:131:PRO:HG2  | 1.96                     | 0.46              |
| 38:d:192:ALA:HA   | 38:d:195:GLN:OE1  | 2.16                     | 0.46              |
| 8:7:513:A:H1'     | 54:t:11:ARG:NH1   | 2.30                     | 0.46              |
| 8:7:569:U:H1'     | 8:7:947:A:O4'     | 2.15                     | 0.46              |
| 8:7:995:C:O2      | 47:m:3:THR:OG1    | 2.20                     | 0.46              |
| 8:7:2233:U:H2'    | 8:7:2234:G:C8     | 2.51                     | 0.46              |
| 8:7:2394:C:N3     | 33:X:77:A:O2'     | 2.49                     | 0.46              |
| 10:A:1219:A:H2'   | 10:A:1220:G:C8    | 2.50                     | 0.46              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 12:C:167:TRP:HZ3 | 12:C:169:ARG:HG2  | 1.79                     | 0.46              |
| 33:X:35:I:H3'    | 33:X:36:C:H6      | 1.78                     | 0.46              |
| 36:b:124:ILE:O   | 36:b:124:ILE:HG13 | 2.15                     | 0.46              |
| 36:b:225:MET:SD  | 36:b:230:HIS:HB2  | 2.55                     | 0.46              |
| 40:f:15:VAL:HG11 | 40:f:76:VAL:HG23  | 1.96                     | 0.46              |
| 8:7:210:C:OP1    | 46:l:29:GLN:NE2   | 2.46                     | 0.46              |
| 8:7:1856:U:H2'   | 8:7:1857:G:C5'    | 2.44                     | 0.46              |
| 8:7:1971:U:OP2   | 8:7:1971:U:H4'    | 2.15                     | 0.46              |
| 10:A:109:A:H2'   | 10:A:326:G:N2     | 2.31                     | 0.46              |
| 10:A:200:G:H2'   | 10:A:201:G:C8     | 2.50                     | 0.46              |
| 10:A:218:U:H2'   | 10:A:219:U:C6     | 2.51                     | 0.46              |
| 10:A:1060:U:H3   | 10:A:1197:A:H61   | 1.63                     | 0.46              |
| 11:B:47:VAL:HB   | 11:B:48:PRO:HD3   | 1.96                     | 0.46              |
| 12:C:22:TRP:HZ2  | 12:C:33:LEU:HD23  | 1.80                     | 0.46              |
| 32:W:7:G:O2'     | 32:W:49:G:O5'     | 2.33                     | 0.46              |
| 8:7:1019:U:H3    | 8:7:1142:A:H62    | 1.64                     | 0.46              |
| 8:7:1275:A:OP2   | 8:7:1646:C:N4     | 2.49                     | 0.46              |
| 8:7:1367:A:C2'   | 46:l:25:LYS:HZ3   | 2.29                     | 0.46              |
| 8:7:2204:G:O2'   | 36:b:148:PRO:O    | 2.32                     | 0.46              |
| 10:A:94:G:H4'    | 10:A:95:C:H5'     | 1.97                     | 0.46              |
| 10:A:1027:C:H2'  | 10:A:1028:C:C6    | 2.51                     | 0.46              |
| 14:E:83:HIS:CE1  | 17:H:96:MET:HE1   | 2.50                     | 0.46              |
| 25:P:61:VAL:HG22 | 25:P:67:ILE:HD11  | 1.96                     | 0.46              |
| 34:Y:9:A:H1'     | 34:Y:45:G:O2'     | 2.16                     | 0.46              |
| 36:b:78:VAL:HG21 | 36:b:110:LEU:HD21 | 1.98                     | 0.46              |
| 56:v:4:ILE:HG13  | 56:v:106:VAL:HG22 | 1.98                     | 0.46              |
| 8:7:512:G:OP1    | 8:7:1234:U:O2'    | 2.34                     | 0.46              |
| 8:7:1029:A:N1    | 8:7:2465:C:O2'    | 2.48                     | 0.46              |
| 8:7:2432:A:H1'   | 33:X:76:C:O4'     | 2.15                     | 0.46              |
| 10:A:1319:A:O2'  | 10:A:1323:G:N7    | 2.48                     | 0.46              |
| 17:H:41:LYS:HE2  | 17:H:48:ASP:HA    | 1.98                     | 0.46              |
| 44:j:36:ASP:OD1  | 45:k:118:THR:OG1  | 2.34                     | 0.46              |
| 51:q:87:PHE:CE2  | 51:q:115:LEU:HD23 | 2.51                     | 0.46              |
| 52:r:30:ARG:HA   | 52:r:35:ILE:HD12  | 1.97                     | 0.46              |
| 53:s:43:PHE:CZ   | 53:s:63:LYS:HE3   | 2.50                     | 0.46              |
| 8:7:597:G:O2'    | 49:o:11:GLY:O     | 2.25                     | 0.45              |
| 8:7:1796:U:H2'   | 8:7:1797:G:C8     | 2.50                     | 0.45              |
| 8:7:1820:U:C4    | 36:b:159:GLY:HA3  | 2.51                     | 0.45              |
| 10:A:488:C:H2'   | 10:A:489:C:C6     | 2.52                     | 0.45              |
| 10:A:997:U:H2'   | 10:A:998:C:C6     | 2.51                     | 0.45              |
| 10:A:1043:G:H2'  | 10:A:1044:A:H8    | 1.80                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:A:1119:C:H2'   | 10:A:1120:C:H6    | 1.82                     | 0.45              |
| 21:L:13:ALA:O     | 21:L:15:LYS:NZ    | 2.47                     | 0.45              |
| 34:Y:75:C:H2'     | 34:Y:76:A:C5      | 2.50                     | 0.45              |
| 51:q:28:LEU:HD13  | 51:q:34:ILE:HG22  | 1.98                     | 0.45              |
| 7:6:13:ARG:NH1    | 49:o:59:ARG:HA    | 2.31                     | 0.45              |
| 8:7:797:G:OP1     | 38:d:55:SER:OG    | 2.23                     | 0.45              |
| 10:A:105:G:H2'    | 10:A:106:C:C6     | 2.51                     | 0.45              |
| 10:A:262:A:H2'    | 10:A:263:A:C8     | 2.51                     | 0.45              |
| 10:A:354:G:O2'    | 10:A:389:A:OP1    | 2.28                     | 0.45              |
| 10:A:844:G:C8     | 10:A:845:A:H3'    | 2.50                     | 0.45              |
| 10:A:1030:U:O2    | 10:A:1030:U:H2'   | 2.14                     | 0.45              |
| 29:T:57:ILE:HG23  | 29:T:61:GLN:HE22  | 1.81                     | 0.45              |
| 30:U:64:ASN:C     | 30:U:66:ARG:H     | 2.23                     | 0.45              |
| 38:d:6:LYS:NZ     | 38:d:141:MET:SD   | 2.87                     | 0.45              |
| 38:d:112:LEU:HD23 | 38:d:115:GLN:HE21 | 1.81                     | 0.45              |
| 39:e:175:PHE:CD1  | 39:e:176:PRO:HD2  | 2.51                     | 0.45              |
| 43:i:75:LEU:HB3   | 43:i:76:GLU:H     | 1.56                     | 0.45              |
| 8:7:554:U:H2'     | 8:7:555:G:O4'     | 2.16                     | 0.45              |
| 8:7:1130:U:N3     | 8:7:2025:C:OP1    | 2.31                     | 0.45              |
| 10:A:38:G:H22     | 10:A:397:A:H5'    | 1.80                     | 0.45              |
| 10:A:162:A:C5     | 10:A:163:C:H1'    | 2.51                     | 0.45              |
| 10:A:322:C:H2'    | 10:A:323:U:C6     | 2.52                     | 0.45              |
| 10:A:322:C:O3'    | 29:T:18:ARG:NH2   | 2.50                     | 0.45              |
| 10:A:539:A:H2'    | 10:A:540:G:C8     | 2.51                     | 0.45              |
| 10:A:1103:C:O2    | 11:B:106:THR:HG21 | 2.17                     | 0.45              |
| 10:A:1147:C:H2'   | 10:A:1148:U:C6    | 2.52                     | 0.45              |
| 10:A:1314:C:N4    | 28:S:2:PRO:O      | 2.48                     | 0.45              |
| 12:C:117:ALA:HB1  | 12:C:187:SER:HB3  | 1.98                     | 0.45              |
| 20:K:113:VAL:O    | 20:K:113:VAL:HG12 | 2.16                     | 0.45              |
| 36:b:35:GLU:OE1   | 36:b:35:GLU:N     | 2.50                     | 0.45              |
| 48:n:68:GLY:HA3   | 48:n:77:ILE:O     | 2.16                     | 0.45              |
| 56:v:86:MET:CG    | 56:v:96:ILE:HG13  | 2.47                     | 0.45              |
| 4:3:12:SER:O      | 4:3:16:ARG:NH2    | 2.50                     | 0.45              |
| 10:A:1095:U:H2'   | 10:A:1096:C:C6    | 2.51                     | 0.45              |
| 28:S:81:ARG:HA    | 28:S:81:ARG:NE    | 2.32                     | 0.45              |
| 37:c:24:VAL:HG12  | 37:c:178:VAL:HG21 | 1.99                     | 0.45              |
| 57:w:47:VAL:HG23  | 57:w:51:PHE:HD2   | 1.82                     | 0.45              |
| 1:0:17:VAL:HG12   | 1:0:19:ARG:H      | 1.81                     | 0.45              |
| 4:3:12:SER:HB2    | 4:3:32:ILE:HD11   | 1.97                     | 0.45              |
| 8:7:468:G:H5''    | 38:d:55:SER:HB2   | 1.98                     | 0.45              |
| 8:7:481:G:O2'     | 8:7:507:A:N1      | 2.49                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:7:567:U:OP2     | 49:o:29:LYS:NZ    | 2.36                     | 0.45              |
| 8:7:2429:G:C8     | 49:o:55:MET:HE3   | 2.51                     | 0.45              |
| 10:A:181:A:H2'    | 10:A:182:A:C8     | 2.52                     | 0.45              |
| 10:A:434:U:H2'    | 10:A:435:A:C8     | 2.51                     | 0.45              |
| 10:A:941:G:H4'    | 10:A:1350:A:H4'   | 1.99                     | 0.45              |
| 10:A:976:G:OP2    | 10:A:1358:U:O2'   | 2.34                     | 0.45              |
| 11:B:90:PHE:HE1   | 11:B:153:ASP:HB2  | 1.81                     | 0.45              |
| 20:K:117:PRO:HG2  | 30:U:35:ARG:HD3   | 1.99                     | 0.45              |
| 29:T:29:ARG:HB3   | 29:T:33:LYS:NZ    | 2.32                     | 0.45              |
| 55:u:6:GLN:HE21   | 55:u:9:GLY:H      | 1.62                     | 0.45              |
| 6:5:6:ASN:HD21    | 8:7:2022:U:H3     | 1.64                     | 0.45              |
| 8:7:1:G:H2'       | 8:7:2:G:C8        | 2.52                     | 0.45              |
| 8:7:2645:G:OP2    | 8:7:2645:G:N2     | 2.30                     | 0.45              |
| 8:7:2845:U:H5''   | 53:s:52:ASN:O     | 2.16                     | 0.45              |
| 10:A:427:U:C3'    | 10:A:428:G:H5''   | 2.44                     | 0.45              |
| 10:A:461:A:H2'    | 10:A:462:G:C8     | 2.52                     | 0.45              |
| 10:A:489:C:H2'    | 10:A:490:C:C6     | 2.50                     | 0.45              |
| 10:A:1119:C:OP1   | 18:I:85:ARG:NH1   | 2.50                     | 0.45              |
| 15:F:15:SER:HA    | 15:F:18:VAL:HG23  | 1.99                     | 0.45              |
| 37:c:16:THR:OG1   | 37:c:18:ASP:OD1   | 2.24                     | 0.45              |
| 38:d:12:LEU:HD21  | 38:d:193:VAL:HG11 | 1.99                     | 0.45              |
| 40:f:76:VAL:O     | 40:f:80:THR:HG23  | 2.17                     | 0.45              |
| 48:n:9:ASN:OD1    | 48:n:18:ARG:NH1   | 2.50                     | 0.45              |
| 54:t:109:LEU:HD23 | 55:u:49:ILE:HD13  | 1.97                     | 0.45              |
| 57:w:66:LYS:O     | 57:w:77:ARG:HG2   | 2.16                     | 0.45              |
| 8:7:2585:U:H5     | 34:Y:76:A:O2'     | 2.00                     | 0.45              |
| 8:7:2788:C:H2'    | 8:7:2789:C:C6     | 2.52                     | 0.45              |
| 10:A:509:A:N3     | 10:A:543:U:O2'    | 2.49                     | 0.45              |
| 10:A:946:A:H2'    | 10:A:947:G:H8     | 1.82                     | 0.45              |
| 10:A:982:U:H4'    | 10:A:983:A:O5'    | 2.17                     | 0.45              |
| 10:A:1367:C:H4'   | 19:J:50:THR:HG21  | 1.98                     | 0.45              |
| 12:C:17:PRO:HA    | 12:C:211:MET:HE1  | 1.99                     | 0.45              |
| 17:H:95:VAL:HG21  | 17:H:102:ALA:HB2  | 1.99                     | 0.45              |
| 43:i:135:HIS:CG   | 43:i:136:SER:H    | 2.34                     | 0.45              |
| 44:j:45:GLY:HA2   | 44:j:50:VAL:HB    | 1.98                     | 0.45              |
| 53:s:9:GLU:O      | 53:s:13:MET:HG3   | 2.15                     | 0.45              |
| 2:1:17:ASN:OD1    | 2:1:27:ARG:HD2    | 2.17                     | 0.45              |
| 6:5:9:THR:CG2     | 8:7:2020:A:H5'    | 2.46                     | 0.45              |
| 8:7:2106:U:H3     | 8:7:2183:A:H61    | 1.64                     | 0.45              |
| 10:A:43:C:H2'     | 10:A:44:A:H8      | 1.82                     | 0.45              |
| 10:A:537:G:O3'    | 21:L:110:ARG:NH2  | 2.49                     | 0.45              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 10:A:1174:G:H2'  | 10:A:1175:G:H8    | 1.82                     | 0.45              |
| 10:A:1268:G:H2'  | 10:A:1269:A:C8    | 2.51                     | 0.45              |
| 10:A:1437:A:P    | 29:T:29:ARG:HH12  | 2.37                     | 0.45              |
| 29:T:3:ASN:OD1   | 29:T:4:ILE:HD12   | 2.16                     | 0.45              |
| 8:7:832:U:H5'    | 49:o:38:GLN:HG2   | 1.98                     | 0.45              |
| 8:7:1338:G:H5''  | 57:w:17:SER:HB3   | 1.99                     | 0.45              |
| 8:7:2238:G:H2'   | 8:7:2238:G:N3     | 2.31                     | 0.45              |
| 10:A:376:G:H5''  | 25:P:5:ARG:HB2    | 1.99                     | 0.45              |
| 10:A:382:A:H2'   | 10:A:383:A:H8     | 1.82                     | 0.45              |
| 10:A:505:G:H4'   | 10:A:534:U:C4     | 2.52                     | 0.45              |
| 10:A:541:G:O2'   | 13:D:40:GLN:OE1   | 2.20                     | 0.45              |
| 10:A:658:C:H1'   | 24:O:22:THR:HG21  | 1.99                     | 0.45              |
| 10:A:1219:A:H2'  | 10:A:1220:G:H8    | 1.82                     | 0.45              |
| 14:E:156:LYS:HE2 | 17:H:71:VAL:HA    | 1.97                     | 0.45              |
| 15:F:21:MET:HA   | 15:F:24:ARG:HH11  | 1.82                     | 0.45              |
| 33:X:38:2MA:H3'  | 33:X:39:A:C8      | 2.52                     | 0.45              |
| 48:n:71:ARG:HB3  | 48:n:72:PRO:HD2   | 1.97                     | 0.45              |
| 48:n:121:GLU:OE1 | 48:n:123:LEU:HD23 | 2.15                     | 0.45              |
| 7:6:26:HIS:HB3   | 7:6:44:LEU:HD22   | 1.99                     | 0.45              |
| 8:7:1542:U:H2'   | 8:7:1543:G:O4'    | 2.17                     | 0.45              |
| 8:7:1782:U:H1'   | 8:7:2609:U:H5''   | 1.99                     | 0.45              |
| 8:7:1820:U:N3    | 36:b:159:GLY:HA3  | 2.32                     | 0.45              |
| 8:7:2142:A:H61   | 8:7:2148:G:H1     | 1.63                     | 0.45              |
| 8:7:2271:G:OP1   | 60:z:18:ALA:HB1   | 2.17                     | 0.45              |
| 8:7:2744:G:N2    | 40:f:143:GLN:OE1  | 2.50                     | 0.45              |
| 10:A:1302:C:C5   | 22:M:17:ILE:HG13  | 2.51                     | 0.45              |
| 29:T:13:GLN:HA   | 29:T:16:LYS:HB2   | 1.99                     | 0.45              |
| 52:r:28:VAL:HG11 | 52:r:103:VAL:HG13 | 1.98                     | 0.45              |
| 8:7:1020:A:H1'   | 8:7:1021:A:OP2    | 2.17                     | 0.44              |
| 10:A:385:C:H2'   | 10:A:386:C:C6     | 2.53                     | 0.44              |
| 10:A:1265:C:H2'  | 10:A:1266:G:C8    | 2.53                     | 0.44              |
| 10:A:1500:A:H5'' | 10:A:1508:A:H5''  | 1.99                     | 0.44              |
| 14:E:83:HIS:CE1  | 14:E:147:MET:HG3  | 2.52                     | 0.44              |
| 20:K:27:PHE:CE1  | 20:K:89:PRO:HG2   | 2.48                     | 0.44              |
| 44:j:65:GLU:OE1  | 44:j:65:GLU:N     | 2.41                     | 0.44              |
| 45:k:13:VAL:HB   | 45:k:54:PRO:HB3   | 1.97                     | 0.44              |
| 8:7:1881:C:H2'   | 8:7:1882:U:O4'    | 2.17                     | 0.44              |
| 8:7:2000:C:OP1   | 51:q:5:LYS:NZ     | 2.46                     | 0.44              |
| 10:A:187:G:N2    | 10:A:189:A:H3'    | 2.32                     | 0.44              |
| 10:A:1043:G:H2'  | 10:A:1044:A:C8    | 2.52                     | 0.44              |
| 10:A:1368:A:OP1  | 19:J:64:GLN:NE2   | 2.50                     | 0.44              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 13:D:87:GLY:HA3  | 13:D:197:GLU:OE1  | 2.17                     | 0.44              |
| 19:J:63:ASP:OD1  | 23:N:98:LYS:HG3   | 2.17                     | 0.44              |
| 25:P:68:SER:HB3  | 25:P:71:VAL:HG22  | 1.99                     | 0.44              |
| 37:c:32:ASN:ND2  | 37:c:52:THR:HB    | 2.32                     | 0.44              |
| 37:c:176:ASP:HB3 | 37:c:190:LYS:HB3  | 1.97                     | 0.44              |
| 40:f:72:LEU:HA   | 40:f:72:LEU:HD13  | 1.84                     | 0.44              |
| 47:m:39:LYS:HE2  | 47:m:39:LYS:HB3   | 1.80                     | 0.44              |
| 47:m:102:GLU:O   | 47:m:103:ILE:C    | 2.59                     | 0.44              |
| 51:q:18:GLN:OE1  | 51:q:22:ARG:NH2   | 2.50                     | 0.44              |
| 4:3:10:THR:HG21  | 4:3:56:LYS:HG2    | 1.99                     | 0.44              |
| 8:7:833:A:H2'    | 8:7:834:G:C8      | 2.52                     | 0.44              |
| 10:A:67:C:H2'    | 10:A:68:G:H8      | 1.83                     | 0.44              |
| 10:A:243:A:H62   | 10:A:281:G:H1'    | 1.82                     | 0.44              |
| 10:A:1176:A:H2'  | 10:A:1177:G:C8    | 2.52                     | 0.44              |
| 18:I:6:TYR:HB2   | 18:I:21:ILE:HB    | 1.99                     | 0.44              |
| 32:W:23:A:H2'    | 32:W:24:G:C8      | 2.51                     | 0.44              |
| 39:e:5:HIS:O     | 39:e:8:TYR:HB3    | 2.17                     | 0.44              |
| 47:m:45:THR:HB   | 47:m:48:VAL:HB    | 1.99                     | 0.44              |
| 56:v:3:THR:HG21  | 56:v:58:ALA:HB2   | 1.98                     | 0.44              |
| 6:5:55:ILE:HG22  | 6:5:57:LYS:H      | 1.81                     | 0.44              |
| 10:A:222:C:H2'   | 10:A:223:A:H8     | 1.81                     | 0.44              |
| 10:A:320:A:H2'   | 10:A:321:A:C8     | 2.51                     | 0.44              |
| 10:A:331:G:H2'   | 29:T:4:ILE:HD11   | 2.00                     | 0.44              |
| 10:A:643:C:H5''  | 17:H:32:LEU:HD11  | 2.00                     | 0.44              |
| 10:A:972:C:O2'   | 19:J:57:VAL:O     | 2.35                     | 0.44              |
| 10:A:1114:C:H2'  | 10:A:1115:U:H6    | 1.83                     | 0.44              |
| 13:D:26:ARG:HD3  | 13:D:31:LYS:HD2   | 2.00                     | 0.44              |
| 15:F:6:ILE:HG23  | 15:F:89:VAL:HG22  | 1.97                     | 0.44              |
| 32:W:10:G:H2'    | 32:W:11:U:C6      | 2.52                     | 0.44              |
| 35:a:170:ILE:HB  | 35:a:172:HIS:CE1  | 2.52                     | 0.44              |
| 45:k:81:LYS:HD3  | 45:k:85:GLY:HA2   | 2.00                     | 0.44              |
| 8:7:2112:G:N1    | 8:7:2168:G:OP1    | 2.51                     | 0.44              |
| 8:7:2124:G:H3'   | 8:7:2125:G:H8     | 1.83                     | 0.44              |
| 8:7:2142:A:N6    | 8:7:2148:G:H1     | 2.14                     | 0.44              |
| 8:7:2547:A:H4'   | 48:n:29:HIS:NE2   | 2.33                     | 0.44              |
| 10:A:182:A:N1    | 10:A:223:A:O2'    | 2.51                     | 0.44              |
| 10:A:323:U:H2'   | 10:A:324:G:O4'    | 2.18                     | 0.44              |
| 10:A:461:A:H2'   | 10:A:462:G:H8     | 1.82                     | 0.44              |
| 16:G:113:ASP:HB3 | 16:G:118:LEU:HG   | 2.00                     | 0.44              |
| 21:L:63:VAL:HG21 | 21:L:95:TYR:CE2   | 2.52                     | 0.44              |
| 21:L:81:LEU:HB2  | 21:L:102:LEU:HD13 | 1.99                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 43:i:72:ILE:HG12  | 43:i:142:VAL:HG21 | 1.99                     | 0.44              |
| 44:j:56:ARG:HE    | 44:j:57:ASN:H     | 1.64                     | 0.44              |
| 56:v:74:ILE:HD12  | 56:v:105:VAL:HG22 | 1.99                     | 0.44              |
| 8:7:587:C:C6      | 49:o:19:LEU:HD11  | 2.52                     | 0.44              |
| 8:7:894:U:H2'     | 8:7:895:U:O4'     | 2.18                     | 0.44              |
| 8:7:2687:U:H2'    | 8:7:2688:G:O4'    | 2.17                     | 0.44              |
| 10:A:87:C:C4      | 10:A:88:U:H1'     | 2.53                     | 0.44              |
| 10:A:1397:C:H5'   | 31:V:28:A:H61     | 1.81                     | 0.44              |
| 12:C:16:LYS:HD3   | 12:C:17:PRO:HD2   | 2.00                     | 0.44              |
| 15:F:50:PRO:HG3   | 15:F:55:HIS:NE2   | 2.33                     | 0.44              |
| 22:M:15:ALA:O     | 22:M:19:LEU:HD23  | 2.17                     | 0.44              |
| 36:b:220:VAL:HG13 | 36:b:225:MET:HE3  | 1.99                     | 0.44              |
| 5:4:44:PHE:H      | 5:4:44:PHE:HD1    | 1.66                     | 0.44              |
| 10:A:545:C:H5'    | 13:D:69:GLU:CB    | 2.48                     | 0.44              |
| 10:A:553:A:H2'    | 10:A:554:A:C8     | 2.53                     | 0.44              |
| 10:A:1173:U:H2'   | 10:A:1174:G:O4'   | 2.18                     | 0.44              |
| 10:A:1326:U:H2'   | 10:A:1327:C:H6    | 1.82                     | 0.44              |
| 12:C:26:THR:HA    | 23:N:76:LYS:HE2   | 1.99                     | 0.44              |
| 23:N:69:ARG:CZ    | 23:N:81:ARG:HH21  | 2.31                     | 0.44              |
| 37:c:124:ARG:HA   | 37:c:165:MET:SD   | 2.58                     | 0.44              |
| 37:c:181:ASP:OD1  | 37:c:183:GLU:HG3  | 2.18                     | 0.44              |
| 37:c:183:GLU:CD   | 37:c:184:ARG:HG3  | 2.43                     | 0.44              |
| 39:e:148:ARG:NH1  | 39:e:148:ARG:HB2  | 2.33                     | 0.44              |
| 54:t:45:TYR:HA    | 54:t:48:ARG:HH12  | 1.82                     | 0.44              |
| 2:1:59:ILE:HD13   | 2:1:67:VAL:HG11   | 2.00                     | 0.44              |
| 8:7:570:G:H2'     | 8:7:2030:6MZ:N7   | 2.33                     | 0.44              |
| 8:7:859:G:O2'     | 8:7:916:G:O6      | 2.22                     | 0.44              |
| 8:7:1035:U:H2'    | 8:7:1036:G:H8     | 1.81                     | 0.44              |
| 10:A:123:U:H5''   | 10:A:311:C:O2'    | 2.18                     | 0.44              |
| 10:A:178:C:H2'    | 10:A:179:A:H8     | 1.83                     | 0.44              |
| 10:A:328:C:H4'    | 10:A:329:A:H5''   | 2.00                     | 0.44              |
| 10:A:339:C:H3'    | 48:n:98:ARG:NH2   | 2.33                     | 0.44              |
| 10:A:361:G:H2'    | 10:A:362:G:O4'    | 2.16                     | 0.44              |
| 10:A:555:U:H2'    | 10:A:556:C:C6     | 2.53                     | 0.44              |
| 10:A:1120:C:H2'   | 10:A:1121:U:C6    | 2.52                     | 0.44              |
| 10:A:1174:G:H2'   | 10:A:1175:G:C8    | 2.53                     | 0.44              |
| 10:A:1492:A:H2'   | 10:A:1493:A:C4    | 2.52                     | 0.44              |
| 12:C:23:PHE:CE1   | 19:J:97:ASP:HB2   | 2.53                     | 0.44              |
| 22:M:42:ASP:OD1   | 22:M:42:ASP:N     | 2.49                     | 0.44              |
| 44:j:8:LYS:HD2    | 44:j:59:LEU:HD21  | 2.00                     | 0.44              |
| 56:v:76:VAL:HG13  | 56:v:103:ILE:HG13 | 2.00                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 58:x:86:ARG:NH1   | 58:x:100:SER:OG   | 2.46                     | 0.44              |
| 4:3:12:SER:C      | 4:3:16:ARG:HH21   | 2.25                     | 0.44              |
| 4:3:19:LYS:HZ1    | 8:7:851:C:H5'     | 1.82                     | 0.44              |
| 8:7:500:G:N1      | 8:7:503:A:OP2     | 2.49                     | 0.44              |
| 8:7:922:C:O2'     | 60:z:29:GLU:OE2   | 2.33                     | 0.44              |
| 8:7:1344:U:O2     | 8:7:1385:A:H5'    | 2.17                     | 0.44              |
| 8:7:1597:A:H5''   | 8:7:1598:A:H5'    | 1.99                     | 0.44              |
| 8:7:2636:C:O2'    | 37:c:45:TYR:OH    | 2.24                     | 0.44              |
| 10:A:562:U:H1'    | 21:L:12:ARG:HD2   | 1.99                     | 0.44              |
| 10:A:1157:A:H4'   | 10:A:1158:C:O5'   | 2.18                     | 0.44              |
| 12:C:185:ASN:CG   | 12:C:186:THR:H    | 2.23                     | 0.44              |
| 15:F:42:TRP:HZ3   | 15:F:103:VAL:HG13 | 1.82                     | 0.44              |
| 49:o:90:VAL:HB    | 49:o:122:VAL:HA   | 2.00                     | 0.44              |
| 52:r:13:ARG:HG2   | 52:r:17:LYS:HZ2   | 1.83                     | 0.44              |
| 59:y:61:LEU:N     | 59:y:72:VAL:O     | 2.46                     | 0.44              |
| 10:A:62:U:H2'     | 10:A:63:C:C6      | 2.53                     | 0.43              |
| 10:A:128:G:H2'    | 10:A:129:A:C8     | 2.53                     | 0.43              |
| 10:A:139:A:H2'    | 10:A:140:U:C6     | 2.53                     | 0.43              |
| 12:C:42:TYR:CE1   | 12:C:90:VAL:HG11  | 2.52                     | 0.43              |
| 18:I:84:THR:HG23  | 18:I:98:LEU:HD13  | 2.00                     | 0.43              |
| 34:Y:18:G:H1      | 34:Y:55:PSU:H1'   | 1.83                     | 0.43              |
| 8:7:2291:U:H2'    | 8:7:2292:U:C6     | 2.52                     | 0.43              |
| 10:A:190:A:H3'    | 10:A:191:G:H8     | 1.83                     | 0.43              |
| 10:A:235:C:H2'    | 10:A:236:A:C8     | 2.52                     | 0.43              |
| 10:A:1172:C:H2'   | 10:A:1173:U:C6    | 2.54                     | 0.43              |
| 12:C:123:GLN:HG3  | 12:C:126:ARG:HH22 | 1.83                     | 0.43              |
| 12:C:186:THR:HG22 | 12:C:199:LYS:HG2  | 2.00                     | 0.43              |
| 13:D:47:ARG:HH22  | 31:V:34:A:N6      | 2.17                     | 0.43              |
| 13:D:202:GLU:HB2  | 14:E:112:ARG:HH22 | 1.82                     | 0.43              |
| 36:b:6:CYS:SG     | 36:b:13:ARG:NH2   | 2.91                     | 0.43              |
| 36:b:122:ALA:O    | 36:b:130:LEU:HD21 | 2.18                     | 0.43              |
| 42:h:33:LEU:HD13  | 42:h:117:PHE:HB3  | 2.00                     | 0.43              |
| 45:k:72:LYS:HG3   | 45:k:73:THR:N     | 2.29                     | 0.43              |
| 48:n:76:VAL:HG22  | 53:s:73:VAL:HG21  | 2.00                     | 0.43              |
| 56:v:86:MET:HG2   | 56:v:96:ILE:HG13  | 1.99                     | 0.43              |
| 57:w:3:ARG:HG3    | 57:w:5:GLU:H      | 1.83                     | 0.43              |
| 4:3:19:LYS:NZ     | 8:7:851:C:H5'     | 2.34                     | 0.43              |
| 10:A:165:G:H2'    | 10:A:166:U:C6     | 2.54                     | 0.43              |
| 10:A:255:G:H4'    | 26:Q:19:LYS:HD3   | 2.00                     | 0.43              |
| 10:A:778:G:O2'    | 20:K:121:CYS:HB3  | 2.18                     | 0.43              |
| 10:A:911:U:OP2    | 21:L:94:ARG:NH2   | 2.52                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 12:C:60:PRO:HG2   | 12:C:63:SER:HB3   | 2.00                     | 0.43              |
| 18:I:97:GLU:HG2   | 18:I:98:LEU:N     | 2.34                     | 0.43              |
| 32:W:51:G:H1      | 32:W:63:C:H42     | 1.64                     | 0.43              |
| 5:4:6:HIS:ND1     | 39:e:62:GLY:O     | 2.47                     | 0.43              |
| 8:7:2127:G:N2     | 8:7:2162:G:O4'    | 2.43                     | 0.43              |
| 8:7:2182:U:H2'    | 8:7:2183:A:N7     | 2.34                     | 0.43              |
| 10:A:1464:U:OP2   | 53:s:109:ARG:NH1  | 2.47                     | 0.43              |
| 33:X:47:G7M:O2'   | 33:X:48:3AU:H5'A  | 2.18                     | 0.43              |
| 36:b:98:ASP:OD1   | 36:b:98:ASP:O     | 2.36                     | 0.43              |
| 42:h:81:ARG:HD2   | 60:z:4:LYS:HE3    | 2.00                     | 0.43              |
| 47:m:103:ILE:HG13 | 47:m:104:ALA:N    | 2.33                     | 0.43              |
| 8:7:1818:U:H5     | 36:b:156:ARG:HH22 | 1.66                     | 0.43              |
| 10:A:88:U:H2'     | 10:A:89:U:C6      | 2.54                     | 0.43              |
| 10:A:337:G:H2'    | 10:A:338:A:C8     | 2.54                     | 0.43              |
| 10:A:399:G:H2'    | 10:A:400:C:C6     | 2.53                     | 0.43              |
| 10:A:496:A:O2'    | 10:A:497:G:H3'    | 2.19                     | 0.43              |
| 10:A:1258:G:H2'   | 10:A:1259:C:C6    | 2.53                     | 0.43              |
| 10:A:1264:U:H2'   | 10:A:1265:C:C6    | 2.54                     | 0.43              |
| 10:A:1327:C:H2'   | 10:A:1328:C:C6    | 2.53                     | 0.43              |
| 23:N:79:LEU:HD13  | 23:N:84:VAL:HA    | 2.00                     | 0.43              |
| 29:T:27:MET:HB3   | 29:T:57:ILE:HG21  | 1.99                     | 0.43              |
| 34:Y:35:G:H2'     | 34:Y:36:C:O4'     | 2.18                     | 0.43              |
| 42:h:105:MET:SD   | 42:h:108:VAL:HG21 | 2.58                     | 0.43              |
| 5:4:64:PHE:HB2    | 5:4:66:ILE:HG23   | 2.01                     | 0.43              |
| 8:7:600:G:H1'     | 38:d:100:MET:CE   | 2.47                     | 0.43              |
| 8:7:698:C:O2'     | 8:7:734:A:N6      | 2.51                     | 0.43              |
| 8:7:700:G:O2'     | 8:7:1632:A:N3     | 2.47                     | 0.43              |
| 8:7:1939:5MU:OP1  | 8:7:2604:PSU:O2'  | 2.37                     | 0.43              |
| 10:A:8:A:N6       | 13:D:202:GLU:O    | 2.51                     | 0.43              |
| 10:A:41:G:H2'     | 10:A:42:G:C8      | 2.53                     | 0.43              |
| 10:A:76:G:H2'     | 10:A:77:A:C8      | 2.54                     | 0.43              |
| 10:A:943:U:H3     | 10:A:1340:A:H61   | 1.66                     | 0.43              |
| 10:A:1106:G:H5''  | 12:C:172:ARG:HG3  | 2.00                     | 0.43              |
| 34:Y:54:5MU:H6    | 34:Y:54:5MU:C5'   | 2.31                     | 0.43              |
| 40:f:87:LEU:HB2   | 40:f:131:ILE:HB   | 2.01                     | 0.43              |
| 43:i:93:SER:OG    | 43:i:123:ARG:NH2  | 2.51                     | 0.43              |
| 47:m:134:ALA:O    | 47:m:136:GLN:NE2  | 2.51                     | 0.43              |
| 8:7:663:G:H5''    | 49:o:17:LYS:NZ    | 2.34                     | 0.43              |
| 8:7:1076:C:H2'    | 8:7:1077:A:C8     | 2.54                     | 0.43              |
| 8:7:1182:G:H2'    | 8:7:1183:U:O4'    | 2.19                     | 0.43              |
| 8:7:1645:G:H5''   | 8:7:1646:C:H5'    | 2.00                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:7:1791:A:C5'    | 36:b:205:LEU:HD11 | 2.49                     | 0.43              |
| 8:7:1969:A:O2'    | 8:7:1972:G:N3     | 2.47                     | 0.43              |
| 8:7:2116:G:H5''   | 8:7:2117:A:OP1    | 2.19                     | 0.43              |
| 10:A:41:G:H2'     | 10:A:42:G:H8      | 1.84                     | 0.43              |
| 10:A:70:U:H3      | 10:A:98:A:N6      | 2.15                     | 0.43              |
| 10:A:84:U:H4'     | 10:A:85:U:H3'     | 2.00                     | 0.43              |
| 10:A:209:U:H3'    | 10:A:210:C:H6     | 1.83                     | 0.43              |
| 10:A:417:G:N2     | 10:A:427:U:C2     | 2.87                     | 0.43              |
| 10:A:419:C:H2'    | 10:A:420:U:O4'    | 2.19                     | 0.43              |
| 17:H:18:GLN:NE2   | 17:H:72:VAL:H     | 2.16                     | 0.43              |
| 17:H:127:CYS:SG   | 17:H:128:TYR:N    | 2.91                     | 0.43              |
| 39:e:111:ILE:HD13 | 39:e:137:ILE:HG21 | 2.01                     | 0.43              |
| 8:7:296:U:H2'     | 8:7:297:G:C8      | 2.53                     | 0.43              |
| 8:7:967:U:H2'     | 8:7:968:C:C6      | 2.54                     | 0.43              |
| 8:7:2119:A:C2     | 8:7:2170:A:H1'    | 2.53                     | 0.43              |
| 8:7:2182:U:H2'    | 8:7:2183:A:C8     | 2.53                     | 0.43              |
| 10:A:67:C:H2'     | 10:A:68:G:C8      | 2.54                     | 0.43              |
| 10:A:404:G:OP2    | 13:D:115:ARG:NH1  | 2.52                     | 0.43              |
| 10:A:692:U:O2'    | 10:A:694:A:N7     | 2.39                     | 0.43              |
| 12:C:29:PHE:HE1   | 12:C:33:LEU:HD21  | 1.84                     | 0.43              |
| 18:I:60:LYS:HG3   | 18:I:61:LEU:HD12  | 2.00                     | 0.43              |
| 27:R:57:ARG:O     | 27:R:61:ARG:HG3   | 2.19                     | 0.43              |
| 33:X:51:G:H2'     | 33:X:52:A:H8      | 1.84                     | 0.43              |
| 34:Y:45:G:H3'     | 34:Y:46:G7M:H5''  | 2.01                     | 0.43              |
| 6:5:8:PRO:HD2     | 8:7:1263:U:O2'    | 2.18                     | 0.43              |
| 6:5:32:LYS:NZ     | 8:7:2885:G:N3     | 2.63                     | 0.43              |
| 8:7:598:U:H2'     | 8:7:599:A:C8      | 2.54                     | 0.43              |
| 8:7:1064:C:H4'    | 45:k:91:GLY:HA2   | 2.01                     | 0.43              |
| 8:7:1759:A:O2'    | 8:7:2714:G:O2'    | 2.34                     | 0.43              |
| 8:7:2176:A:H4'    | 35:a:219:GLY:O    | 2.19                     | 0.43              |
| 10:A:230:G:OP1    | 25:P:31:ARG:NH2   | 2.52                     | 0.43              |
| 10:A:300:A:C6     | 10:A:301:G:H1'    | 2.54                     | 0.43              |
| 10:A:462:G:H3'    | 10:A:463:U:C6     | 2.54                     | 0.43              |
| 10:A:554:A:H2'    | 10:A:555:U:C6     | 2.54                     | 0.43              |
| 25:P:78:VAL:HG13  | 25:P:79:ASN:N     | 2.33                     | 0.43              |
| 35:a:26:ALA:HB1   | 35:a:214:ILE:HD11 | 2.01                     | 0.43              |
| 36:b:135:ILE:O    | 36:b:167:ARG:NH2  | 2.42                     | 0.43              |
| 6:5:13:ARG:NH2    | 8:7:517:C:OP1     | 2.48                     | 0.43              |
| 8:7:743:A:OP1     | 37:c:135:GLY:HA2  | 2.19                     | 0.43              |
| 8:7:859:G:OP2     | 8:7:859:G:H8      | 2.01                     | 0.43              |
| 8:7:1000:A:OP2    | 8:7:1154:G:N1     | 2.35                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:7:1108:U:OP2    | 44:j:56:ARG:NH2   | 2.35                     | 0.43              |
| 8:7:1614:A:C2     | 56:v:93:ALA:HB2   | 2.54                     | 0.43              |
| 8:7:2016:U:H2'    | 8:7:2017:U:C6     | 2.54                     | 0.43              |
| 10:A:342:C:H2'    | 10:A:343:U:C6     | 2.54                     | 0.43              |
| 10:A:376:G:H1     | 10:A:387:U:H3     | 1.66                     | 0.43              |
| 10:A:1378:C:H4'   | 16:G:92:ARG:NH1   | 2.34                     | 0.43              |
| 10:A:1384:C:H2'   | 10:A:1385:G:C8    | 2.54                     | 0.43              |
| 15:F:78:PHE:HA    | 15:F:84:VAL:HG11  | 2.00                     | 0.43              |
| 25:P:69:ASP:OD1   | 25:P:70:ARG:N     | 2.52                     | 0.43              |
| 31:V:18:C:H2'     | 31:V:19:G:C8      | 2.53                     | 0.43              |
| 48:n:40:LYS:HE3   | 48:n:57:VAL:HG22  | 2.00                     | 0.43              |
| 53:s:5:ILE:O      | 53:s:9:GLU:HG2    | 2.18                     | 0.43              |
| 8:7:118:A:H5''    | 46:l:22:MET:CE    | 2.49                     | 0.42              |
| 8:7:832:U:H2'     | 8:7:833:A:C8      | 2.54                     | 0.42              |
| 8:7:1475:G:O2'    | 8:7:1476:U:P      | 2.77                     | 0.42              |
| 8:7:2112:G:H3'    | 8:7:2113:U:H6     | 1.83                     | 0.42              |
| 8:7:2129:C:O2'    | 8:7:2159:G:N2     | 2.50                     | 0.42              |
| 8:7:2503:2MA:O2'  | 8:7:2505:G:OP2    | 2.36                     | 0.42              |
| 10:A:360:G:C2'    | 10:A:361:G:H5'    | 2.49                     | 0.42              |
| 10:A:1492:A:H2'   | 10:A:1493:A:C5    | 2.54                     | 0.42              |
| 10:A:1492:A:OP1   | 21:L:44:LYS:N     | 2.52                     | 0.42              |
| 11:B:104:TRP:O    | 11:B:105:LYS:C    | 2.62                     | 0.42              |
| 12:C:64:ILE:HD11  | 12:C:97:VAL:HG23  | 2.00                     | 0.42              |
| 12:C:212:ALA:H    | 19:J:16:ARG:NH1   | 2.15                     | 0.42              |
| 14:E:164:ILE:HG13 | 14:E:165:LEU:N    | 2.35                     | 0.42              |
| 22:M:50:GLU:HA    | 22:M:53:ILE:HD12  | 2.00                     | 0.42              |
| 36:b:141:VAL:HG12 | 36:b:192:LEU:HD13 | 2.01                     | 0.42              |
| 38:d:105:LEU:HD23 | 38:d:105:LEU:HA   | 1.87                     | 0.42              |
| 45:k:24:VAL:HG11  | 45:k:28:LEU:HD23  | 2.00                     | 0.42              |
| 8:7:1504:A:H2'    | 8:7:1505:A:C8     | 2.54                     | 0.42              |
| 8:7:2148:G:OP2    | 8:7:2148:G:H8     | 2.02                     | 0.42              |
| 8:7:2747:G:O6     | 8:7:2755:C:H5''   | 2.20                     | 0.42              |
| 10:A:90:C:H1'     | 10:A:91:U:H5'     | 2.01                     | 0.42              |
| 10:A:158:G:H2'    | 10:A:159:G:H8     | 1.84                     | 0.42              |
| 10:A:221:C:H2'    | 10:A:222:C:C6     | 2.53                     | 0.42              |
| 10:A:258:G:H1     | 10:A:268:U:H3     | 1.67                     | 0.42              |
| 11:B:56:GLU:O     | 11:B:60:ILE:HG13  | 2.19                     | 0.42              |
| 14:E:153:VAL:HG21 | 17:H:99:LEU:HD23  | 2.02                     | 0.42              |
| 20:K:96:THR:O     | 20:K:100:LEU:HD23 | 2.18                     | 0.42              |
| 22:M:77:ILE:HG22  | 22:M:81:MET:HE3   | 2.01                     | 0.42              |
| 26:Q:71:LYS:HE2   | 26:Q:71:LYS:HB3   | 1.82                     | 0.42              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 36:b:92:ALA:N    | 36:b:104:ILE:O    | 2.36                     | 0.42              |
| 36:b:210:ALA:HA  | 36:b:213:TRP:CE3  | 2.54                     | 0.42              |
| 38:d:127:GLU:H   | 38:d:127:GLU:CD   | 2.28                     | 0.42              |
| 48:n:58:LEU:HD11 | 48:n:86:LEU:HG    | 2.01                     | 0.42              |
| 56:v:13:SER:OG   | 56:v:16:LYS:HG3   | 2.19                     | 0.42              |
| 8:7:307:G:N1     | 8:7:310:A:OP2     | 2.53                     | 0.42              |
| 8:7:858:G:H3'    | 8:7:859:G:C8      | 2.53                     | 0.42              |
| 8:7:1367:A:O2'   | 46:l:25:LYS:NZ    | 2.46                     | 0.42              |
| 8:7:2167:U:N3    | 8:7:2170:A:OP2    | 2.48                     | 0.42              |
| 9:8:48:U:H2'     | 9:8:49:C:C6       | 2.54                     | 0.42              |
| 10:A:402:G:O2'   | 10:A:403:C:H5'    | 2.18                     | 0.42              |
| 10:A:830:G:H5'   | 11:B:23:TRP:HE1   | 1.83                     | 0.42              |
| 10:A:1052:U:H3   | 10:A:1206:G:H1    | 1.67                     | 0.42              |
| 37:c:25:THR:HG21 | 37:c:193:VAL:HG22 | 2.01                     | 0.42              |
| 40:f:152:ARG:HD3 | 40:f:152:ARG:HA   | 1.84                     | 0.42              |
| 52:r:62:LEU:HD12 | 52:r:62:LEU:O     | 2.19                     | 0.42              |
| 54:t:58:ARG:HA   | 54:t:61:TRP:CE3   | 2.54                     | 0.42              |
| 1:0:32:LYS:HE3   | 1:0:32:LYS:HB3    | 1.78                     | 0.42              |
| 8:7:859:G:N2     | 8:7:916:G:H2'     | 2.35                     | 0.42              |
| 8:7:1357:C:H2'   | 8:7:1358:G:O4'    | 2.19                     | 0.42              |
| 8:7:1720:U:H2'   | 8:7:1721:G:O4'    | 2.19                     | 0.42              |
| 8:7:1997:C:OP2   | 37:c:129:THR:HG22 | 2.19                     | 0.42              |
| 8:7:2743:U:O2'   | 40:f:153:ARG:NH2  | 2.52                     | 0.42              |
| 10:A:333:U:OP1   | 29:T:2:ALA:N      | 2.52                     | 0.42              |
| 10:A:718:A:H5'   | 20:K:119:ASN:OD1  | 2.20                     | 0.42              |
| 10:A:1273:C:H2'  | 10:A:1274:A:O4'   | 2.19                     | 0.42              |
| 10:A:1442:G:H4'  | 53:s:114:LEU:HD11 | 2.02                     | 0.42              |
| 25:P:25:ARG:HE   | 25:P:25:ARG:HB2   | 1.66                     | 0.42              |
| 36:b:161:TYR:HB3 | 36:b:194:GLU:HG3  | 2.02                     | 0.42              |
| 38:d:164:LEU:HB2 | 38:d:167:VAL:HG22 | 2.01                     | 0.42              |
| 48:n:65:THR:HG22 | 48:n:67:LYS:H     | 1.83                     | 0.42              |
| 52:r:54:VAL:HG23 | 52:r:54:VAL:O     | 2.19                     | 0.42              |
| 2:1:55:GLY:O     | 2:1:58:VAL:HG22   | 2.20                     | 0.42              |
| 8:7:558:U:H2'    | 8:7:559:G:H8      | 1.83                     | 0.42              |
| 8:7:580:U:H2'    | 8:7:581:C:C6      | 2.54                     | 0.42              |
| 8:7:1475:G:H4'   | 8:7:1476:U:H5'    | 2.01                     | 0.42              |
| 10:A:343:U:H2'   | 10:A:345:C:C5     | 2.55                     | 0.42              |
| 10:A:1032:G:H3'  | 10:A:1032:G:N3    | 2.34                     | 0.42              |
| 10:A:1125:U:O2'  | 10:A:1126:U:H3'   | 2.19                     | 0.42              |
| 12:C:64:ILE:O    | 12:C:99:ALA:HB1   | 2.19                     | 0.42              |
| 14:E:81:LEU:HD12 | 14:E:123:VAL:HG23 | 2.00                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:F:5:GLU:HA     | 15:F:63:ASN:HA    | 2.02                     | 0.42              |
| 18:I:119:ARG:HH12 | 18:I:125:PRO:HA   | 1.83                     | 0.42              |
| 19:J:59:LYS:HZ2   | 19:J:62:ARG:NH2   | 2.17                     | 0.42              |
| 8:7:2039:U:H2'    | 8:7:2040:G:H8     | 1.85                     | 0.42              |
| 8:7:2061:G:OP1    | 38:d:63:LYS:NZ    | 2.38                     | 0.42              |
| 8:7:2523:G:O2'    | 8:7:2764:A:O2'    | 2.34                     | 0.42              |
| 10:A:140:U:H3'    | 10:A:141:G:H5''   | 2.00                     | 0.42              |
| 10:A:1302:C:H41   | 22:M:14:HIS:CD2   | 2.38                     | 0.42              |
| 11:B:64:LYS:HA    | 11:B:64:LYS:HD3   | 1.88                     | 0.42              |
| 13:D:107:PHE:CG   | 13:D:145:ILE:HD11 | 2.54                     | 0.42              |
| 26:Q:77:ARG:CZ    | 26:Q:77:ARG:HB3   | 2.50                     | 0.42              |
| 35:a:207:VAL:O    | 35:a:208:TYR:C    | 2.63                     | 0.42              |
| 56:v:82:MET:HE3   | 56:v:84:ARG:HH12  | 1.84                     | 0.42              |
| 4:3:16:ARG:HB3    | 4:3:20:HIS:HB2    | 2.01                     | 0.42              |
| 6:5:29:SER:HB3    | 8:7:2885:G:O6     | 2.20                     | 0.42              |
| 8:7:600:G:H1      | 8:7:657:U:H3      | 1.68                     | 0.42              |
| 8:7:796:C:H2'     | 8:7:797:G:C8      | 2.55                     | 0.42              |
| 8:7:1114:C:N4     | 8:7:1115:G:O6     | 2.53                     | 0.42              |
| 8:7:1548:A:H2'    | 8:7:1549:A:C8     | 2.54                     | 0.42              |
| 8:7:1569:A:H2'    | 8:7:1570:A:C8     | 2.55                     | 0.42              |
| 8:7:1852:U:OP1    | 33:X:72:G:O2'     | 2.38                     | 0.42              |
| 8:7:1931:U:H2'    | 8:7:1932:A:H8     | 1.84                     | 0.42              |
| 8:7:2345:G:N3     | 8:7:2381:A:H2'    | 2.35                     | 0.42              |
| 10:A:1060:U:H2'   | 10:A:1061:G:C8    | 2.52                     | 0.42              |
| 10:A:1132:C:H5'   | 10:A:1133:G:OP2   | 2.19                     | 0.42              |
| 10:A:1227:A:H5'   | 22:M:110:LYS:NZ   | 2.35                     | 0.42              |
| 10:A:1338:G:H2'   | 10:A:1339:A:C8    | 2.54                     | 0.42              |
| 11:B:196:VAL:O    | 11:B:197:ASP:HB2  | 2.20                     | 0.42              |
| 13:D:183:LYS:HG2  | 13:D:184:ARG:HG2  | 2.01                     | 0.42              |
| 16:G:15:ASP:OD2   | 16:G:20:SER:N     | 2.33                     | 0.42              |
| 20:K:76:GLU:OE1   | 20:K:76:GLU:N     | 2.51                     | 0.42              |
| 22:M:69:LEU:HD12  | 22:M:72:GLU:OE2   | 2.19                     | 0.42              |
| 33:X:37:G:H2'     | 33:X:38:2MA:O4'   | 2.20                     | 0.42              |
| 33:X:71:U:H2'     | 33:X:72:G:O4'     | 2.19                     | 0.42              |
| 36:b:133:ARG:HB2  | 36:b:186:ALA:HB1  | 2.02                     | 0.42              |
| 37:c:22:ILE:HG23  | 37:c:190:LYS:HG3  | 2.02                     | 0.42              |
| 37:c:175:LEU:HD12 | 37:c:190:LYS:O    | 2.20                     | 0.42              |
| 45:k:76:ALA:HB2   | 45:k:113:LYS:HE2  | 2.01                     | 0.42              |
| 48:n:44:LYS:O     | 48:n:54:LYS:NZ    | 2.53                     | 0.42              |
| 52:r:58:ILE:HG13  | 52:r:58:ILE:O     | 2.19                     | 0.42              |
| 54:t:9:ILE:HG13   | 54:t:10:ALA:N     | 2.35                     | 0.42              |

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| Atom-1          | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-------------------|--------------------------|-------------------|
| 58:x:4:LYS:O    | 58:x:94:ARG:NH1   | 2.45                     | 0.42              |
| 8:7:1059:G:N2   | 45:k:132:THR:OG1  | 2.52                     | 0.42              |
| 8:7:1827:U:OP1  | 8:7:1971:U:O2'    | 2.35                     | 0.42              |
| 8:7:1827:U:OP2  | 36:b:221:ARG:NE   | 2.52                     | 0.42              |
| 8:7:2183:A:H2'  | 8:7:2184:A:C8     | 2.54                     | 0.42              |
| 9:8:66:A:H61    | 9:8:107:G:H2'     | 1.84                     | 0.42              |
| 10:A:202:G:O2'  | 10:A:468:A:N3     | 2.52                     | 0.42              |
| 10:A:222:C:H2'  | 10:A:223:A:C8     | 2.54                     | 0.42              |
| 10:A:471:U:H2'  | 10:A:472:U:C6     | 2.55                     | 0.42              |
| 10:A:506:G:H2'  | 10:A:507:C:C6     | 2.55                     | 0.42              |
| 10:A:824:G:H2'  | 10:A:825:A:C8     | 2.55                     | 0.42              |
| 10:A:1140:C:O2' | 10:A:1141:C:H6    | 2.02                     | 0.42              |
| 11:B:15:HIS:HD2 | 11:B:40:ILE:HG23  | 1.84                     | 0.42              |
| 21:L:123:LYS:HA | 21:L:123:LYS:HE3  | 2.02                     | 0.42              |
| 22:M:4:ILE:HG13 | 22:M:57:ARG:HG2   | 2.01                     | 0.42              |
| 2:1:30:LEU:HD23 | 2:1:30:LEU:H      | 1.85                     | 0.42              |
| 2:1:56:MET:HE3  | 2:1:56:MET:HB3    | 1.92                     | 0.42              |
| 4:3:19:LYS:O    | 4:3:19:LYS:HD2    | 2.20                     | 0.42              |
| 6:5:16:ARG:NH1  | 8:7:1266:G:OP1    | 2.53                     | 0.42              |
| 6:5:42:HIS:HD2  | 51:q:101:GLY:H    | 1.68                     | 0.42              |
| 7:6:40:ARG:HD2  | 8:7:2363:G:OP2    | 2.20                     | 0.42              |
| 8:7:558:U:H2'   | 8:7:559:G:C8      | 2.55                     | 0.42              |
| 8:7:948:C:H6    | 8:7:948:C:O5'     | 2.03                     | 0.42              |
| 8:7:1188:U:H2'  | 8:7:1189:A:H8     | 1.84                     | 0.42              |
| 8:7:1779:U:H5   | 8:7:1784:A:N7     | 2.18                     | 0.42              |
| 8:7:2107:G:H2'  | 8:7:2108:A:O4'    | 2.19                     | 0.42              |
| 8:7:2286:G:N2   | 41:g:24:THR:O     | 2.34                     | 0.42              |
| 9:8:66:A:N6     | 9:8:107:G:H2'     | 2.35                     | 0.42              |
| 10:A:518:C:H4'  | 10:A:519:C:H5''   | 2.01                     | 0.42              |
| 10:A:578:C:O2'  | 10:A:728:A:N3     | 2.48                     | 0.42              |
| 10:A:1025:U:O5' | 10:A:1025:U:H6    | 2.01                     | 0.42              |
| 10:A:1401:G:H2' | 10:A:1402:4OC:O4' | 2.20                     | 0.42              |
| 17:H:22:LYS:O   | 17:H:65:TYR:OH    | 2.31                     | 0.42              |
| 26:Q:45:HIS:HB3 | 26:Q:71:LYS:HG2   | 2.02                     | 0.42              |
| 32:W:17:H2U:H3' | 32:W:17:H2U:H61   | 2.01                     | 0.42              |
| 33:X:1:G:HO2'   | 33:X:2:C:P        | 2.41                     | 0.42              |
| 39:e:49:LEU:HA  | 39:e:52:ASN:ND2   | 2.35                     | 0.42              |
| 39:e:117:LEU:C  | 39:e:178:ARG:H    | 2.24                     | 0.42              |
| 4:3:27:LEU:HD11 | 4:3:47:MET:HB3    | 2.01                     | 0.42              |
| 8:7:43:G:O2'    | 8:7:44:A:OP1      | 2.34                     | 0.42              |
| 8:7:878:A:H3'   | 8:7:879:G:H8      | 1.85                     | 0.42              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 8:7:2106:U:H2'   | 8:7:2107:G:C8     | 2.55                     | 0.42              |
| 8:7:2162:G:H4'   | 8:7:2173:A:C4     | 2.55                     | 0.42              |
| 8:7:2502:G:N7    | 66:7:3303:HOH:O   | 2.37                     | 0.42              |
| 9:8:13:G:N7      | 9:8:70:C:H4'      | 2.35                     | 0.42              |
| 10:A:691:G:O2'   | 10:A:797:C:H4'    | 2.20                     | 0.42              |
| 10:A:1019:A:H5'  | 10:A:1020:G:OP2   | 2.20                     | 0.42              |
| 12:C:129:MET:HB2 | 12:C:132:ARG:HG3  | 2.02                     | 0.42              |
| 14:E:83:HIS:NE2  | 14:E:147:MET:HG3  | 2.35                     | 0.42              |
| 21:L:100:GLY:HA3 | 21:L:118:GLY:HA3  | 2.02                     | 0.42              |
| 28:S:62:VAL:HA   | 28:S:66:MET:SD    | 2.60                     | 0.42              |
| 43:i:12:LEU:HD23 | 43:i:12:LEU:HA    | 1.87                     | 0.42              |
| 60:z:40:GLN:OE1  | 60:z:44:LYS:HB2   | 2.20                     | 0.42              |
| 8:7:639:U:H2'    | 8:7:640:C:C6      | 2.55                     | 0.41              |
| 8:7:2131:U:H5'   | 8:7:2132:U:H2'    | 2.02                     | 0.41              |
| 9:8:88:C:O5'     | 9:8:88:C:H6       | 2.03                     | 0.41              |
| 10:A:368:U:H6    | 10:A:368:U:H2'    | 1.64                     | 0.41              |
| 10:A:408:A:H3'   | 10:A:409:U:H6     | 1.84                     | 0.41              |
| 10:A:831:A:H2'   | 10:A:832:G:H8     | 1.85                     | 0.41              |
| 10:A:1064:G:OP1  | 10:A:1386:G:H4'   | 2.20                     | 0.41              |
| 10:A:1095:U:OP1  | 10:A:1108:G:N2    | 2.47                     | 0.41              |
| 10:A:1112:C:C2   | 12:C:178:LEU:HD23 | 2.55                     | 0.41              |
| 10:A:1247:U:C2'  | 10:A:1248:A:H5''  | 2.49                     | 0.41              |
| 12:C:169:ARG:HE  | 12:C:169:ARG:HB2  | 1.70                     | 0.41              |
| 16:G:10:ARG:O    | 16:G:11:LYS:HB2   | 2.20                     | 0.41              |
| 26:Q:16:LYS:O    | 26:Q:16:LYS:HD3   | 2.20                     | 0.41              |
| 37:c:61:THR:OG1  | 37:c:64:GLU:HG2   | 2.20                     | 0.41              |
| 39:e:111:ILE:HB  | 39:e:114:PHE:HB2  | 2.02                     | 0.41              |
| 59:y:58:SER:O    | 59:y:73:LYS:NZ    | 2.52                     | 0.41              |
| 1:0:30:GLU:HG3   | 1:0:32:LYS:HB2    | 2.03                     | 0.41              |
| 3:2:5:GLU:OE1    | 3:2:6:LEU:HD22    | 2.20                     | 0.41              |
| 7:6:45:ARG:NH2   | 8:7:2349:G:OP1    | 2.52                     | 0.41              |
| 8:7:881:G:H1     | 8:7:895:U:H3      | 1.68                     | 0.41              |
| 8:7:1084:A:OP2   | 44:j:53:ARG:NH2   | 2.53                     | 0.41              |
| 8:7:1324:G:OP1   | 63:7:3003:SPD:N10 | 2.53                     | 0.41              |
| 8:7:2150:C:H2'   | 8:7:2151:U:O4'    | 2.20                     | 0.41              |
| 8:7:2899:A:H5'   | 47:m:136:GLN:HE21 | 1.85                     | 0.41              |
| 10:A:1:A:H3'     | 10:A:2:A:C8       | 2.55                     | 0.41              |
| 10:A:40:C:H2'    | 10:A:41:G:H8      | 1.84                     | 0.41              |
| 10:A:343:U:H3'   | 10:A:345:C:H41    | 1.85                     | 0.41              |
| 10:A:451:A:H62   | 10:A:481:G:H5'    | 1.85                     | 0.41              |
| 10:A:452:A:H3'   | 10:A:453:G:H8     | 1.84                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:A:990:C:H2'    | 10:A:991:U:C6     | 2.55                     | 0.41              |
| 10:A:1105:A:H2'   | 10:A:1106:G:C8    | 2.55                     | 0.41              |
| 10:A:1160:G:H5''  | 11:B:131:LYS:HD2  | 2.01                     | 0.41              |
| 12:C:63:SER:C     | 12:C:64:ILE:HG13  | 2.45                     | 0.41              |
| 17:H:96:MET:HB3   | 17:H:100:GLY:N    | 2.30                     | 0.41              |
| 25:P:76:LYS:C     | 25:P:78:VAL:H     | 2.28                     | 0.41              |
| 34:Y:53:G:C3'     | 34:Y:54:5MU:H5'   | 2.49                     | 0.41              |
| 38:d:115:GLN:CD   | 38:d:117:ARG:HD3  | 2.45                     | 0.41              |
| 39:e:49:LEU:HD23  | 39:e:52:ASN:HD21  | 1.84                     | 0.41              |
| 45:k:14:ALA:N     | 45:k:54:PRO:HA    | 2.32                     | 0.41              |
| 45:k:109:ILE:HG23 | 45:k:113:LYS:HZ3  | 1.85                     | 0.41              |
| 47:m:105:VAL:O    | 47:m:109:LEU:HD13 | 2.20                     | 0.41              |
| 47:m:110:PRO:O    | 47:m:115:GLY:HA3  | 2.20                     | 0.41              |
| 49:o:9:ALA:O      | 49:o:12:SER:OG    | 2.29                     | 0.41              |
| 1:0:32:LYS:NZ     | 8:7:2478:A:OP1    | 2.53                     | 0.41              |
| 6:5:21:ALA:HA     | 56:v:19:LEU:HD12  | 2.02                     | 0.41              |
| 8:7:542:C:H2'     | 8:7:543:G:C8      | 2.55                     | 0.41              |
| 8:7:2574:G:H1'    | 37:c:148:GLN:NE2  | 2.35                     | 0.41              |
| 10:A:116:A:H2'    | 10:A:117:G:O4'    | 2.20                     | 0.41              |
| 10:A:409:U:H2'    | 10:A:410:G:O4'    | 2.20                     | 0.41              |
| 10:A:417:G:H1     | 10:A:426:U:H3     | 1.69                     | 0.41              |
| 10:A:452:A:H3'    | 10:A:453:G:C8     | 2.55                     | 0.41              |
| 10:A:1307:U:H2'   | 10:A:1308:U:C6    | 2.55                     | 0.41              |
| 17:H:87:LYS:HB2   | 17:H:87:LYS:HE2   | 1.68                     | 0.41              |
| 22:M:110:LYS:HE3  | 22:M:110:LYS:HB3  | 1.84                     | 0.41              |
| 29:T:10:ARG:HA    | 29:T:13:GLN:HE22  | 1.83                     | 0.41              |
| 29:T:13:GLN:O     | 29:T:17:ALA:N     | 2.45                     | 0.41              |
| 41:g:11:LEU:HD23  | 41:g:51:GLU:HA    | 2.01                     | 0.41              |
| 43:i:8:LYS:HE3    | 43:i:8:LYS:HB2    | 1.89                     | 0.41              |
| 43:i:42:LYS:O     | 43:i:45:GLU:HG2   | 2.19                     | 0.41              |
| 56:v:2:GLU:HG3    | 56:v:108:SER:HB3  | 2.02                     | 0.41              |
| 56:v:78:GLU:OE1   | 56:v:78:GLU:N     | 2.51                     | 0.41              |
| 8:7:466:A:N1      | 8:7:795:C:O2'     | 2.50                     | 0.41              |
| 8:7:1847:A:O2'    | 8:7:1848:A:P      | 2.78                     | 0.41              |
| 8:7:2051:A:H5'    | 8:7:2578:G:O4'    | 2.21                     | 0.41              |
| 8:7:2516:A:O2'    | 8:7:2517:C:H5'    | 2.21                     | 0.41              |
| 8:7:2698:U:H2'    | 8:7:2699:C:C6     | 2.56                     | 0.41              |
| 8:7:2872:A:H2'    | 8:7:2873:A:H5''   | 2.02                     | 0.41              |
| 10:A:202:G:H2'    | 10:A:203:G:O4'    | 2.20                     | 0.41              |
| 10:A:748:G:H2'    | 10:A:749:A:C8     | 2.55                     | 0.41              |
| 10:A:1156:G:O2'   | 10:A:1180:A:N1    | 2.40                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:B:148:LEU:O    | 11:B:151:ILE:HG12 | 2.20                     | 0.41              |
| 12:C:169:ARG:NH2  | 12:C:171:GLY:O    | 2.54                     | 0.41              |
| 15:F:70:VAL:HA    | 15:F:73:GLU:OE2   | 2.21                     | 0.41              |
| 18:I:118:LEU:HD23 | 18:I:124:ARG:HG2  | 2.02                     | 0.41              |
| 23:N:62:ASN:OD1   | 23:N:75:ARG:NE    | 2.54                     | 0.41              |
| 25:P:51:ARG:O     | 25:P:52:LEU:HD23  | 2.20                     | 0.41              |
| 35:a:208:TYR:CD2  | 35:a:209:ILE:HG23 | 2.55                     | 0.41              |
| 37:c:9:VAL:HG11   | 53:s:4:ILE:HB     | 2.01                     | 0.41              |
| 39:e:103:LEU:HD12 | 39:e:107:ALA:HB3  | 2.02                     | 0.41              |
| 47:m:109:LEU:HD23 | 47:m:118:MET:HB2  | 2.02                     | 0.41              |
| 8:7:371:A:OP1     | 8:7:371:A:H3'     | 2.21                     | 0.41              |
| 8:7:773:U:O2'     | 36:b:48:ARG:HD3   | 2.20                     | 0.41              |
| 8:7:1416:G:O2'    | 8:7:1417:C:P      | 2.79                     | 0.41              |
| 8:7:1880:U:H2'    | 8:7:1881:C:C6     | 2.55                     | 0.41              |
| 10:A:279:A:H5''   | 10:A:281:G:O4'    | 2.20                     | 0.41              |
| 10:A:409:U:H3     | 10:A:433:G:H1     | 1.68                     | 0.41              |
| 10:A:1019:A:C2    | 10:A:1020:G:H1'   | 2.55                     | 0.41              |
| 10:A:1035:A:H2'   | 10:A:1036:A:C8    | 2.55                     | 0.41              |
| 10:A:1228:C:H2'   | 10:A:1229:A:H8    | 1.85                     | 0.41              |
| 10:A:1271:A:H2'   | 10:A:1272:G:C8    | 2.56                     | 0.41              |
| 10:A:1318:A:H5''  | 28:S:3:ARG:NH1    | 2.34                     | 0.41              |
| 11:B:15:HIS:HA    | 11:B:41:ILE:HB    | 2.03                     | 0.41              |
| 11:B:128:LYS:HA   | 11:B:128:LYS:HD2  | 1.86                     | 0.41              |
| 19:J:19:ASP:HA    | 19:J:22:THR:HG22  | 2.01                     | 0.41              |
| 29:T:36:TYR:HA    | 29:T:39:ILE:HD12  | 2.01                     | 0.41              |
| 39:e:175:PHE:HB3  | 39:e:177:PHE:CE2  | 2.56                     | 0.41              |
| 40:f:73:ASN:O     | 40:f:76:VAL:HG12  | 2.20                     | 0.41              |
| 46:l:10:LEU:HD11  | 46:l:14:ARG:NH2   | 2.35                     | 0.41              |
| 51:q:96:ARG:O     | 51:q:113:ILE:HD12 | 2.21                     | 0.41              |
| 60:z:50:ASN:HB2   | 60:z:82:ILE:HB    | 2.02                     | 0.41              |
| 5:4:57:VAL:HG22   | 28:S:67:VAL:HG21  | 2.02                     | 0.41              |
| 8:7:1326:U:O2'    | 8:7:2010:G:O2'    | 2.35                     | 0.41              |
| 8:7:1677:A:H2'    | 8:7:1678:A:C8     | 2.55                     | 0.41              |
| 8:7:2357:G:N2     | 8:7:2360:G:OP2    | 2.47                     | 0.41              |
| 10:A:19:A:H2'     | 10:A:20:U:C6      | 2.55                     | 0.41              |
| 10:A:70:U:H4'     | 10:A:71:A:C8      | 2.56                     | 0.41              |
| 10:A:341:C:H2'    | 10:A:342:C:C6     | 2.55                     | 0.41              |
| 10:A:402:G:H2'    | 10:A:403:C:C6     | 2.56                     | 0.41              |
| 10:A:673:A:H2'    | 10:A:674:G:C8     | 2.56                     | 0.41              |
| 10:A:950:U:H2'    | 10:A:951:G:C8     | 2.55                     | 0.41              |
| 10:A:1012:A:H2'   | 10:A:1013:G:C8    | 2.55                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:B:28:LYS:N     | 11:B:29:PRO:HD2   | 2.35                     | 0.41              |
| 11:B:213:TYR:O    | 11:B:217:VAL:HG22 | 2.20                     | 0.41              |
| 25:P:17:TYR:CE2   | 25:P:41:PRO:HG3   | 2.55                     | 0.41              |
| 29:T:18:ARG:NE    | 29:T:18:ARG:HA    | 2.35                     | 0.41              |
| 29:T:71:LYS:HA    | 29:T:74:ARG:HE    | 1.85                     | 0.41              |
| 37:c:150:GLN:HE21 | 37:c:150:GLN:HB3  | 1.67                     | 0.41              |
| 38:d:188:MET:HE1  | 38:d:193:VAL:HG22 | 2.03                     | 0.41              |
| 40:f:55:ARG:HD3   | 40:f:55:ARG:HA    | 1.87                     | 0.41              |
| 50:p:31:VAL:C     | 50:p:33:ASN:N     | 2.78                     | 0.41              |
| 4:3:47:MET:O      | 4:3:51:VAL:HG22   | 2.20                     | 0.41              |
| 7:6:52:LYS:NZ     | 8:7:937:C:OP1     | 2.39                     | 0.41              |
| 8:7:1447:C:H2'    | 8:7:1448:G:C8     | 2.56                     | 0.41              |
| 8:7:1744:A:H3'    | 8:7:1745:A:H8     | 1.86                     | 0.41              |
| 8:7:2112:G:H1'    | 33:X:20:A:C5      | 2.55                     | 0.41              |
| 8:7:2590:A:H2'    | 8:7:2591:C:C6     | 2.55                     | 0.41              |
| 9:8:48:U:H4'      | 52:r:100:HIS:CE1  | 2.55                     | 0.41              |
| 10:A:491:G:O2'    | 10:A:492:C:H5'    | 2.20                     | 0.41              |
| 10:A:1064:G:H21   | 10:A:1190:G:H1'   | 1.85                     | 0.41              |
| 10:A:1071:C:H2'   | 10:A:1072:G:C8    | 2.54                     | 0.41              |
| 11:B:27:MET:HE2   | 11:B:188:ASP:O    | 2.21                     | 0.41              |
| 39:e:66:LEU:HD23  | 39:e:88:LYS:HD3   | 2.03                     | 0.41              |
| 43:i:68:ARG:O     | 43:i:72:ILE:HG22  | 2.20                     | 0.41              |
| 45:k:125:MET:O    | 45:k:129:ILE:HG12 | 2.21                     | 0.41              |
| 50:p:32:ARG:C     | 50:p:34:ALA:N     | 2.79                     | 0.41              |
| 52:r:51:ALA:HB3   | 52:r:78:VAL:HB    | 2.03                     | 0.41              |
| 7:6:33:LEU:H      | 7:6:33:LEU:HD23   | 1.86                     | 0.41              |
| 8:7:276:U:O2'     | 8:7:278:A:N7      | 2.52                     | 0.41              |
| 8:7:1095:A:N6     | 45:k:26:PRO:HB2   | 2.35                     | 0.41              |
| 8:7:1410:G:H1     | 8:7:1592:C:H42    | 1.69                     | 0.41              |
| 8:7:1486:U:H2'    | 8:7:1487:U:C6     | 2.55                     | 0.41              |
| 8:7:1701:A:OP1    | 8:7:1763:G:N2     | 2.46                     | 0.41              |
| 8:7:1753:G:N2     | 8:7:1756:G:O5'    | 2.51                     | 0.41              |
| 10:A:31:G:C8      | 10:A:306:A:H1'    | 2.56                     | 0.41              |
| 10:A:202:G:H21    | 10:A:466:A:H61    | 1.69                     | 0.41              |
| 10:A:816:A:OP1    | 10:A:1526:G:O2'   | 2.34                     | 0.41              |
| 10:A:1073:U:H2'   | 10:A:1074:G:O4'   | 2.20                     | 0.41              |
| 10:A:1317:C:O5'   | 23:N:28:LYS:NZ    | 2.51                     | 0.41              |
| 10:A:1398:A:H5''  | 10:A:1401:G:H4'   | 2.03                     | 0.41              |
| 10:A:1530:G:H2'   | 10:A:1531:A:C8    | 2.56                     | 0.41              |
| 14:E:134:ILE:HG13 | 14:E:135:ASN:N    | 2.36                     | 0.41              |
| 15:F:79:ARG:HG2   | 15:F:80:PHE:CE1   | 2.56                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 20:K:12:VAL:O    | 20:K:13:ARG:HG2   | 2.20                     | 0.41              |
| 22:M:17:ILE:HD13 | 22:M:17:ILE:HA    | 1.93                     | 0.41              |
| 34:Y:54:5MU:OP1  | 42:h:55:ARG:HB2   | 2.20                     | 0.41              |
| 49:o:132:ARG:HG3 | 49:o:142:ILE:HD12 | 2.02                     | 0.41              |
| 52:r:60:GLU:OE1  | 52:r:60:GLU:N     | 2.54                     | 0.41              |
| 58:x:98:SER:C    | 58:x:100:SER:H    | 2.27                     | 0.41              |
| 4:3:9:GLN:HA     | 4:3:55:VAL:HA     | 2.03                     | 0.41              |
| 4:3:27:LEU:HG    | 4:3:47:MET:HG3    | 2.01                     | 0.41              |
| 4:3:47:MET:HE1   | 8:7:851:C:O4'     | 2.20                     | 0.41              |
| 8:7:320:A:N3     | 38:d:163:ASN:ND2  | 2.58                     | 0.41              |
| 8:7:414:C:H2'    | 8:7:415:A:C8      | 2.56                     | 0.41              |
| 8:7:476:G:H22    | 8:7:479:A:C5'     | 2.33                     | 0.41              |
| 8:7:1046:A:O4'   | 44:j:62:ARG:NH2   | 2.54                     | 0.41              |
| 8:7:1796:U:H2'   | 8:7:1797:G:H8     | 1.85                     | 0.41              |
| 8:7:2108:A:H2'   | 8:7:2109:U:C6     | 2.56                     | 0.41              |
| 8:7:2236:U:H2'   | 8:7:2237:G:O4'    | 2.21                     | 0.41              |
| 8:7:2329:U:H2'   | 8:7:2330:G:C8     | 2.55                     | 0.41              |
| 8:7:2336:A:H61   | 60:z:43:THR:HG21  | 1.86                     | 0.41              |
| 8:7:2707:U:O2    | 51:q:71:ARG:NH1   | 2.45                     | 0.41              |
| 10:A:94:G:H4'    | 10:A:95:C:C5'     | 2.51                     | 0.41              |
| 10:A:151:A:H2'   | 10:A:152:A:C8     | 2.55                     | 0.41              |
| 10:A:389:A:H3'   | 10:A:390:U:C6     | 2.54                     | 0.41              |
| 10:A:440:C:C2    | 10:A:441:A:C8     | 3.08                     | 0.41              |
| 10:A:501:C:H2'   | 10:A:502:A:O4'    | 2.21                     | 0.41              |
| 10:A:748:G:H2'   | 10:A:749:A:H8     | 1.86                     | 0.41              |
| 10:A:923:A:N6    | 10:A:1392:G:O6    | 2.54                     | 0.41              |
| 10:A:945:G:N3    | 10:A:945:G:H2'    | 2.36                     | 0.41              |
| 10:A:1005:A:H2'  | 10:A:1006:G:O4'   | 2.20                     | 0.41              |
| 10:A:1105:A:H2'  | 10:A:1106:G:H8    | 1.86                     | 0.41              |
| 10:A:1237:C:H4'  | 10:A:1300:G:H22   | 1.86                     | 0.41              |
| 10:A:1269:A:O5'  | 10:A:1269:A:H8    | 2.03                     | 0.41              |
| 12:C:22:TRP:CZ2  | 12:C:33:LEU:HD23  | 2.55                     | 0.41              |
| 12:C:88:ARG:HG2  | 12:C:101:ILE:HG12 | 2.02                     | 0.41              |
| 14:E:83:HIS:CG   | 17:H:96:MET:HE1   | 2.55                     | 0.41              |
| 19:J:15:HIS:HB3  | 19:J:70:HIS:NE2   | 2.35                     | 0.41              |
| 19:J:36:VAL:HG12 | 19:J:76:ILE:HG13  | 2.03                     | 0.41              |
| 21:L:43:LYS:HG2  | 21:L:44:LYS:H     | 1.86                     | 0.41              |
| 24:O:3:LEU:HD23  | 24:O:8:THR:HG22   | 2.03                     | 0.41              |
| 24:O:64:ARG:HD2  | 24:O:67:LEU:HD21  | 2.02                     | 0.41              |
| 33:X:72:G:H5'    | 33:X:73:C:OP2     | 2.20                     | 0.41              |
| 36:b:227:PRO:HA  | 36:b:233:GLY:HA2  | 2.02                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 38:d:111:GLU:HG2  | 49:o:1:MET:HG2    | 2.03                     | 0.41              |
| 39:e:58:ALA:HB2   | 39:e:65:PRO:HD3   | 2.02                     | 0.41              |
| 40:f:98:VAL:HG22  | 40:f:100:GLY:H    | 1.86                     | 0.41              |
| 41:g:50:LYS:HE2   | 41:g:50:LYS:HB2   | 1.88                     | 0.41              |
| 42:h:53:MET:SD    | 42:h:120:ALA:HB2  | 2.61                     | 0.41              |
| 43:i:29:PHE:CZ    | 43:i:35:LYS:HE2   | 2.55                     | 0.41              |
| 44:j:111:ALA:HB3  | 44:j:118:ILE:HB   | 2.02                     | 0.41              |
| 48:n:45:GLU:HA    | 48:n:54:LYS:HZ1   | 1.86                     | 0.41              |
| 49:o:51:GLU:O     | 49:o:51:GLU:HG3   | 2.20                     | 0.41              |
| 52:r:11:ALA:O     | 52:r:12:THR:C     | 2.63                     | 0.41              |
| 4:3:24:LEU:HD21   | 4:3:54:MET:SD     | 2.61                     | 0.41              |
| 8:7:124:G:OP1     | 8:7:1376:C:O2'    | 2.27                     | 0.41              |
| 8:7:655:A:H8      | 8:7:655:A:OP1     | 2.04                     | 0.41              |
| 8:7:1935:G:H21    | 8:7:1964:G:H5'    | 1.86                     | 0.41              |
| 8:7:2134:A:H8     | 8:7:2134:A:O5'    | 2.04                     | 0.41              |
| 8:7:2723:C:H2'    | 8:7:2724:U:O4'    | 2.21                     | 0.41              |
| 10:A:21:G:H2'     | 10:A:22:G:H8      | 1.85                     | 0.41              |
| 10:A:504:C:N3     | 10:A:511:C:N4     | 2.69                     | 0.41              |
| 10:A:512:U:H2'    | 10:A:513:C:C6     | 2.56                     | 0.41              |
| 10:A:865:A:H5'    | 10:A:1078:U:C5    | 2.56                     | 0.41              |
| 10:A:1047:G:H4'   | 23:N:4:GLN:NE2    | 2.36                     | 0.41              |
| 10:A:1080:A:OP1   | 14:E:52:LYS:HE2   | 2.20                     | 0.41              |
| 10:A:1379:G:O6    | 16:G:2:PRO:HB3    | 2.20                     | 0.41              |
| 23:N:76:LYS:HG3   | 23:N:77:PHE:CD2   | 2.54                     | 0.41              |
| 40:f:105:LEU:HD21 | 40:f:148:LEU:HD12 | 2.03                     | 0.41              |
| 42:h:34:LYS:HD3   | 59:y:82:TYR:HA    | 2.03                     | 0.41              |
| 7:6:45:ARG:NH1    | 8:7:2418:A:OP1    | 2.54                     | 0.40              |
| 8:7:552:U:H2'     | 8:7:553:G:C8      | 2.56                     | 0.40              |
| 8:7:668:A:H2'     | 8:7:670:A:H62     | 1.86                     | 0.40              |
| 8:7:979:A:H2'     | 8:7:982:C:H42     | 1.85                     | 0.40              |
| 8:7:2145:C:H3'    | 8:7:2146:C:C2     | 2.55                     | 0.40              |
| 8:7:2305:U:C2     | 39:e:151:GLY:HA3  | 2.57                     | 0.40              |
| 8:7:2899:A:H5'    | 47:m:136:GLN:NE2  | 2.36                     | 0.40              |
| 10:A:1271:A:H2'   | 10:A:1272:G:H8    | 1.85                     | 0.40              |
| 10:A:1315:U:H2'   | 10:A:1316:G:C8    | 2.56                     | 0.40              |
| 10:A:1347:G:N7    | 18:I:13:LYS:HE2   | 2.36                     | 0.40              |
| 13:D:11:LEU:HD23  | 13:D:63:ARG:HG2   | 2.03                     | 0.40              |
| 36:b:67:PHE:HE1   | 36:b:156:ARG:HD2  | 1.85                     | 0.40              |
| 40:f:35:ARG:HD3   | 40:f:71:LEU:HD13  | 2.03                     | 0.40              |
| 40:f:117:LEU:HD13 | 40:f:121:ILE:HG22 | 2.02                     | 0.40              |
| 57:w:4:GLU:HG3    | 57:w:49:LYS:HE2   | 2.03                     | 0.40              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 60:z:25:ARG:HH21 | 60:z:29:GLU:HB3   | 1.85                     | 0.40              |
| 5:4:6:HIS:CE1    | 39:e:63:GLN:HA    | 2.41                     | 0.40              |
| 7:6:25:LYS:O     | 49:o:61:LEU:HD12  | 2.21                     | 0.40              |
| 8:7:558:U:H5'    | 47:m:114:LEU:HD13 | 2.03                     | 0.40              |
| 8:7:1283:G:N1    | 8:7:1286:A:OP2    | 2.53                     | 0.40              |
| 8:7:1367:A:O3'   | 46:l:25:LYS:NZ    | 2.53                     | 0.40              |
| 8:7:1386:C:H2'   | 8:7:1387:A:C8     | 2.56                     | 0.40              |
| 8:7:2676:C:P     | 48:n:31:ARG:HH22  | 2.44                     | 0.40              |
| 10:A:57:G:H2'    | 10:A:58:C:O4'     | 2.21                     | 0.40              |
| 10:A:82:G:H3'    | 10:A:83:C:H6      | 1.87                     | 0.40              |
| 10:A:203:G:H1'   | 10:A:465:A:H61    | 1.87                     | 0.40              |
| 10:A:310:G:H5''  | 25:P:31:ARG:HB2   | 2.02                     | 0.40              |
| 10:A:551:U:H2'   | 10:A:552:U:C6     | 2.56                     | 0.40              |
| 10:A:993:G:O2'   | 10:A:994:A:N7     | 2.50                     | 0.40              |
| 10:A:1157:A:H5'  | 10:A:1158:C:C6    | 2.56                     | 0.40              |
| 11:B:100:MET:HE2 | 11:B:100:MET:HB2  | 1.91                     | 0.40              |
| 12:C:49:LYS:HE2  | 12:C:49:LYS:HB3   | 1.93                     | 0.40              |
| 15:F:12:PRO:HG3  | 15:F:56:LYS:O     | 2.22                     | 0.40              |
| 16:G:15:ASP:OD1  | 16:G:18:PHE:N     | 2.55                     | 0.40              |
| 16:G:47:LEU:HD23 | 16:G:47:LEU:HA    | 1.90                     | 0.40              |
| 16:G:69:VAL:O    | 16:G:138:ARG:HG3  | 2.21                     | 0.40              |
| 25:P:19:VAL:HG12 | 25:P:36:VAL:HG23  | 2.03                     | 0.40              |
| 34:Y:58:A:O2'    | 34:Y:60:C:OP2     | 2.26                     | 0.40              |
| 49:o:79:LEU:HG   | 49:o:111:ILE:O    | 2.20                     | 0.40              |
| 3:2:14:LEU:HD22  | 3:2:53:VAL:HG23   | 2.03                     | 0.40              |
| 7:6:33:LEU:O     | 7:6:41:LYS:HD2    | 2.22                     | 0.40              |
| 8:7:627:A:H4'    | 8:7:628:G:H5'     | 2.04                     | 0.40              |
| 8:7:1054:A:H2'   | 8:7:1055:G:C8     | 2.57                     | 0.40              |
| 8:7:1799:G:C2    | 36:b:154:LEU:HD13 | 2.56                     | 0.40              |
| 9:8:48:U:H5'     | 52:r:98:GLN:NE2   | 2.37                     | 0.40              |
| 10:A:1456:A:H2'  | 10:A:1457:G:O4'   | 2.21                     | 0.40              |
| 16:G:58:GLU:H    | 16:G:58:GLU:CD    | 2.21                     | 0.40              |
| 22:M:71:ARG:HD3  | 39:e:115:ARG:HD2  | 2.04                     | 0.40              |
| 30:U:28:VAL:O    | 30:U:32:VAL:HG23  | 2.20                     | 0.40              |
| 33:X:48:3AU:O5'  | 33:X:48:3AU:H6    | 2.21                     | 0.40              |
| 40:f:47:ASP:CG   | 40:f:48:ASN:H     | 2.29                     | 0.40              |
| 52:r:3:LYS:HE3   | 52:r:3:LYS:HB3    | 1.84                     | 0.40              |
| 52:r:78:VAL:HA   | 52:r:81:ARG:HD2   | 2.03                     | 0.40              |
| 8:7:489:G:H22    | 8:7:1320:C:H3'    | 1.87                     | 0.40              |
| 8:7:997:G:OP1    | 54:t:92:ARG:HD2   | 2.21                     | 0.40              |
| 8:7:1088:A:N6    | 45:k:132:THR:OG1  | 2.55                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 8:7:1487:U:H2'   | 8:7:1488:C:C6    | 2.56                     | 0.40              |
| 8:7:2156:G:H8    | 8:7:2156:G:O5'   | 2.05                     | 0.40              |
| 10:A:266:G:H1'   | 10:A:268:U:OP2   | 2.22                     | 0.40              |
| 10:A:519:C:H3'   | 10:A:520:A:C8    | 2.55                     | 0.40              |
| 10:A:696:A:H2'   | 10:A:697:U:C6    | 2.57                     | 0.40              |
| 10:A:1064:G:N2   | 10:A:1190:G:H1'  | 2.36                     | 0.40              |
| 19:J:56:HIS:ND1  | 19:J:57:VAL:HG13 | 2.36                     | 0.40              |
| 26:Q:30:LYS:HE3  | 26:Q:35:GLY:HA2  | 2.04                     | 0.40              |
| 34:Y:75:C:H2'    | 34:Y:76:A:C4     | 2.57                     | 0.40              |
| 35:a:3:LYS:HE2   | 35:a:3:LYS:HB3   | 1.94                     | 0.40              |
| 46:l:25:LYS:HA   | 46:l:28:ARG:HB2  | 2.04                     | 0.40              |
| 49:o:37:GLY:O    | 49:o:41:ARG:HG2  | 2.21                     | 0.40              |
| 8:7:898:C:H2'    | 8:7:899:A:O4'    | 2.21                     | 0.40              |
| 10:A:200:G:H1    | 10:A:217:C:H42   | 1.68                     | 0.40              |
| 10:A:203:G:H1    | 10:A:214:C:N4    | 2.16                     | 0.40              |
| 10:A:663:A:O3'   | 27:R:53:ARG:NH2  | 2.53                     | 0.40              |
| 10:A:1144:G:H21  | 10:A:1146:A:H62  | 1.69                     | 0.40              |
| 11:B:56:GLU:HG3  | 11:B:198:PHE:CE1 | 2.56                     | 0.40              |
| 12:C:30:ALA:HA   | 12:C:33:LEU:HD12 | 2.04                     | 0.40              |
| 12:C:185:ASN:OD1 | 12:C:186:THR:N   | 2.47                     | 0.40              |
| 14:E:80:THR:HG23 | 14:E:122:ASN:O   | 2.22                     | 0.40              |
| 33:X:74:A:H2'    | 33:X:74:A:N3     | 2.36                     | 0.40              |
| 37:c:49:GLN:OE1  | 37:c:67:HIS:NE2  | 2.46                     | 0.40              |
| 38:d:77:ILE:H    | 38:d:77:ILE:HD12 | 1.86                     | 0.40              |
| 56:v:24:ILE:O    | 56:v:24:ILE:HG22 | 2.20                     | 0.40              |
| 56:v:26:GLY:H    | 56:v:71:VAL:HG23 | 1.85                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed      | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|------------|----------|----------|-------------|-----|
| 1   | 0     | 36/38 (95%)   | 33 (92%)   | 3 (8%)   | 0        | 100         | 100 |
| 2   | 1     | 75/78 (96%)   | 74 (99%)   | 1 (1%)   | 0        | 100         | 100 |
| 3   | 2     | 61/63 (97%)   | 60 (98%)   | 1 (2%)   | 0        | 100         | 100 |
| 4   | 3     | 56/59 (95%)   | 54 (96%)   | 2 (4%)   | 0        | 100         | 100 |
| 5   | 4     | 66/70 (94%)   | 56 (85%)   | 9 (14%)  | 1 (2%)   | 8           | 32  |
| 6   | 5     | 54/57 (95%)   | 54 (100%)  | 0        | 0        | 100         | 100 |
| 7   | 6     | 62/65 (95%)   | 60 (97%)   | 2 (3%)   | 0        | 100         | 100 |
| 11  | B     | 225/241 (93%) | 189 (84%)  | 29 (13%) | 7 (3%)   | 3           | 18  |
| 12  | C     | 210/233 (90%) | 186 (89%)  | 23 (11%) | 1 (0%)   | 24          | 57  |
| 13  | D     | 203/206 (98%) | 200 (98%)  | 3 (2%)   | 0        | 100         | 100 |
| 14  | E     | 156/167 (93%) | 152 (97%)  | 4 (3%)   | 0        | 100         | 100 |
| 15  | F     | 104/135 (77%) | 84 (81%)   | 19 (18%) | 1 (1%)   | 12          | 41  |
| 16  | G     | 151/179 (84%) | 140 (93%)  | 10 (7%)  | 1 (1%)   | 18          | 49  |
| 17  | H     | 127/130 (98%) | 127 (100%) | 0        | 0        | 100         | 100 |
| 18  | I     | 125/130 (96%) | 117 (94%)  | 8 (6%)   | 0        | 100         | 100 |
| 19  | J     | 98/103 (95%)  | 89 (91%)   | 8 (8%)   | 1 (1%)   | 12          | 41  |
| 20  | K     | 116/129 (90%) | 102 (88%)  | 14 (12%) | 0        | 100         | 100 |
| 21  | L     | 121/124 (98%) | 116 (96%)  | 5 (4%)   | 0        | 100         | 100 |
| 22  | M     | 115/118 (98%) | 108 (94%)  | 7 (6%)   | 0        | 100         | 100 |
| 23  | N     | 98/101 (97%)  | 95 (97%)   | 3 (3%)   | 0        | 100         | 100 |
| 24  | O     | 86/89 (97%)   | 84 (98%)   | 2 (2%)   | 0        | 100         | 100 |
| 25  | P     | 80/82 (98%)   | 75 (94%)   | 5 (6%)   | 0        | 100         | 100 |
| 26  | Q     | 78/84 (93%)   | 77 (99%)   | 1 (1%)   | 0        | 100         | 100 |
| 27  | R     | 64/75 (85%)   | 52 (81%)   | 12 (19%) | 0        | 100         | 100 |
| 28  | S     | 81/92 (88%)   | 78 (96%)   | 3 (4%)   | 0        | 100         | 100 |
| 29  | T     | 84/87 (97%)   | 84 (100%)  | 0        | 0        | 100         | 100 |
| 30  | U     | 68/71 (96%)   | 64 (94%)   | 3 (4%)   | 1 (2%)   | 8           | 32  |
| 35  | a     | 130/234 (56%) | 123 (95%)  | 7 (5%)   | 0        | 100         | 100 |
| 36  | b     | 269/273 (98%) | 265 (98%)  | 4 (2%)   | 0        | 100         | 100 |
| 37  | c     | 207/209 (99%) | 202 (98%)  | 5 (2%)   | 0        | 100         | 100 |
| 38  | d     | 199/201 (99%) | 194 (98%)  | 5 (2%)   | 0        | 100         | 100 |
| 39  | e     | 176/179 (98%) | 170 (97%)  | 6 (3%)   | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 40  | f     | 174/177 (98%)   | 170 (98%)  | 4 (2%)   | 0        | 100         | 100 |
| 41  | g     | 50/55 (91%)     | 50 (100%)  | 0        | 0        | 100         | 100 |
| 42  | h     | 135/136 (99%)   | 135 (100%) | 0        | 0        | 100         | 100 |
| 43  | i     | 147/149 (99%)   | 122 (83%)  | 25 (17%) | 0        | 100         | 100 |
| 44  | j     | 133/165 (81%)   | 122 (92%)  | 11 (8%)  | 0        | 100         | 100 |
| 45  | k     | 132/142 (93%)   | 123 (93%)  | 9 (7%)   | 0        | 100         | 100 |
| 46  | l     | 44/46 (96%)     | 44 (100%)  | 0        | 0        | 100         | 100 |
| 47  | m     | 140/142 (99%)   | 137 (98%)  | 2 (1%)   | 1 (1%)   | 18          | 49  |
| 48  | n     | 121/123 (98%)   | 119 (98%)  | 2 (2%)   | 0        | 100         | 100 |
| 49  | o     | 142/144 (99%)   | 138 (97%)  | 4 (3%)   | 0        | 100         | 100 |
| 50  | p     | 5/36 (14%)      | 2 (40%)    | 2 (40%)  | 1 (20%)  | 0           | 0   |
| 51  | q     | 118/127 (93%)   | 115 (98%)  | 3 (2%)   | 0        | 100         | 100 |
| 52  | r     | 114/117 (97%)   | 110 (96%)  | 3 (3%)   | 1 (1%)   | 14          | 44  |
| 53  | s     | 112/115 (97%)   | 111 (99%)  | 1 (1%)   | 0        | 100         | 100 |
| 54  | t     | 115/118 (98%)   | 114 (99%)  | 1 (1%)   | 0        | 100         | 100 |
| 55  | u     | 101/103 (98%)   | 94 (93%)   | 7 (7%)   | 0        | 100         | 100 |
| 56  | v     | 108/110 (98%)   | 99 (92%)   | 8 (7%)   | 1 (1%)   | 14          | 44  |
| 57  | w     | 91/100 (91%)    | 89 (98%)   | 2 (2%)   | 0        | 100         | 100 |
| 58  | x     | 100/104 (96%)   | 94 (94%)   | 6 (6%)   | 0        | 100         | 100 |
| 59  | y     | 92/94 (98%)     | 92 (100%)  | 0        | 0        | 100         | 100 |
| 60  | z     | 82/85 (96%)     | 79 (96%)   | 3 (4%)   | 0        | 100         | 100 |
| All | All   | 6037/6490 (93%) | 5723 (95%) | 297 (5%) | 17 (0%)  | 37          | 67  |

All (17) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 30  | U     | 64  | ASN  |
| 11  | B     | 117 | LEU  |
| 11  | B     | 118 | GLU  |
| 15  | F     | 38  | ARG  |
| 19  | J     | 94  | ALA  |
| 47  | m     | 95  | ARG  |
| 16  | G     | 10  | ARG  |
| 11  | B     | 74  | ARG  |
| 11  | B     | 119 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11  | B     | 187 | VAL  |
| 11  | B     | 188 | ASP  |
| 12  | C     | 60  | PRO  |
| 52  | r     | 12  | THR  |
| 56  | v     | 65  | ASP  |
| 5   | 4     | 7   | PRO  |
| 11  | B     | 156 | GLY  |
| 50  | p     | 31  | VAL  |

### 5.3.2 Protein sidechains [i](#)

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

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

| Mol | Chain | Analysed      | Rotameric  | Outliers | Percentiles |     |
|-----|-------|---------------|------------|----------|-------------|-----|
| 1   | 0     | 34/34 (100%)  | 34 (100%)  | 0        | 100         | 100 |
| 2   | 1     | 67/68 (98%)   | 67 (100%)  | 0        | 100         | 100 |
| 3   | 2     | 55/55 (100%)  | 55 (100%)  | 0        | 100         | 100 |
| 4   | 3     | 48/49 (98%)   | 48 (100%)  | 0        | 100         | 100 |
| 5   | 4     | 60/62 (97%)   | 60 (100%)  | 0        | 100         | 100 |
| 6   | 5     | 47/48 (98%)   | 47 (100%)  | 0        | 100         | 100 |
| 7   | 6     | 51/52 (98%)   | 51 (100%)  | 0        | 100         | 100 |
| 11  | B     | 189/199 (95%) | 189 (100%) | 0        | 100         | 100 |
| 12  | C     | 172/190 (90%) | 171 (99%)  | 1 (1%)   | 78          | 83  |
| 13  | D     | 172/173 (99%) | 172 (100%) | 0        | 100         | 100 |
| 14  | E     | 120/126 (95%) | 120 (100%) | 0        | 100         | 100 |
| 15  | F     | 92/116 (79%)  | 92 (100%)  | 0        | 100         | 100 |
| 16  | G     | 126/147 (86%) | 124 (98%)  | 2 (2%)   | 55          | 75  |
| 17  | H     | 104/105 (99%) | 104 (100%) | 0        | 100         | 100 |
| 18  | I     | 105/107 (98%) | 105 (100%) | 0        | 100         | 100 |
| 19  | J     | 88/90 (98%)   | 88 (100%)  | 0        | 100         | 100 |
| 20  | K     | 91/99 (92%)   | 91 (100%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 21  | L     | 103/104 (99%)  | 103 (100%) | 0        | 100         | 100 |
| 22  | M     | 95/96 (99%)    | 95 (100%)  | 0        | 100         | 100 |
| 23  | N     | 83/84 (99%)    | 83 (100%)  | 0        | 100         | 100 |
| 24  | O     | 76/77 (99%)    | 76 (100%)  | 0        | 100         | 100 |
| 25  | P     | 65/65 (100%)   | 65 (100%)  | 0        | 100         | 100 |
| 26  | Q     | 74/78 (95%)    | 74 (100%)  | 0        | 100         | 100 |
| 27  | R     | 57/65 (88%)    | 55 (96%)   | 2 (4%)   | 32          | 62  |
| 28  | S     | 72/79 (91%)    | 72 (100%)  | 0        | 100         | 100 |
| 29  | T     | 65/66 (98%)    | 65 (100%)  | 0        | 100         | 100 |
| 30  | U     | 59/61 (97%)    | 59 (100%)  | 0        | 100         | 100 |
| 35  | a     | 110/181 (61%)  | 110 (100%) | 0        | 100         | 100 |
| 36  | b     | 216/218 (99%)  | 216 (100%) | 0        | 100         | 100 |
| 37  | c     | 164/164 (100%) | 164 (100%) | 0        | 100         | 100 |
| 38  | d     | 165/165 (100%) | 165 (100%) | 0        | 100         | 100 |
| 39  | e     | 149/150 (99%)  | 148 (99%)  | 1 (1%)   | 76          | 82  |
| 40  | f     | 137/138 (99%)  | 135 (98%)  | 2 (2%)   | 57          | 75  |
| 41  | g     | 47/49 (96%)    | 47 (100%)  | 0        | 100         | 100 |
| 42  | h     | 110/109 (101%) | 110 (100%) | 0        | 100         | 100 |
| 43  | i     | 114/114 (100%) | 114 (100%) | 0        | 100         | 100 |
| 44  | j     | 103/123 (84%)  | 103 (100%) | 0        | 100         | 100 |
| 45  | k     | 104/110 (94%)  | 104 (100%) | 0        | 100         | 100 |
| 46  | l     | 38/38 (100%)   | 38 (100%)  | 0        | 100         | 100 |
| 47  | m     | 116/116 (100%) | 115 (99%)  | 1 (1%)   | 70          | 80  |
| 48  | n     | 104/104 (100%) | 104 (100%) | 0        | 100         | 100 |
| 49  | o     | 103/103 (100%) | 103 (100%) | 0        | 100         | 100 |
| 50  | p     | 5/5 (100%)     | 5 (100%)   | 0        | 100         | 100 |
| 51  | q     | 100/103 (97%)  | 100 (100%) | 0        | 100         | 100 |
| 52  | r     | 86/87 (99%)    | 86 (100%)  | 0        | 100         | 100 |
| 53  | s     | 99/100 (99%)   | 99 (100%)  | 0        | 100         | 100 |
| 54  | t     | 89/90 (99%)    | 89 (100%)  | 0        | 100         | 100 |
| 55  | u     | 84/84 (100%)   | 84 (100%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Rotameric   | Outliers | Percentiles |     |
|-----|-------|-----------------|-------------|----------|-------------|-----|
| 56  | v     | 93/93 (100%)    | 93 (100%)   | 0        | 100         | 100 |
| 57  | w     | 80/84 (95%)     | 80 (100%)   | 0        | 100         | 100 |
| 58  | x     | 83/85 (98%)     | 83 (100%)   | 0        | 100         | 100 |
| 59  | y     | 78/78 (100%)    | 78 (100%)   | 0        | 100         | 100 |
| 60  | z     | 62/63 (98%)     | 62 (100%)   | 0        | 100         | 100 |
| All | All   | 5009/5249 (95%) | 5000 (100%) | 9 (0%)   | 85          | 89  |

All (9) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 12  | C     | 64  | ILE  |
| 16  | G     | 2   | PRO  |
| 16  | G     | 126 | ASP  |
| 27  | R     | 11  | CYS  |
| 27  | R     | 74  | HIS  |
| 39  | e     | 175 | PHE  |
| 40  | f     | 69  | ARG  |
| 40  | f     | 72  | LEU  |
| 47  | m     | 99  | ARG  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | 1     | 20  | HIS  |
| 3   | 2     | 15  | ASN  |
| 3   | 2     | 25  | GLN  |
| 3   | 2     | 38  | GLN  |
| 4   | 3     | 9   | GLN  |
| 6   | 5     | 4   | GLN  |
| 11  | B     | 89  | GLN  |
| 11  | B     | 122 | GLN  |
| 14  | E     | 89  | HIS  |
| 14  | E     | 122 | ASN  |
| 16  | G     | 148 | ASN  |
| 19  | J     | 58  | ASN  |
| 19  | J     | 99  | GLN  |
| 20  | K     | 22  | HIS  |
| 20  | K     | 119 | ASN  |
| 21  | L     | 29  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 21  | L     | 46  | ASN  |
| 29  | T     | 55  | GLN  |
| 36  | b     | 143 | ASN  |
| 36  | b     | 200 | HIS  |
| 36  | b     | 243 | HIS  |
| 36  | b     | 260 | ASN  |
| 37  | c     | 150 | GLN  |
| 37  | c     | 173 | GLN  |
| 38  | d     | 9   | GLN  |
| 38  | d     | 115 | GLN  |
| 39  | e     | 5   | HIS  |
| 40  | f     | 73  | ASN  |
| 40  | f     | 101 | ASN  |
| 40  | f     | 115 | HIS  |
| 41  | g     | 19  | HIS  |
| 42  | h     | 13  | HIS  |
| 43  | i     | 43  | ASN  |
| 43  | i     | 133 | GLN  |
| 45  | k     | 43  | ASN  |
| 45  | k     | 105 | GLN  |
| 47  | m     | 47  | HIS  |
| 47  | m     | 80  | HIS  |
| 48  | n     | 82  | ASN  |
| 49  | o     | 99  | ASN  |
| 49  | o     | 104 | GLN  |
| 53  | s     | 10  | GLN  |
| 53  | s     | 77  | HIS  |
| 54  | t     | 59  | GLN  |
| 57  | w     | 59  | ASN  |
| 57  | w     | 72  | GLN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 10  | A     | 1534/1535 (99%) | 396 (25%)         | 30 (1%)         |
| 31  | V     | 23/24 (95%)     | 13 (56%)          | 3 (13%)         |
| 32  | W     | 75/76 (98%)     | 24 (32%)          | 4 (5%)          |
| 33  | X     | 76/77 (98%)     | 28 (36%)          | 6 (7%)          |
| 34  | Y     | 75/76 (98%)     | 22 (29%)          | 2 (2%)          |
| 8   | 7     | 2903/2921 (99%) | 465 (16%)         | 31 (1%)         |
| 9   | 8     | 119/120 (99%)   | 14 (11%)          | 3 (2%)          |

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| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| All | All   | 4805/4829 (99%) | 962 (20%)         | 79 (1%)         |

All (962) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8   | 7     | 10  | A    |
| 8   | 7     | 15  | G    |
| 8   | 7     | 34  | U    |
| 8   | 7     | 44  | A    |
| 8   | 7     | 46  | G    |
| 8   | 7     | 55  | G    |
| 8   | 7     | 71  | A    |
| 8   | 7     | 74  | A    |
| 8   | 7     | 75  | G    |
| 8   | 7     | 101 | A    |
| 8   | 7     | 102 | U    |
| 8   | 7     | 103 | A    |
| 8   | 7     | 110 | G    |
| 8   | 7     | 118 | A    |
| 8   | 7     | 119 | A    |
| 8   | 7     | 120 | U    |
| 8   | 7     | 125 | A    |
| 8   | 7     | 135 | U    |
| 8   | 7     | 139 | U    |
| 8   | 7     | 141 | G    |
| 8   | 7     | 142 | A    |
| 8   | 7     | 159 | G    |
| 8   | 7     | 163 | C    |
| 8   | 7     | 174 | U    |
| 8   | 7     | 177 | G    |
| 8   | 7     | 178 | G    |
| 8   | 7     | 181 | A    |
| 8   | 7     | 196 | A    |
| 8   | 7     | 199 | A    |
| 8   | 7     | 215 | G    |
| 8   | 7     | 216 | A    |
| 8   | 7     | 221 | A    |
| 8   | 7     | 222 | A    |
| 8   | 7     | 248 | G    |
| 8   | 7     | 252 | G    |
| 8   | 7     | 275 | C    |
| 8   | 7     | 277 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8   | 7     | 278 | A    |
| 8   | 7     | 279 | A    |
| 8   | 7     | 283 | G    |
| 8   | 7     | 284 | U    |
| 8   | 7     | 285 | G    |
| 8   | 7     | 286 | U    |
| 8   | 7     | 311 | A    |
| 8   | 7     | 330 | A    |
| 8   | 7     | 345 | A    |
| 8   | 7     | 353 | C    |
| 8   | 7     | 359 | G    |
| 8   | 7     | 361 | G    |
| 8   | 7     | 362 | A    |
| 8   | 7     | 386 | G    |
| 8   | 7     | 395 | U    |
| 8   | 7     | 396 | G    |
| 8   | 7     | 401 | A    |
| 8   | 7     | 405 | U    |
| 8   | 7     | 412 | A    |
| 8   | 7     | 455 | C    |
| 8   | 7     | 456 | C    |
| 8   | 7     | 457 | A    |
| 8   | 7     | 470 | A    |
| 8   | 7     | 473 | G    |
| 8   | 7     | 481 | G    |
| 8   | 7     | 491 | G    |
| 8   | 7     | 505 | A    |
| 8   | 7     | 506 | G    |
| 8   | 7     | 509 | C    |
| 8   | 7     | 513 | A    |
| 8   | 7     | 527 | C    |
| 8   | 7     | 532 | A    |
| 8   | 7     | 547 | A    |
| 8   | 7     | 549 | G    |
| 8   | 7     | 563 | A    |
| 8   | 7     | 573 | U    |
| 8   | 7     | 575 | A    |
| 8   | 7     | 578 | G    |
| 8   | 7     | 603 | A    |
| 8   | 7     | 613 | A    |
| 8   | 7     | 614 | A    |
| 8   | 7     | 615 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8   | 7     | 637 | A    |
| 8   | 7     | 645 | C    |
| 8   | 7     | 646 | U    |
| 8   | 7     | 647 | G    |
| 8   | 7     | 654 | A    |
| 8   | 7     | 655 | A    |
| 8   | 7     | 686 | U    |
| 8   | 7     | 717 | C    |
| 8   | 7     | 726 | G    |
| 8   | 7     | 729 | G    |
| 8   | 7     | 730 | A    |
| 8   | 7     | 747 | 5MU  |
| 8   | 7     | 748 | G    |
| 8   | 7     | 749 | A    |
| 8   | 7     | 764 | A    |
| 8   | 7     | 765 | C    |
| 8   | 7     | 775 | G    |
| 8   | 7     | 776 | G    |
| 8   | 7     | 782 | A    |
| 8   | 7     | 784 | G    |
| 8   | 7     | 785 | G    |
| 8   | 7     | 789 | A    |
| 8   | 7     | 805 | G    |
| 8   | 7     | 812 | C    |
| 8   | 7     | 819 | A    |
| 8   | 7     | 827 | U    |
| 8   | 7     | 828 | U    |
| 8   | 7     | 830 | G    |
| 8   | 7     | 845 | A    |
| 8   | 7     | 846 | U    |
| 8   | 7     | 847 | U    |
| 8   | 7     | 858 | G    |
| 8   | 7     | 859 | G    |
| 8   | 7     | 869 | G    |
| 8   | 7     | 878 | A    |
| 8   | 7     | 883 | G    |
| 8   | 7     | 885 | C    |
| 8   | 7     | 887 | U    |
| 8   | 7     | 888 | C    |
| 8   | 7     | 891 | G    |
| 8   | 7     | 895 | U    |
| 8   | 7     | 896 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 8   | 7     | 897  | C    |
| 8   | 7     | 902  | C    |
| 8   | 7     | 907  | G    |
| 8   | 7     | 910  | A    |
| 8   | 7     | 917  | A    |
| 8   | 7     | 919  | U    |
| 8   | 7     | 931  | U    |
| 8   | 7     | 932  | U    |
| 8   | 7     | 941  | A    |
| 8   | 7     | 946  | C    |
| 8   | 7     | 961  | C    |
| 8   | 7     | 962  | G    |
| 8   | 7     | 974  | G    |
| 8   | 7     | 983  | A    |
| 8   | 7     | 995  | C    |
| 8   | 7     | 996  | A    |
| 8   | 7     | 999  | U    |
| 8   | 7     | 1005 | C    |
| 8   | 7     | 1012 | U    |
| 8   | 7     | 1013 | C    |
| 8   | 7     | 1021 | A    |
| 8   | 7     | 1026 | G    |
| 8   | 7     | 1033 | U    |
| 8   | 7     | 1046 | A    |
| 8   | 7     | 1047 | G    |
| 8   | 7     | 1055 | G    |
| 8   | 7     | 1060 | U    |
| 8   | 7     | 1070 | A    |
| 8   | 7     | 1081 | U    |
| 8   | 7     | 1083 | U    |
| 8   | 7     | 1084 | A    |
| 8   | 7     | 1085 | A    |
| 8   | 7     | 1087 | G    |
| 8   | 7     | 1088 | A    |
| 8   | 7     | 1090 | A    |
| 8   | 7     | 1097 | U    |
| 8   | 7     | 1112 | G    |
| 8   | 7     | 1130 | U    |
| 8   | 7     | 1131 | G    |
| 8   | 7     | 1132 | U    |
| 8   | 7     | 1133 | A    |
| 8   | 7     | 1134 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 8   | 7     | 1135 | C    |
| 8   | 7     | 1136 | G    |
| 8   | 7     | 1142 | A    |
| 8   | 7     | 1149 | G    |
| 8   | 7     | 1161 | C    |
| 8   | 7     | 1169 | A    |
| 8   | 7     | 1172 | C    |
| 8   | 7     | 1173 | U    |
| 8   | 7     | 1174 | U    |
| 8   | 7     | 1176 | U    |
| 8   | 7     | 1178 | C    |
| 8   | 7     | 1179 | G    |
| 8   | 7     | 1180 | U    |
| 8   | 7     | 1212 | G    |
| 8   | 7     | 1235 | G    |
| 8   | 7     | 1236 | G    |
| 8   | 7     | 1238 | G    |
| 8   | 7     | 1247 | A    |
| 8   | 7     | 1249 | U    |
| 8   | 7     | 1250 | G    |
| 8   | 7     | 1253 | A    |
| 8   | 7     | 1256 | G    |
| 8   | 7     | 1262 | A    |
| 8   | 7     | 1266 | G    |
| 8   | 7     | 1267 | U    |
| 8   | 7     | 1271 | G    |
| 8   | 7     | 1272 | A    |
| 8   | 7     | 1273 | U    |
| 8   | 7     | 1300 | G    |
| 8   | 7     | 1301 | A    |
| 8   | 7     | 1321 | A    |
| 8   | 7     | 1329 | U    |
| 8   | 7     | 1345 | C    |
| 8   | 7     | 1352 | U    |
| 8   | 7     | 1365 | A    |
| 8   | 7     | 1368 | G    |
| 8   | 7     | 1379 | U    |
| 8   | 7     | 1380 | G    |
| 8   | 7     | 1383 | A    |
| 8   | 7     | 1395 | A    |
| 8   | 7     | 1396 | U    |
| 8   | 7     | 1416 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 8   | 7     | 1417 | C    |
| 8   | 7     | 1419 | A    |
| 8   | 7     | 1420 | A    |
| 8   | 7     | 1428 | C    |
| 8   | 7     | 1434 | A    |
| 8   | 7     | 1452 | G    |
| 8   | 7     | 1453 | A    |
| 8   | 7     | 1461 | C    |
| 8   | 7     | 1476 | U    |
| 8   | 7     | 1482 | G    |
| 8   | 7     | 1488 | C    |
| 8   | 7     | 1490 | A    |
| 8   | 7     | 1491 | G    |
| 8   | 7     | 1493 | C    |
| 8   | 7     | 1494 | A    |
| 8   | 7     | 1497 | U    |
| 8   | 7     | 1503 | A    |
| 8   | 7     | 1508 | A    |
| 8   | 7     | 1509 | A    |
| 8   | 7     | 1515 | A    |
| 8   | 7     | 1524 | G    |
| 8   | 7     | 1532 | A    |
| 8   | 7     | 1539 | U    |
| 8   | 7     | 1566 | A    |
| 8   | 7     | 1569 | A    |
| 8   | 7     | 1578 | U    |
| 8   | 7     | 1581 | G    |
| 8   | 7     | 1583 | A    |
| 8   | 7     | 1584 | U    |
| 8   | 7     | 1608 | A    |
| 8   | 7     | 1610 | A    |
| 8   | 7     | 1618 | 6MZ  |
| 8   | 7     | 1619 | G    |
| 8   | 7     | 1647 | U    |
| 8   | 7     | 1648 | U    |
| 8   | 7     | 1649 | G    |
| 8   | 7     | 1674 | G    |
| 8   | 7     | 1715 | G    |
| 8   | 7     | 1727 | C    |
| 8   | 7     | 1729 | U    |
| 8   | 7     | 1730 | C    |
| 8   | 7     | 1731 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 8   | 7     | 1738 | G    |
| 8   | 7     | 1764 | C    |
| 8   | 7     | 1773 | A    |
| 8   | 7     | 1782 | U    |
| 8   | 7     | 1784 | A    |
| 8   | 7     | 1786 | A    |
| 8   | 7     | 1791 | A    |
| 8   | 7     | 1799 | G    |
| 8   | 7     | 1800 | C    |
| 8   | 7     | 1801 | A    |
| 8   | 7     | 1807 | G    |
| 8   | 7     | 1808 | A    |
| 8   | 7     | 1816 | C    |
| 8   | 7     | 1848 | A    |
| 8   | 7     | 1870 | C    |
| 8   | 7     | 1872 | A    |
| 8   | 7     | 1873 | G    |
| 8   | 7     | 1901 | A    |
| 8   | 7     | 1906 | G    |
| 8   | 7     | 1907 | G    |
| 8   | 7     | 1913 | A    |
| 8   | 7     | 1920 | C    |
| 8   | 7     | 1929 | G    |
| 8   | 7     | 1930 | G    |
| 8   | 7     | 1937 | A    |
| 8   | 7     | 1938 | A    |
| 8   | 7     | 1940 | U    |
| 8   | 7     | 1955 | U    |
| 8   | 7     | 1956 | U    |
| 8   | 7     | 1960 | A    |
| 8   | 7     | 1963 | U    |
| 8   | 7     | 1964 | G    |
| 8   | 7     | 1966 | A    |
| 8   | 7     | 1967 | C    |
| 8   | 7     | 1970 | A    |
| 8   | 7     | 1971 | U    |
| 8   | 7     | 1972 | G    |
| 8   | 7     | 1975 | G    |
| 8   | 7     | 1982 | U    |
| 8   | 7     | 1991 | U    |
| 8   | 7     | 1993 | U    |
| 8   | 7     | 1997 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 8   | 7     | 2022 | U    |
| 8   | 7     | 2023 | C    |
| 8   | 7     | 2030 | 6MZ  |
| 8   | 7     | 2031 | A    |
| 8   | 7     | 2032 | G    |
| 8   | 7     | 2033 | A    |
| 8   | 7     | 2043 | C    |
| 8   | 7     | 2055 | C    |
| 8   | 7     | 2056 | G    |
| 8   | 7     | 2059 | A    |
| 8   | 7     | 2060 | A    |
| 8   | 7     | 2061 | G    |
| 8   | 7     | 2062 | A    |
| 8   | 7     | 2069 | G7M  |
| 8   | 7     | 2072 | C    |
| 8   | 7     | 2093 | G    |
| 8   | 7     | 2098 | U    |
| 8   | 7     | 2100 | G    |
| 8   | 7     | 2101 | A    |
| 8   | 7     | 2104 | C    |
| 8   | 7     | 2109 | U    |
| 8   | 7     | 2110 | G    |
| 8   | 7     | 2111 | U    |
| 8   | 7     | 2112 | G    |
| 8   | 7     | 2113 | U    |
| 8   | 7     | 2114 | A    |
| 8   | 7     | 2115 | G    |
| 8   | 7     | 2116 | G    |
| 8   | 7     | 2117 | A    |
| 8   | 7     | 2118 | U    |
| 8   | 7     | 2119 | A    |
| 8   | 7     | 2120 | G    |
| 8   | 7     | 2126 | A    |
| 8   | 7     | 2130 | U    |
| 8   | 7     | 2131 | U    |
| 8   | 7     | 2132 | U    |
| 8   | 7     | 2133 | G    |
| 8   | 7     | 2134 | A    |
| 8   | 7     | 2139 | U    |
| 8   | 7     | 2140 | G    |
| 8   | 7     | 2141 | G    |
| 8   | 7     | 2145 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 8   | 7     | 2146 | C    |
| 8   | 7     | 2149 | U    |
| 8   | 7     | 2154 | A    |
| 8   | 7     | 2158 | A    |
| 8   | 7     | 2161 | C    |
| 8   | 7     | 2162 | G    |
| 8   | 7     | 2164 | C    |
| 8   | 7     | 2165 | C    |
| 8   | 7     | 2166 | U    |
| 8   | 7     | 2167 | U    |
| 8   | 7     | 2170 | A    |
| 8   | 7     | 2171 | A    |
| 8   | 7     | 2172 | U    |
| 8   | 7     | 2173 | A    |
| 8   | 7     | 2179 | C    |
| 8   | 7     | 2182 | U    |
| 8   | 7     | 2183 | A    |
| 8   | 7     | 2198 | A    |
| 8   | 7     | 2204 | G    |
| 8   | 7     | 2211 | A    |
| 8   | 7     | 2225 | A    |
| 8   | 7     | 2238 | G    |
| 8   | 7     | 2239 | G    |
| 8   | 7     | 2243 | U    |
| 8   | 7     | 2251 | OMG  |
| 8   | 7     | 2268 | A    |
| 8   | 7     | 2278 | A    |
| 8   | 7     | 2279 | G    |
| 8   | 7     | 2283 | C    |
| 8   | 7     | 2287 | A    |
| 8   | 7     | 2305 | U    |
| 8   | 7     | 2308 | G    |
| 8   | 7     | 2309 | A    |
| 8   | 7     | 2311 | A    |
| 8   | 7     | 2312 | U    |
| 8   | 7     | 2319 | G    |
| 8   | 7     | 2321 | U    |
| 8   | 7     | 2322 | A    |
| 8   | 7     | 2325 | G    |
| 8   | 7     | 2333 | A    |
| 8   | 7     | 2336 | A    |
| 8   | 7     | 2345 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 8   | 7     | 2347 | C    |
| 8   | 7     | 2350 | C    |
| 8   | 7     | 2361 | G    |
| 8   | 7     | 2372 | U    |
| 8   | 7     | 2375 | G    |
| 8   | 7     | 2379 | G    |
| 8   | 7     | 2383 | G    |
| 8   | 7     | 2385 | C    |
| 8   | 7     | 2391 | G    |
| 8   | 7     | 2402 | U    |
| 8   | 7     | 2403 | C    |
| 8   | 7     | 2406 | A    |
| 8   | 7     | 2410 | G    |
| 8   | 7     | 2423 | U    |
| 8   | 7     | 2425 | A    |
| 8   | 7     | 2429 | G    |
| 8   | 7     | 2430 | A    |
| 8   | 7     | 2431 | U    |
| 8   | 7     | 2441 | U    |
| 8   | 7     | 2448 | A    |
| 8   | 7     | 2457 | PSU  |
| 8   | 7     | 2464 | G    |
| 8   | 7     | 2475 | C    |
| 8   | 7     | 2476 | A    |
| 8   | 7     | 2478 | A    |
| 8   | 7     | 2482 | A    |
| 8   | 7     | 2484 | G    |
| 8   | 7     | 2491 | U    |
| 8   | 7     | 2494 | G    |
| 8   | 7     | 2498 | OMC  |
| 8   | 7     | 2502 | G    |
| 8   | 7     | 2503 | 2MA  |
| 8   | 7     | 2505 | G    |
| 8   | 7     | 2507 | C    |
| 8   | 7     | 2514 | U    |
| 8   | 7     | 2518 | A    |
| 8   | 7     | 2529 | G    |
| 8   | 7     | 2535 | G    |
| 8   | 7     | 2537 | U    |
| 8   | 7     | 2547 | A    |
| 8   | 7     | 2549 | G    |
| 8   | 7     | 2554 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 8   | 7     | 2556 | C    |
| 8   | 7     | 2566 | A    |
| 8   | 7     | 2567 | G    |
| 8   | 7     | 2571 | U    |
| 8   | 7     | 2572 | A    |
| 8   | 7     | 2573 | C    |
| 8   | 7     | 2581 | G    |
| 8   | 7     | 2582 | G    |
| 8   | 7     | 2586 | U    |
| 8   | 7     | 2602 | A    |
| 8   | 7     | 2608 | G    |
| 8   | 7     | 2609 | U    |
| 8   | 7     | 2613 | U    |
| 8   | 7     | 2614 | A    |
| 8   | 7     | 2615 | U    |
| 8   | 7     | 2629 | U    |
| 8   | 7     | 2630 | G    |
| 8   | 7     | 2663 | G    |
| 8   | 7     | 2689 | U    |
| 8   | 7     | 2690 | U    |
| 8   | 7     | 2714 | G    |
| 8   | 7     | 2726 | A    |
| 8   | 7     | 2732 | G    |
| 8   | 7     | 2733 | A    |
| 8   | 7     | 2743 | U    |
| 8   | 7     | 2744 | G    |
| 8   | 7     | 2748 | A    |
| 8   | 7     | 2751 | G    |
| 8   | 7     | 2757 | A    |
| 8   | 7     | 2765 | A    |
| 8   | 7     | 2778 | A    |
| 8   | 7     | 2779 | U    |
| 8   | 7     | 2798 | U    |
| 8   | 7     | 2800 | A    |
| 8   | 7     | 2818 | U    |
| 8   | 7     | 2820 | A    |
| 8   | 7     | 2821 | A    |
| 8   | 7     | 2832 | U    |
| 8   | 7     | 2835 | A    |
| 8   | 7     | 2861 | U    |
| 8   | 7     | 2867 | G    |
| 8   | 7     | 2873 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 8   | 7     | 2879 | A    |
| 8   | 7     | 2880 | C    |
| 8   | 7     | 2883 | A    |
| 8   | 7     | 2884 | U    |
| 8   | 7     | 2885 | G    |
| 8   | 7     | 2886 | A    |
| 8   | 7     | 2891 | U    |
| 8   | 7     | 2904 | U    |
| 9   | 8     | 4    | C    |
| 9   | 8     | 9    | G    |
| 9   | 8     | 13   | G    |
| 9   | 8     | 35   | C    |
| 9   | 8     | 50   | A    |
| 9   | 8     | 51   | G    |
| 9   | 8     | 66   | A    |
| 9   | 8     | 67   | G    |
| 9   | 8     | 87   | U    |
| 9   | 8     | 89   | U    |
| 9   | 8     | 90   | C    |
| 9   | 8     | 91   | C    |
| 9   | 8     | 99   | A    |
| 9   | 8     | 109  | A    |
| 10  | A     | 2    | A    |
| 10  | A     | 4    | U    |
| 10  | A     | 7    | A    |
| 10  | A     | 8    | A    |
| 10  | A     | 9    | G    |
| 10  | A     | 16   | A    |
| 10  | A     | 26   | A    |
| 10  | A     | 30   | U    |
| 10  | A     | 31   | G    |
| 10  | A     | 32   | A    |
| 10  | A     | 39   | G    |
| 10  | A     | 40   | C    |
| 10  | A     | 47   | C    |
| 10  | A     | 48   | C    |
| 10  | A     | 51   | A    |
| 10  | A     | 64   | G    |
| 10  | A     | 70   | U    |
| 10  | A     | 71   | A    |
| 10  | A     | 72   | A    |
| 10  | A     | 73   | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10  | A     | 74  | A    |
| 10  | A     | 75  | G    |
| 10  | A     | 76  | G    |
| 10  | A     | 78  | A    |
| 10  | A     | 82  | G    |
| 10  | A     | 85  | U    |
| 10  | A     | 86  | G    |
| 10  | A     | 88  | U    |
| 10  | A     | 90  | C    |
| 10  | A     | 91  | U    |
| 10  | A     | 94  | G    |
| 10  | A     | 95  | C    |
| 10  | A     | 97  | G    |
| 10  | A     | 98  | A    |
| 10  | A     | 116 | A    |
| 10  | A     | 120 | A    |
| 10  | A     | 121 | U    |
| 10  | A     | 129 | A    |
| 10  | A     | 131 | A    |
| 10  | A     | 137 | U    |
| 10  | A     | 138 | G    |
| 10  | A     | 141 | G    |
| 10  | A     | 143 | A    |
| 10  | A     | 148 | G    |
| 10  | A     | 150 | U    |
| 10  | A     | 155 | A    |
| 10  | A     | 163 | C    |
| 10  | A     | 164 | G    |
| 10  | A     | 173 | U    |
| 10  | A     | 174 | A    |
| 10  | A     | 176 | C    |
| 10  | A     | 177 | G    |
| 10  | A     | 182 | A    |
| 10  | A     | 183 | C    |
| 10  | A     | 184 | G    |
| 10  | A     | 186 | C    |
| 10  | A     | 187 | G    |
| 10  | A     | 188 | C    |
| 10  | A     | 193 | C    |
| 10  | A     | 195 | A    |
| 10  | A     | 197 | A    |
| 10  | A     | 199 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10  | A     | 202 | G    |
| 10  | A     | 204 | G    |
| 10  | A     | 205 | A    |
| 10  | A     | 207 | C    |
| 10  | A     | 208 | U    |
| 10  | A     | 209 | U    |
| 10  | A     | 210 | C    |
| 10  | A     | 215 | C    |
| 10  | A     | 216 | U    |
| 10  | A     | 218 | U    |
| 10  | A     | 224 | U    |
| 10  | A     | 240 | G    |
| 10  | A     | 245 | U    |
| 10  | A     | 247 | G    |
| 10  | A     | 250 | A    |
| 10  | A     | 251 | G    |
| 10  | A     | 252 | U    |
| 10  | A     | 253 | A    |
| 10  | A     | 257 | G    |
| 10  | A     | 262 | A    |
| 10  | A     | 263 | A    |
| 10  | A     | 266 | G    |
| 10  | A     | 267 | C    |
| 10  | A     | 269 | C    |
| 10  | A     | 275 | G    |
| 10  | A     | 276 | G    |
| 10  | A     | 278 | G    |
| 10  | A     | 279 | A    |
| 10  | A     | 281 | G    |
| 10  | A     | 282 | A    |
| 10  | A     | 289 | G    |
| 10  | A     | 301 | G    |
| 10  | A     | 305 | G    |
| 10  | A     | 307 | C    |
| 10  | A     | 316 | C    |
| 10  | A     | 323 | U    |
| 10  | A     | 328 | C    |
| 10  | A     | 329 | A    |
| 10  | A     | 330 | C    |
| 10  | A     | 331 | G    |
| 10  | A     | 351 | G    |
| 10  | A     | 352 | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10  | A     | 354 | G    |
| 10  | A     | 355 | C    |
| 10  | A     | 356 | A    |
| 10  | A     | 361 | G    |
| 10  | A     | 367 | U    |
| 10  | A     | 368 | U    |
| 10  | A     | 370 | C    |
| 10  | A     | 372 | C    |
| 10  | A     | 373 | A    |
| 10  | A     | 374 | A    |
| 10  | A     | 375 | U    |
| 10  | A     | 387 | U    |
| 10  | A     | 388 | G    |
| 10  | A     | 391 | G    |
| 10  | A     | 393 | A    |
| 10  | A     | 397 | A    |
| 10  | A     | 398 | U    |
| 10  | A     | 405 | U    |
| 10  | A     | 406 | G    |
| 10  | A     | 408 | A    |
| 10  | A     | 409 | U    |
| 10  | A     | 411 | A    |
| 10  | A     | 412 | A    |
| 10  | A     | 413 | G    |
| 10  | A     | 414 | A    |
| 10  | A     | 415 | A    |
| 10  | A     | 416 | G    |
| 10  | A     | 422 | C    |
| 10  | A     | 423 | G    |
| 10  | A     | 424 | G    |
| 10  | A     | 426 | U    |
| 10  | A     | 428 | G    |
| 10  | A     | 429 | U    |
| 10  | A     | 431 | A    |
| 10  | A     | 437 | U    |
| 10  | A     | 439 | U    |
| 10  | A     | 440 | C    |
| 10  | A     | 442 | G    |
| 10  | A     | 443 | C    |
| 10  | A     | 444 | G    |
| 10  | A     | 445 | G    |
| 10  | A     | 448 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10  | A     | 450 | G    |
| 10  | A     | 452 | A    |
| 10  | A     | 456 | A    |
| 10  | A     | 457 | G    |
| 10  | A     | 458 | U    |
| 10  | A     | 459 | A    |
| 10  | A     | 460 | A    |
| 10  | A     | 461 | A    |
| 10  | A     | 462 | G    |
| 10  | A     | 464 | U    |
| 10  | A     | 465 | A    |
| 10  | A     | 466 | A    |
| 10  | A     | 467 | U    |
| 10  | A     | 468 | A    |
| 10  | A     | 469 | C    |
| 10  | A     | 472 | U    |
| 10  | A     | 473 | U    |
| 10  | A     | 474 | G    |
| 10  | A     | 475 | C    |
| 10  | A     | 478 | A    |
| 10  | A     | 479 | U    |
| 10  | A     | 480 | U    |
| 10  | A     | 481 | G    |
| 10  | A     | 482 | A    |
| 10  | A     | 484 | G    |
| 10  | A     | 492 | C    |
| 10  | A     | 495 | A    |
| 10  | A     | 496 | A    |
| 10  | A     | 497 | G    |
| 10  | A     | 498 | A    |
| 10  | A     | 499 | A    |
| 10  | A     | 501 | C    |
| 10  | A     | 506 | G    |
| 10  | A     | 511 | C    |
| 10  | A     | 512 | U    |
| 10  | A     | 513 | C    |
| 10  | A     | 516 | U    |
| 10  | A     | 518 | C    |
| 10  | A     | 520 | A    |
| 10  | A     | 521 | G    |
| 10  | A     | 524 | G    |
| 10  | A     | 527 | G7M  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10  | A     | 528 | C    |
| 10  | A     | 530 | G    |
| 10  | A     | 531 | U    |
| 10  | A     | 532 | A    |
| 10  | A     | 533 | A    |
| 10  | A     | 534 | U    |
| 10  | A     | 536 | C    |
| 10  | A     | 538 | G    |
| 10  | A     | 539 | A    |
| 10  | A     | 542 | G    |
| 10  | A     | 547 | A    |
| 10  | A     | 549 | C    |
| 10  | A     | 551 | U    |
| 10  | A     | 558 | G    |
| 10  | A     | 559 | A    |
| 10  | A     | 562 | U    |
| 10  | A     | 572 | A    |
| 10  | A     | 573 | A    |
| 10  | A     | 575 | G    |
| 10  | A     | 576 | C    |
| 10  | A     | 577 | G    |
| 10  | A     | 633 | G    |
| 10  | A     | 653 | U    |
| 10  | A     | 665 | A    |
| 10  | A     | 703 | G    |
| 10  | A     | 717 | U    |
| 10  | A     | 718 | A    |
| 10  | A     | 721 | G    |
| 10  | A     | 723 | U    |
| 10  | A     | 724 | G    |
| 10  | A     | 731 | G    |
| 10  | A     | 733 | G    |
| 10  | A     | 734 | G    |
| 10  | A     | 735 | C    |
| 10  | A     | 748 | G    |
| 10  | A     | 755 | G    |
| 10  | A     | 777 | A    |
| 10  | A     | 788 | U    |
| 10  | A     | 790 | A    |
| 10  | A     | 793 | U    |
| 10  | A     | 794 | A    |
| 10  | A     | 815 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 10  | A     | 817  | C    |
| 10  | A     | 821  | G    |
| 10  | A     | 828  | U    |
| 10  | A     | 829  | G    |
| 10  | A     | 841  | C    |
| 10  | A     | 842  | U    |
| 10  | A     | 843  | U    |
| 10  | A     | 844  | G    |
| 10  | A     | 845  | A    |
| 10  | A     | 846  | G    |
| 10  | A     | 902  | G    |
| 10  | A     | 914  | A    |
| 10  | A     | 926  | G    |
| 10  | A     | 933  | G    |
| 10  | A     | 934  | C    |
| 10  | A     | 935  | A    |
| 10  | A     | 945  | G    |
| 10  | A     | 953  | G    |
| 10  | A     | 960  | U    |
| 10  | A     | 961  | U    |
| 10  | A     | 969  | A    |
| 10  | A     | 972  | C    |
| 10  | A     | 974  | A    |
| 10  | A     | 975  | A    |
| 10  | A     | 976  | G    |
| 10  | A     | 977  | A    |
| 10  | A     | 989  | U    |
| 10  | A     | 991  | U    |
| 10  | A     | 992  | U    |
| 10  | A     | 993  | G    |
| 10  | A     | 994  | A    |
| 10  | A     | 996  | A    |
| 10  | A     | 1004 | A    |
| 10  | A     | 1006 | G    |
| 10  | A     | 1008 | U    |
| 10  | A     | 1009 | U    |
| 10  | A     | 1011 | C    |
| 10  | A     | 1014 | A    |
| 10  | A     | 1017 | U    |
| 10  | A     | 1018 | G    |
| 10  | A     | 1019 | A    |
| 10  | A     | 1020 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 10  | A     | 1021 | A    |
| 10  | A     | 1022 | A    |
| 10  | A     | 1023 | U    |
| 10  | A     | 1029 | U    |
| 10  | A     | 1030 | U    |
| 10  | A     | 1031 | C    |
| 10  | A     | 1032 | G    |
| 10  | A     | 1033 | G    |
| 10  | A     | 1034 | G    |
| 10  | A     | 1044 | A    |
| 10  | A     | 1046 | A    |
| 10  | A     | 1056 | U    |
| 10  | A     | 1063 | C    |
| 10  | A     | 1064 | G    |
| 10  | A     | 1065 | U    |
| 10  | A     | 1067 | A    |
| 10  | A     | 1074 | G    |
| 10  | A     | 1081 | A    |
| 10  | A     | 1085 | U    |
| 10  | A     | 1086 | U    |
| 10  | A     | 1094 | G    |
| 10  | A     | 1095 | U    |
| 10  | A     | 1098 | C    |
| 10  | A     | 1101 | A    |
| 10  | A     | 1102 | A    |
| 10  | A     | 1108 | G    |
| 10  | A     | 1113 | C    |
| 10  | A     | 1124 | G    |
| 10  | A     | 1125 | U    |
| 10  | A     | 1127 | G    |
| 10  | A     | 1128 | C    |
| 10  | A     | 1129 | C    |
| 10  | A     | 1130 | A    |
| 10  | A     | 1131 | G    |
| 10  | A     | 1133 | G    |
| 10  | A     | 1134 | G    |
| 10  | A     | 1136 | C    |
| 10  | A     | 1137 | C    |
| 10  | A     | 1138 | G    |
| 10  | A     | 1139 | G    |
| 10  | A     | 1140 | C    |
| 10  | A     | 1141 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 10  | A     | 1146 | A    |
| 10  | A     | 1152 | A    |
| 10  | A     | 1157 | A    |
| 10  | A     | 1158 | C    |
| 10  | A     | 1159 | U    |
| 10  | A     | 1160 | G    |
| 10  | A     | 1168 | U    |
| 10  | A     | 1169 | A    |
| 10  | A     | 1182 | G    |
| 10  | A     | 1184 | G    |
| 10  | A     | 1185 | G    |
| 10  | A     | 1191 | A    |
| 10  | A     | 1196 | A    |
| 10  | A     | 1197 | A    |
| 10  | A     | 1201 | A    |
| 10  | A     | 1202 | U    |
| 10  | A     | 1212 | U    |
| 10  | A     | 1213 | A    |
| 10  | A     | 1215 | G    |
| 10  | A     | 1217 | C    |
| 10  | A     | 1218 | C    |
| 10  | A     | 1225 | A    |
| 10  | A     | 1226 | C    |
| 10  | A     | 1227 | A    |
| 10  | A     | 1238 | A    |
| 10  | A     | 1241 | G    |
| 10  | A     | 1248 | A    |
| 10  | A     | 1249 | C    |
| 10  | A     | 1253 | G    |
| 10  | A     | 1256 | A    |
| 10  | A     | 1268 | G    |
| 10  | A     | 1270 | G    |
| 10  | A     | 1271 | A    |
| 10  | A     | 1279 | G    |
| 10  | A     | 1280 | A    |
| 10  | A     | 1281 | C    |
| 10  | A     | 1282 | C    |
| 10  | A     | 1286 | U    |
| 10  | A     | 1287 | A    |
| 10  | A     | 1291 | U    |
| 10  | A     | 1297 | G    |
| 10  | A     | 1298 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 10  | A     | 1300 | G    |
| 10  | A     | 1305 | G    |
| 10  | A     | 1317 | C    |
| 10  | A     | 1318 | A    |
| 10  | A     | 1319 | A    |
| 10  | A     | 1320 | C    |
| 10  | A     | 1332 | A    |
| 10  | A     | 1336 | C    |
| 10  | A     | 1338 | G    |
| 10  | A     | 1340 | A    |
| 10  | A     | 1346 | A    |
| 10  | A     | 1348 | U    |
| 10  | A     | 1351 | U    |
| 10  | A     | 1353 | G    |
| 10  | A     | 1360 | A    |
| 10  | A     | 1363 | A    |
| 10  | A     | 1364 | U    |
| 10  | A     | 1368 | A    |
| 10  | A     | 1370 | G    |
| 10  | A     | 1375 | A    |
| 10  | A     | 1379 | G    |
| 10  | A     | 1397 | C    |
| 10  | A     | 1398 | A    |
| 10  | A     | 1429 | A    |
| 10  | A     | 1441 | A    |
| 10  | A     | 1446 | A    |
| 10  | A     | 1448 | C    |
| 10  | A     | 1454 | G    |
| 10  | A     | 1487 | G    |
| 10  | A     | 1492 | A    |
| 10  | A     | 1499 | A    |
| 10  | A     | 1503 | A    |
| 10  | A     | 1506 | U    |
| 10  | A     | 1517 | G    |
| 10  | A     | 1519 | MA6  |
| 10  | A     | 1520 | C    |
| 10  | A     | 1529 | G    |
| 10  | A     | 1530 | G    |
| 10  | A     | 1534 | A    |
| 10  | A     | 1535 | C    |
| 31  | V     | 17   | G    |
| 31  | V     | 18   | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 31  | V     | 20  | C    |
| 31  | V     | 23  | G    |
| 31  | V     | 24  | G    |
| 31  | V     | 27  | A    |
| 31  | V     | 28  | A    |
| 31  | V     | 31  | U    |
| 31  | V     | 32  | C    |
| 31  | V     | 33  | G    |
| 31  | V     | 34  | A    |
| 31  | V     | 36  | A    |
| 31  | V     | 37  | A    |
| 32  | W     | 2   | G    |
| 32  | W     | 4   | G    |
| 32  | W     | 8   | 4SU  |
| 32  | W     | 11  | U    |
| 32  | W     | 15  | A    |
| 32  | W     | 16  | H2U  |
| 32  | W     | 17  | H2U  |
| 32  | W     | 18  | G    |
| 32  | W     | 19  | G    |
| 32  | W     | 20  | H2U  |
| 32  | W     | 22  | G    |
| 32  | W     | 34  | C    |
| 32  | W     | 44  | G    |
| 32  | W     | 46  | G7M  |
| 32  | W     | 47  | U    |
| 32  | W     | 48  | U    |
| 32  | W     | 49  | G    |
| 32  | W     | 52  | A    |
| 32  | W     | 54  | 5MU  |
| 32  | W     | 58  | A    |
| 32  | W     | 59  | G    |
| 32  | W     | 60  | U    |
| 32  | W     | 72  | U    |
| 32  | W     | 76  | A    |
| 33  | X     | 2   | C    |
| 33  | X     | 3   | A    |
| 33  | X     | 8   | 4SU  |
| 33  | X     | 9   | A    |
| 33  | X     | 13  | C    |
| 33  | X     | 15  | G    |
| 33  | X     | 16  | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 33  | X     | 18  | G    |
| 33  | X     | 19  | G    |
| 33  | X     | 20  | A    |
| 33  | X     | 21  | H2U  |
| 33  | X     | 22  | A    |
| 33  | X     | 33  | RSP  |
| 33  | X     | 38  | 2MA  |
| 33  | X     | 39  | A    |
| 33  | X     | 47  | G7M  |
| 33  | X     | 48  | 3AU  |
| 33  | X     | 49  | C    |
| 33  | X     | 50  | G    |
| 33  | X     | 55  | 5MU  |
| 33  | X     | 60  | A    |
| 33  | X     | 66  | C    |
| 33  | X     | 71  | U    |
| 33  | X     | 72  | G    |
| 33  | X     | 73  | C    |
| 33  | X     | 74  | A    |
| 33  | X     | 76  | C    |
| 33  | X     | 77  | A    |
| 34  | Y     | 15  | G    |
| 34  | Y     | 16  | C    |
| 34  | Y     | 17  | H2U  |
| 34  | Y     | 18  | G    |
| 34  | Y     | 19  | G    |
| 34  | Y     | 20  | G    |
| 34  | Y     | 21  | A    |
| 34  | Y     | 22  | G    |
| 34  | Y     | 34  | G    |
| 34  | Y     | 36  | C    |
| 34  | Y     | 39  | G    |
| 34  | Y     | 45  | G    |
| 34  | Y     | 46  | G7M  |
| 34  | Y     | 48  | C    |
| 34  | Y     | 49  | A    |
| 34  | Y     | 54  | 5MU  |
| 34  | Y     | 56  | C    |
| 34  | Y     | 64  | C    |
| 34  | Y     | 72  | C    |
| 34  | Y     | 73  | A    |
| 34  | Y     | 74  | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 34  | Y     | 76  | A    |

All (79) RNA pucker outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 8   | 7     | 43   | G    |
| 8   | 7     | 134  | G    |
| 8   | 7     | 158  | U    |
| 8   | 7     | 277  | G    |
| 8   | 7     | 285  | G    |
| 8   | 7     | 352  | A    |
| 8   | 7     | 404  | A    |
| 8   | 7     | 504  | A    |
| 8   | 7     | 512  | G    |
| 8   | 7     | 613  | A    |
| 8   | 7     | 748  | G    |
| 8   | 7     | 784  | G    |
| 8   | 7     | 827  | U    |
| 8   | 7     | 1020 | A    |
| 8   | 7     | 1046 | A    |
| 8   | 7     | 1130 | U    |
| 8   | 7     | 1211 | C    |
| 8   | 7     | 1266 | G    |
| 8   | 7     | 1416 | G    |
| 8   | 7     | 1475 | G    |
| 8   | 7     | 1490 | A    |
| 8   | 7     | 1580 | A    |
| 8   | 7     | 1847 | A    |
| 8   | 7     | 2031 | A    |
| 8   | 7     | 2061 | G    |
| 8   | 7     | 2118 | U    |
| 8   | 7     | 2172 | U    |
| 8   | 7     | 2430 | A    |
| 8   | 7     | 2474 | U    |
| 8   | 7     | 2581 | G    |
| 8   | 7     | 2756 | U    |
| 9   | 8     | 3    | C    |
| 9   | 8     | 15   | A    |
| 9   | 8     | 88   | C    |
| 10  | A     | 7    | A    |
| 10  | A     | 13   | U    |
| 10  | A     | 30   | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 10  | A     | 70   | U    |
| 10  | A     | 183  | C    |
| 10  | A     | 208  | U    |
| 10  | A     | 209  | U    |
| 10  | A     | 251  | G    |
| 10  | A     | 367  | U    |
| 10  | A     | 411  | A    |
| 10  | A     | 428  | G    |
| 10  | A     | 438  | U    |
| 10  | A     | 532  | A    |
| 10  | A     | 537  | G    |
| 10  | A     | 717  | U    |
| 10  | A     | 845  | A    |
| 10  | A     | 992  | U    |
| 10  | A     | 993  | G    |
| 10  | A     | 1085 | U    |
| 10  | A     | 1101 | A    |
| 10  | A     | 1129 | C    |
| 10  | A     | 1136 | C    |
| 10  | A     | 1140 | C    |
| 10  | A     | 1168 | U    |
| 10  | A     | 1190 | G    |
| 10  | A     | 1201 | A    |
| 10  | A     | 1256 | A    |
| 10  | A     | 1281 | C    |
| 10  | A     | 1297 | G    |
| 10  | A     | 1319 | A    |
| 31  | V     | 16   | C    |
| 31  | V     | 17   | G    |
| 31  | V     | 23   | G    |
| 32  | W     | 10   | G    |
| 32  | W     | 18   | G    |
| 32  | W     | 19   | G    |
| 32  | W     | 43   | G    |
| 33  | X     | 1    | G    |
| 33  | X     | 15   | G    |
| 33  | X     | 17   | H2U  |
| 33  | X     | 35   | I    |
| 33  | X     | 47   | G7M  |
| 33  | X     | 49   | C    |
| 34  | Y     | 17   | H2U  |
| 34  | Y     | 63   | G    |

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

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

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

| Mol | Type | Chain | Res  | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |      |      | Counts       | RMSZ | # $ Z  > 2$ | Counts      | RMSZ | # $ Z  > 2$ |
| 34  | 5MU  | Y     | 54   | 34   | 19,22,23     | 0.27 | 0           | 28,32,35    | 0.29 | 0           |
| 10  | 5MC  | A     | 1407 | 10   | 18,22,23     | 4.04 | 7 (38%)     | 26,32,35    | 1.00 | 2 (7%)      |
| 33  | 5MU  | X     | 55   | 33   | 19,22,23     | 7.20 | 7 (36%)     | 28,32,35    | 3.32 | 10 (35%)    |
| 34  | PSU  | Y     | 55   | 34   | 18,21,22     | 4.66 | 8 (44%)     | 22,30,33    | 1.87 | 5 (22%)     |
| 10  | UR3  | A     | 1498 | 10   | 19,22,23     | 2.76 | 8 (42%)     | 26,32,35    | 1.32 | 2 (7%)      |
| 33  | PSU  | X     | 56   | 33   | 18,21,22     | 4.69 | 8 (44%)     | 22,30,33    | 1.81 | 5 (22%)     |
| 10  | 5MC  | A     | 967  | 10   | 18,22,23     | 4.04 | 7 (38%)     | 26,32,35    | 1.01 | 2 (7%)      |
| 33  | RSP  | X     | 33   | 33   | 17,21,22     | 4.13 | 7 (41%)     | 22,30,33    | 0.82 | 0           |
| 8   | 5MU  | 7     | 747  | 8    | 19,22,23     | 0.23 | 0           | 28,32,35    | 0.34 | 0           |
| 32  | G7M  | W     | 46   | 32   | 23,26,27     | 2.85 | 9 (39%)     | 35,39,42    | 1.94 | 8 (22%)     |
| 8   | PSU  | 7     | 2504 | 8    | 18,21,22     | 4.67 | 8 (44%)     | 22,30,33    | 1.84 | 5 (22%)     |
| 8   | OMG  | 7     | 2251 | 32,8 | 23,26,27     | 2.57 | 7 (30%)     | 33,38,41    | 2.43 | 10 (30%)    |
| 8   | PSU  | 7     | 2605 | 8    | 18,21,22     | 4.65 | 8 (44%)     | 22,30,33    | 1.80 | 5 (22%)     |
| 8   | 2MA  | 7     | 2503 | 8,64 | 22,25,26     | 4.06 | 8 (36%)     | 33,37,40    | 3.39 | 12 (36%)    |
| 10  | G7M  | A     | 527  | 10   | 23,26,27     | 2.84 | 9 (39%)     | 35,39,42    | 1.75 | 8 (22%)     |
| 8   | 2MG  | 7     | 1835 | 8    | 23,26,27     | 0.35 | 0           | 32,38,41    | 0.46 | 0           |
| 32  | 5MU  | W     | 54   | 32   | 19,22,23     | 7.19 | 7 (36%)     | 28,32,35    | 3.31 | 9 (32%)     |
| 33  | H2U  | X     | 17   | 33   | 18,21,22     | 3.10 | 5 (27%)     | 21,30,33    | 1.95 | 4 (19%)     |
| 34  | H2U  | Y     | 17   | 34   | 18,21,22     | 3.09 | 5 (27%)     | 21,30,33    | 2.03 | 5 (23%)     |
| 32  | PSU  | W     | 32   | 32   | 18,21,22     | 4.66 | 8 (44%)     | 22,30,33    | 1.87 | 5 (22%)     |
| 8   | PSU  | 7     | 746  | 8,64 | 18,21,22     | 4.67 | 9 (50%)     | 22,30,33    | 1.78 | 5 (22%)     |
| 32  | MIA  | W     | 37   | 32   | 28,31,32     | 2.42 | 5 (17%)     | 40,44,47    | 2.74 | 17 (42%)    |
| 33  | H2U  | X     | 21   | 33   | 18,21,22     | 3.09 | 5 (27%)     | 21,30,33    | 1.99 | 5 (23%)     |
| 10  | MA6  | A     | 1518 | 10   | 23,26,27     | 1.35 | 3 (13%)     | 34,38,41    | 3.31 | 14 (41%)    |
| 8   | OMC  | 7     | 2498 | 8,64 | 19,22,23     | 3.24 | 8 (42%)     | 26,31,34    | 0.77 | 0           |
| 33  | 4SU  | X     | 8    | 33   | 18,21,22     | 3.79 | 7 (38%)     | 26,30,33    | 2.26 | 4 (15%)     |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 33  | 2MA  | X     | 38   | 33   | 22,25,26     | 4.15 | 8 (36%)  | 33,37,40    | 3.60 | 10 (30%) |
| 32  | H2U  | W     | 20   | 32   | 18,21,22     | 3.06 | 5 (27%)  | 21,30,33    | 2.01 | 5 (23%)  |
| 10  | MA6  | A     | 1519 | 10   | 23,26,27     | 1.35 | 4 (17%)  | 34,38,41    | 3.34 | 14 (41%) |
| 8   | G7M  | 7     | 2069 | 8    | 23,26,27     | 2.82 | 9 (39%)  | 35,39,42    | 1.73 | 7 (20%)  |
| 8   | 5MC  | 7     | 1962 | 8    | 18,22,23     | 4.03 | 7 (38%)  | 26,32,35    | 1.03 | 2 (7%)   |
| 10  | 2MG  | A     | 1207 | 10   | 23,26,27     | 3.10 | 8 (34%)  | 32,38,41    | 2.50 | 11 (34%) |
| 10  | 4OC  | A     | 1402 | 10   | 20,23,24     | 3.24 | 8 (40%)  | 26,32,35    | 0.90 | 1 (3%)   |
| 8   | 6MZ  | 7     | 2030 | 8    | 22,25,26     | 2.85 | 5 (22%)  | 30,36,39    | 2.42 | 11 (36%) |
| 8   | 6MZ  | 7     | 1618 | 8    | 22,25,26     | 2.75 | 4 (18%)  | 30,36,39    | 2.48 | 10 (33%) |
| 8   | 3TD  | 7     | 1915 | 8    | 19,22,23     | 4.04 | 7 (36%)  | 21,32,35    | 1.72 | 2 (9%)   |
| 33  | 3AU  | X     | 48   | 33   | 24,28,29     | 2.84 | 7 (29%)  | 33,40,43    | 1.30 | 3 (9%)   |
| 8   | PSU  | 7     | 955  | 8    | 18,21,22     | 4.63 | 8 (44%)  | 22,30,33    | 1.87 | 5 (22%)  |
| 8   | 1MG  | 7     | 745  | 8    | 22,26,27     | 2.72 | 5 (22%)  | 33,39,42    | 2.31 | 8 (24%)  |
| 8   | 5MU  | 7     | 1939 | 8    | 19,22,23     | 0.27 | 0        | 28,32,35    | 0.27 | 0        |
| 10  | 2MG  | A     | 1516 | 10   | 23,26,27     | 3.11 | 8 (34%)  | 32,38,41    | 2.49 | 11 (34%) |
| 8   | PSU  | 7     | 2580 | 8    | 18,21,22     | 4.62 | 9 (50%)  | 22,30,33    | 1.89 | 6 (27%)  |
| 8   | H2U  | 7     | 2449 | 8    | 18,21,22     | 3.02 | 5 (27%)  | 21,30,33    | 2.04 | 5 (23%)  |
| 8   | PSU  | 7     | 2457 | 8    | 18,21,22     | 4.62 | 8 (44%)  | 22,30,33    | 1.94 | 5 (22%)  |
| 32  | H2U  | W     | 17   | 32   | 18,21,22     | 3.08 | 5 (27%)  | 21,30,33    | 2.00 | 5 (23%)  |
| 32  | PSU  | W     | 55   | 32   | 18,21,22     | 4.68 | 8 (44%)  | 22,30,33    | 1.84 | 5 (22%)  |
| 32  | H2U  | W     | 16   | 32   | 18,21,22     | 3.07 | 5 (27%)  | 21,30,33    | 1.94 | 5 (23%)  |
| 8   | PSU  | 7     | 2604 | 8    | 18,21,22     | 4.63 | 8 (44%)  | 22,30,33    | 1.85 | 5 (22%)  |
| 10  | 2MG  | A     | 966  | 10   | 23,26,27     | 3.13 | 8 (34%)  | 32,38,41    | 2.50 | 11 (34%) |
| 32  | 4SU  | W     | 8    | 32   | 18,21,22     | 3.79 | 7 (38%)  | 26,30,33    | 2.25 | 5 (19%)  |
| 8   | 2MG  | 7     | 2445 | 8    | 23,26,27     | 3.09 | 8 (34%)  | 32,38,41    | 2.50 | 11 (34%) |
| 34  | G7M  | Y     | 46   | 34   | 23,26,27     | 2.84 | 9 (39%)  | 35,39,42    | 1.74 | 7 (20%)  |
| 8   | OMU  | 7     | 2552 | 8    | 19,22,23     | 3.20 | 8 (42%)  | 26,31,34    | 1.71 | 5 (19%)  |
| 33  | G7M  | X     | 47   | 33   | 23,26,27     | 2.85 | 8 (34%)  | 35,39,42    | 1.95 | 8 (22%)  |

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   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 34  | 5MU  | Y     | 54  | 34   | -       | 2/7/25/26 | 0/2/2/2 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|------|------|---------|------------|---------|
| 10  | 5MC  | A     | 1407 | 10   | -       | 0/7/25/26  | 0/2/2/2 |
| 33  | 5MU  | X     | 55   | 33   | -       | 2/7/25/26  | 0/2/2/2 |
| 34  | PSU  | Y     | 55   | 34   | -       | 0/7/25/26  | 0/2/2/2 |
| 10  | UR3  | A     | 1498 | 10   | -       | 2/7/25/26  | 0/2/2/2 |
| 33  | PSU  | X     | 56   | 33   | -       | 1/7/25/26  | 0/2/2/2 |
| 10  | 5MC  | A     | 967  | 10   | -       | 0/7/25/26  | 0/2/2/2 |
| 33  | RSP  | X     | 33   | 33   | -       | 1/7/25/26  | 0/2/2/2 |
| 8   | 5MU  | 7     | 747  | 8    | -       | 1/7/25/26  | 0/2/2/2 |
| 32  | G7M  | W     | 46   | 32   | -       | 5/7/25/26  | 0/3/3/3 |
| 8   | PSU  | 7     | 2504 | 8    | -       | 0/7/25/26  | 0/2/2/2 |
| 8   | OMG  | 7     | 2251 | 32,8 | -       | 3/9/27/28  | 0/3/3/3 |
| 8   | PSU  | 7     | 2605 | 8    | -       | 0/7/25/26  | 0/2/2/2 |
| 8   | 2MA  | 7     | 2503 | 8,64 | -       | 1/7/25/26  | 0/3/3/3 |
| 10  | G7M  | A     | 527  | 10   | -       | 2/7/25/26  | 0/3/3/3 |
| 8   | 2MG  | 7     | 1835 | 8    | -       | 0/9/27/28  | 0/3/3/3 |
| 32  | 5MU  | W     | 54   | 32   | -       | 2/7/25/26  | 0/2/2/2 |
| 33  | H2U  | X     | 17   | 33   | -       | 5/7/38/39  | 0/2/2/2 |
| 34  | H2U  | Y     | 17   | 34   | -       | 7/7/38/39  | 0/2/2/2 |
| 32  | PSU  | W     | 32   | 32   | -       | 0/7/25/26  | 0/2/2/2 |
| 8   | PSU  | 7     | 746  | 8,64 | -       | 1/7/25/26  | 0/2/2/2 |
| 32  | MIA  | W     | 37   | 32   | -       | 3/15/33/34 | 0/3/3/3 |
| 33  | H2U  | X     | 21   | 33   | -       | 2/7/38/39  | 0/2/2/2 |
| 10  | MA6  | A     | 1518 | 10   | -       | 0/11/29/30 | 0/3/3/3 |
| 8   | OMC  | 7     | 2498 | 8,64 | -       | 2/9/27/28  | 0/2/2/2 |
| 33  | 4SU  | X     | 8    | 33   | -       | 2/7/25/26  | 0/2/2/2 |
| 33  | 2MA  | X     | 38   | 33   | -       | 5/7/25/26  | 0/3/3/3 |
| 32  | H2U  | W     | 20   | 32   | -       | 1/7/38/39  | 0/2/2/2 |
| 10  | MA6  | A     | 1519 | 10   | -       | 3/11/29/30 | 0/3/3/3 |
| 8   | G7M  | 7     | 2069 | 8    | -       | 3/7/25/26  | 0/3/3/3 |
| 8   | 5MC  | 7     | 1962 | 8    | -       | 0/7/25/26  | 0/2/2/2 |
| 10  | 2MG  | A     | 1207 | 10   | -       | 0/9/27/28  | 0/3/3/3 |
| 10  | 4OC  | A     | 1402 | 10   | -       | 0/9/29/30  | 0/2/2/2 |
| 8   | 6MZ  | 7     | 2030 | 8    | -       | 3/9/27/28  | 0/3/3/3 |
| 8   | 6MZ  | 7     | 1618 | 8    | -       | 4/9/27/28  | 0/3/3/3 |
| 8   | 3TD  | 7     | 1915 | 8    | -       | 2/7/25/26  | 0/2/2/2 |
| 33  | 3AU  | X     | 48   | 33   | -       | 4/16/34/35 | 0/2/2/2 |
| 8   | PSU  | 7     | 955  | 8    | -       | 0/7/25/26  | 0/2/2/2 |
| 8   | 1MG  | 7     | 745  | 8    | -       | 0/7/25/26  | 0/3/3/3 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|------|------|---------|-----------|---------|
| 8   | 5MU  | 7     | 1939 | 8    | -       | 0/7/25/26 | 0/2/2/2 |
| 10  | 2MG  | A     | 1516 | 10   | -       | 0/9/27/28 | 0/3/3/3 |
| 8   | PSU  | 7     | 2580 | 8    | -       | 0/7/25/26 | 0/2/2/2 |
| 8   | H2U  | 7     | 2449 | 8    | -       | 0/7/38/39 | 0/2/2/2 |
| 8   | PSU  | 7     | 2457 | 8    | -       | 1/7/25/26 | 0/2/2/2 |
| 32  | H2U  | W     | 17   | 32   | -       | 2/7/38/39 | 0/2/2/2 |
| 32  | PSU  | W     | 55   | 32   | -       | 0/7/25/26 | 0/2/2/2 |
| 32  | H2U  | W     | 16   | 32   | -       | 1/7/38/39 | 0/2/2/2 |
| 8   | PSU  | 7     | 2604 | 8    | -       | 0/7/25/26 | 0/2/2/2 |
| 10  | 2MG  | A     | 966  | 10   | -       | 0/9/27/28 | 0/3/3/3 |
| 32  | 4SU  | W     | 8    | 32   | -       | 2/7/25/26 | 0/2/2/2 |
| 8   | 2MG  | 7     | 2445 | 8    | -       | 0/9/27/28 | 0/3/3/3 |
| 34  | G7M  | Y     | 46   | 34   | -       | 2/7/25/26 | 0/3/3/3 |
| 8   | OMU  | 7     | 2552 | 8    | -       | 0/9/27/28 | 0/2/2/2 |
| 33  | G7M  | X     | 47   | 33   | -       | 3/7/25/26 | 0/3/3/3 |

All (352) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|--------|-------------|----------|
| 33  | X     | 55   | 5MU  | C4-C5 | 21.25  | 1.80        | 1.44     |
| 32  | W     | 54   | 5MU  | C4-C5 | 21.10  | 1.79        | 1.44     |
| 32  | W     | 54   | 5MU  | C6-N1 | 15.74  | 1.64        | 1.38     |
| 33  | X     | 55   | 5MU  | C6-N1 | 15.72  | 1.64        | 1.38     |
| 33  | X     | 38   | 2MA  | C4-N3 | 12.66  | 1.50        | 1.34     |
| 8   | 7     | 1915 | 3TD  | C6-C5 | 12.53  | 1.49        | 1.35     |
| 33  | X     | 56   | PSU  | C6-C5 | 12.33  | 1.49        | 1.35     |
| 32  | W     | 55   | PSU  | C6-C5 | 12.24  | 1.49        | 1.35     |
| 8   | 7     | 2503 | 2MA  | C4-N3 | 12.17  | 1.49        | 1.34     |
| 32  | W     | 32   | PSU  | C6-C5 | 12.15  | 1.49        | 1.35     |
| 34  | Y     | 55   | PSU  | C6-C5 | 12.14  | 1.49        | 1.35     |
| 8   | 7     | 2504 | PSU  | C6-C5 | 12.14  | 1.49        | 1.35     |
| 8   | 7     | 2605 | PSU  | C6-C5 | 12.11  | 1.49        | 1.35     |
| 8   | 7     | 746  | PSU  | C6-C5 | 12.11  | 1.49        | 1.35     |
| 8   | 7     | 2580 | PSU  | C6-C5 | 12.06  | 1.49        | 1.35     |
| 8   | 7     | 2457 | PSU  | C6-C5 | 12.05  | 1.49        | 1.35     |
| 8   | 7     | 955  | PSU  | C6-C5 | 12.05  | 1.49        | 1.35     |
| 8   | 7     | 2030 | 6MZ  | C6-N6 | 12.04  | 1.47        | 1.34     |
| 8   | 7     | 2604 | PSU  | C6-C5 | 11.99  | 1.49        | 1.35     |
| 33  | X     | 33   | RSP  | C2-N3 | 11.72  | 1.48        | 1.36     |
| 8   | 7     | 1618 | 6MZ  | C6-N6 | 11.59  | 1.46        | 1.34     |
| 32  | W     | 54   | 5MU  | C6-C5 | -11.00 | 1.16        | 1.34     |

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| Mol | Chain | Res  | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|--------|-------------|----------|
| 33  | X     | 55   | 5MU  | C4-N3 | -10.87 | 1.18        | 1.38     |
| 32  | W     | 54   | 5MU  | C4-N3 | -10.87 | 1.18        | 1.38     |
| 33  | X     | 55   | 5MU  | C6-C5 | -10.84 | 1.16        | 1.34     |
| 10  | A     | 967  | 5MC  | C6-C5 | 9.96   | 1.51        | 1.34     |
| 8   | 7     | 1962 | 5MC  | C6-C5 | 9.94   | 1.50        | 1.34     |
| 10  | A     | 1407 | 5MC  | C6-C5 | 9.94   | 1.50        | 1.34     |
| 33  | X     | 17   | H2U  | C2-N1 | 9.66   | 1.49        | 1.35     |
| 34  | Y     | 55   | PSU  | C2-N1 | 9.66   | 1.49        | 1.36     |
| 8   | 7     | 2504 | PSU  | C2-N1 | 9.63   | 1.49        | 1.36     |
| 32  | W     | 55   | PSU  | C2-N1 | 9.61   | 1.49        | 1.36     |
| 32  | W     | 32   | PSU  | C2-N1 | 9.60   | 1.49        | 1.36     |
| 8   | 7     | 746  | PSU  | C2-N1 | 9.56   | 1.49        | 1.36     |
| 8   | 7     | 2604 | PSU  | C2-N1 | 9.56   | 1.49        | 1.36     |
| 8   | 7     | 2457 | PSU  | C2-N1 | 9.52   | 1.49        | 1.36     |
| 33  | X     | 56   | PSU  | C2-N1 | 9.52   | 1.49        | 1.36     |
| 8   | 7     | 2605 | PSU  | C2-N1 | 9.51   | 1.49        | 1.36     |
| 33  | X     | 21   | H2U  | C2-N1 | 9.48   | 1.49        | 1.35     |
| 8   | 7     | 955  | PSU  | C2-N1 | 9.46   | 1.49        | 1.36     |
| 34  | Y     | 17   | H2U  | C2-N1 | 9.44   | 1.49        | 1.35     |
| 32  | W     | 16   | H2U  | C2-N1 | 9.44   | 1.49        | 1.35     |
| 8   | 7     | 2580 | PSU  | C2-N1 | 9.43   | 1.49        | 1.36     |
| 32  | W     | 17   | H2U  | C2-N1 | 9.41   | 1.49        | 1.35     |
| 32  | W     | 20   | H2U  | C2-N1 | 9.37   | 1.49        | 1.35     |
| 8   | 7     | 2449 | H2U  | C2-N1 | 9.29   | 1.48        | 1.35     |
| 33  | X     | 8    | 4SU  | C4-N3 | 8.87   | 1.47        | 1.37     |
| 8   | 7     | 1915 | 3TD  | C2-N1 | 8.86   | 1.48        | 1.37     |
| 32  | W     | 8    | 4SU  | C4-N3 | 8.85   | 1.47        | 1.37     |
| 10  | A     | 966  | 2MG  | C2-N3 | 8.33   | 1.47        | 1.31     |
| 33  | X     | 56   | PSU  | C2-N3 | 8.28   | 1.51        | 1.37     |
| 10  | A     | 1516 | 2MG  | C2-N3 | 8.26   | 1.47        | 1.31     |
| 8   | 7     | 746  | PSU  | C2-N3 | 8.24   | 1.51        | 1.37     |
| 32  | W     | 55   | PSU  | C2-N3 | 8.24   | 1.51        | 1.37     |
| 8   | 7     | 2504 | PSU  | C2-N3 | 8.24   | 1.51        | 1.37     |
| 8   | 7     | 955  | PSU  | C2-N3 | 8.24   | 1.51        | 1.37     |
| 32  | W     | 32   | PSU  | C2-N3 | 8.21   | 1.51        | 1.37     |
| 34  | Y     | 55   | PSU  | C2-N3 | 8.21   | 1.51        | 1.37     |
| 8   | 7     | 2445 | 2MG  | C2-N3 | 8.18   | 1.47        | 1.31     |
| 10  | A     | 1207 | 2MG  | C2-N3 | 8.17   | 1.47        | 1.31     |
| 8   | 7     | 2580 | PSU  | C2-N3 | 8.17   | 1.51        | 1.37     |
| 33  | X     | 38   | 2MA  | C2-N3 | 8.16   | 1.48        | 1.34     |
| 8   | 7     | 2604 | PSU  | C2-N3 | 8.14   | 1.51        | 1.37     |
| 8   | 7     | 2605 | PSU  | C2-N3 | 8.13   | 1.51        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms  | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|------|-------------|----------|
| 8   | 7     | 2457 | PSU  | C2-N3  | 8.11 | 1.51        | 1.37     |
| 33  | X     | 48   | 3AU  | C2-N1  | 8.08 | 1.50        | 1.38     |
| 32  | W     | 37   | MIA  | C6-N6  | 8.05 | 1.47        | 1.34     |
| 32  | W     | 37   | MIA  | C2-S10 | 7.76 | 1.82        | 1.75     |
| 8   | 7     | 2503 | 2MA  | C2-N3  | 7.74 | 1.47        | 1.34     |
| 10  | A     | 967  | 5MC  | C4-N3  | 7.47 | 1.46        | 1.34     |
| 8   | 7     | 1962 | 5MC  | C4-N3  | 7.43 | 1.46        | 1.34     |
| 10  | A     | 1407 | 5MC  | C4-N3  | 7.39 | 1.46        | 1.34     |
| 8   | 7     | 2251 | OMG  | C2-N2  | 7.17 | 1.51        | 1.34     |
| 10  | A     | 1498 | UR3  | C2-N1  | 7.11 | 1.48        | 1.38     |
| 10  | A     | 1402 | 4OC  | C4-N3  | 7.08 | 1.45        | 1.32     |
| 10  | A     | 966  | 2MG  | C4-N3  | 7.04 | 1.51        | 1.34     |
| 10  | A     | 967  | 5MC  | C2-N3  | 6.97 | 1.50        | 1.36     |
| 8   | 7     | 1962 | 5MC  | C2-N3  | 6.97 | 1.50        | 1.36     |
| 10  | A     | 1407 | 5MC  | C2-N3  | 6.96 | 1.50        | 1.36     |
| 8   | 7     | 2552 | OMU  | C2-N3  | 6.96 | 1.50        | 1.38     |
| 8   | 7     | 745  | 1MG  | C2-N3  | 6.95 | 1.47        | 1.34     |
| 8   | 7     | 2445 | 2MG  | C4-N3  | 6.94 | 1.50        | 1.34     |
| 10  | A     | 1516 | 2MG  | C4-N3  | 6.90 | 1.50        | 1.34     |
| 32  | W     | 8    | 4SU  | C2-N3  | 6.89 | 1.50        | 1.38     |
| 8   | 7     | 2503 | 2MA  | C6-N1  | 6.86 | 1.44        | 1.35     |
| 10  | A     | 1207 | 2MG  | C4-N3  | 6.85 | 1.50        | 1.34     |
| 8   | 7     | 2498 | OMC  | C2-N3  | 6.83 | 1.50        | 1.36     |
| 33  | X     | 33   | RSP  | C6-C5  | 6.83 | 1.50        | 1.35     |
| 33  | X     | 38   | 2MA  | C6-N1  | 6.82 | 1.44        | 1.35     |
| 33  | X     | 8    | 4SU  | C2-N3  | 6.81 | 1.50        | 1.38     |
| 33  | X     | 47   | G7M  | C4-N3  | 6.79 | 1.50        | 1.34     |
| 32  | W     | 46   | G7M  | C4-N3  | 6.76 | 1.50        | 1.34     |
| 33  | X     | 33   | RSP  | C4-N4  | 6.64 | 1.49        | 1.33     |
| 34  | Y     | 46   | G7M  | C4-N3  | 6.60 | 1.50        | 1.34     |
| 33  | X     | 47   | G7M  | C2-N2  | 6.59 | 1.49        | 1.34     |
| 34  | Y     | 46   | G7M  | C2-N2  | 6.58 | 1.49        | 1.34     |
| 10  | A     | 527  | G7M  | C4-N3  | 6.58 | 1.49        | 1.34     |
| 32  | W     | 46   | G7M  | C2-N2  | 6.58 | 1.49        | 1.34     |
| 10  | A     | 527  | G7M  | C2-N2  | 6.56 | 1.49        | 1.34     |
| 34  | Y     | 17   | H2U  | C2-N3  | 6.54 | 1.49        | 1.38     |
| 32  | W     | 17   | H2U  | C2-N3  | 6.53 | 1.49        | 1.38     |
| 8   | 7     | 2069 | G7M  | C4-N3  | 6.52 | 1.49        | 1.34     |
| 32  | W     | 20   | H2U  | C2-N3  | 6.52 | 1.49        | 1.38     |
| 8   | 7     | 2069 | G7M  | C2-N2  | 6.52 | 1.49        | 1.34     |
| 33  | X     | 21   | H2U  | C2-N3  | 6.52 | 1.49        | 1.38     |
| 33  | X     | 17   | H2U  | C2-N3  | 6.51 | 1.49        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 8   | 7     | 2552 | OMU  | C2-N1 | 6.50  | 1.48        | 1.38     |
| 8   | 7     | 745  | 1MG  | C4-N3 | 6.50  | 1.49        | 1.34     |
| 10  | A     | 1207 | 2MG  | C2-N2 | 6.49  | 1.47        | 1.33     |
| 10  | A     | 966  | 2MG  | C2-N2 | 6.49  | 1.47        | 1.33     |
| 32  | W     | 16   | H2U  | C2-N3 | 6.46  | 1.49        | 1.38     |
| 10  | A     | 1516 | 2MG  | C2-N2 | 6.44  | 1.47        | 1.33     |
| 33  | X     | 48   | 3AU  | C2-N3 | 6.42  | 1.50        | 1.38     |
| 8   | 7     | 2445 | 2MG  | C2-N2 | 6.40  | 1.47        | 1.33     |
| 10  | A     | 1402 | 4OC  | C6-C5 | 6.37  | 1.49        | 1.35     |
| 8   | 7     | 2449 | H2U  | C2-N3 | 6.37  | 1.49        | 1.38     |
| 8   | 7     | 745  | 1MG  | C2-N2 | 6.35  | 1.45        | 1.34     |
| 10  | A     | 1402 | 4OC  | C2-N3 | 6.31  | 1.49        | 1.36     |
| 8   | 7     | 2503 | 2MA  | C2-N1 | 6.20  | 1.45        | 1.34     |
| 33  | X     | 38   | 2MA  | C2-N1 | 6.17  | 1.45        | 1.34     |
| 10  | A     | 1498 | UR3  | C6-C5 | 6.15  | 1.49        | 1.35     |
| 33  | X     | 8    | 4SU  | C4-S4 | -6.06 | 1.56        | 1.68     |
| 8   | 7     | 2498 | OMC  | C6-C5 | 6.05  | 1.49        | 1.35     |
| 33  | X     | 48   | 3AU  | C6-C5 | 6.05  | 1.49        | 1.35     |
| 32  | W     | 8    | 4SU  | C4-S4 | -6.04 | 1.56        | 1.68     |
| 8   | 7     | 2251 | OMG  | C4-N3 | 5.94  | 1.48        | 1.34     |
| 33  | X     | 8    | 4SU  | C2-N1 | 5.88  | 1.47        | 1.38     |
| 34  | Y     | 55   | PSU  | C6-N1 | 5.88  | 1.46        | 1.36     |
| 10  | A     | 527  | G7M  | C2-N3 | 5.88  | 1.47        | 1.33     |
| 34  | Y     | 46   | G7M  | C2-N3 | 5.87  | 1.47        | 1.33     |
| 8   | 7     | 2605 | PSU  | C6-N1 | 5.86  | 1.46        | 1.36     |
| 32  | W     | 55   | PSU  | C6-N1 | 5.84  | 1.45        | 1.36     |
| 32  | W     | 8    | 4SU  | C6-C5 | 5.83  | 1.48        | 1.35     |
| 8   | 7     | 2504 | PSU  | C6-N1 | 5.83  | 1.45        | 1.36     |
| 32  | W     | 46   | G7M  | C2-N3 | 5.82  | 1.47        | 1.33     |
| 8   | 7     | 746  | PSU  | C6-N1 | 5.82  | 1.45        | 1.36     |
| 8   | 7     | 2604 | PSU  | C6-N1 | 5.82  | 1.45        | 1.36     |
| 33  | X     | 8    | 4SU  | C6-C5 | 5.81  | 1.48        | 1.35     |
| 33  | X     | 47   | G7M  | C2-N3 | 5.81  | 1.47        | 1.33     |
| 8   | 7     | 2069 | G7M  | C2-N3 | 5.80  | 1.47        | 1.33     |
| 8   | 7     | 2457 | PSU  | C6-N1 | 5.80  | 1.45        | 1.36     |
| 32  | W     | 32   | PSU  | C6-N1 | 5.79  | 1.45        | 1.36     |
| 33  | X     | 56   | PSU  | C6-N1 | 5.79  | 1.45        | 1.36     |
| 8   | 7     | 955  | PSU  | C6-N1 | 5.76  | 1.45        | 1.36     |
| 32  | W     | 8    | 4SU  | C2-N1 | 5.75  | 1.47        | 1.38     |
| 8   | 7     | 2580 | PSU  | C6-N1 | 5.73  | 1.45        | 1.36     |
| 8   | 7     | 1962 | 5MC  | C4-N4 | 5.70  | 1.48        | 1.34     |
| 10  | A     | 1407 | 5MC  | C4-N4 | 5.68  | 1.48        | 1.34     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 10  | A     | 1407 | 5MC  | C6-N1 | 5.67  | 1.47        | 1.38     |
| 10  | A     | 967  | 5MC  | C4-N4 | 5.63  | 1.48        | 1.34     |
| 10  | A     | 967  | 5MC  | C6-N1 | 5.58  | 1.47        | 1.38     |
| 8   | 7     | 2498 | OMC  | C4-N3 | 5.49  | 1.45        | 1.34     |
| 8   | 7     | 1962 | 5MC  | C6-N1 | 5.49  | 1.47        | 1.38     |
| 8   | 7     | 2552 | OMU  | C6-C5 | 5.46  | 1.47        | 1.35     |
| 8   | 7     | 1915 | 3TD  | C6-N1 | 5.46  | 1.45        | 1.36     |
| 10  | A     | 1516 | 2MG  | C2-N1 | 5.42  | 1.45        | 1.36     |
| 10  | A     | 1207 | 2MG  | C2-N1 | 5.42  | 1.45        | 1.36     |
| 10  | A     | 966  | 2MG  | C2-N1 | 5.38  | 1.45        | 1.36     |
| 33  | X     | 38   | 2MA  | C5-C6 | 5.38  | 1.56        | 1.41     |
| 8   | 7     | 2503 | 2MA  | C5-C6 | 5.33  | 1.55        | 1.41     |
| 33  | X     | 33   | RSP  | C4-N3 | 5.29  | 1.45        | 1.34     |
| 8   | 7     | 2445 | 2MG  | C2-N1 | 5.27  | 1.45        | 1.36     |
| 8   | 7     | 2251 | OMG  | C2-N3 | 5.26  | 1.45        | 1.33     |
| 8   | 7     | 2498 | OMC  | C4-N4 | 5.16  | 1.46        | 1.33     |
| 10  | A     | 1498 | UR3  | C2-N3 | 5.14  | 1.49        | 1.39     |
| 10  | A     | 1402 | 4OC  | C4-N4 | 5.13  | 1.46        | 1.35     |
| 32  | W     | 17   | H2U  | C4-N3 | 5.02  | 1.46        | 1.37     |
| 33  | X     | 21   | H2U  | C4-N3 | 5.00  | 1.46        | 1.37     |
| 32  | W     | 20   | H2U  | C4-N3 | 4.96  | 1.46        | 1.37     |
| 34  | Y     | 17   | H2U  | C4-N3 | 4.94  | 1.46        | 1.37     |
| 32  | W     | 16   | H2U  | C4-N3 | 4.89  | 1.45        | 1.37     |
| 33  | X     | 17   | H2U  | C4-N3 | 4.89  | 1.45        | 1.37     |
| 8   | 7     | 2449 | H2U  | C4-N3 | 4.84  | 1.45        | 1.37     |
| 32  | W     | 54   | 5MU  | C2-N1 | 4.65  | 1.45        | 1.38     |
| 10  | A     | 967  | 5MC  | C2-N1 | 4.58  | 1.49        | 1.40     |
| 10  | A     | 1407 | 5MC  | C2-N1 | 4.55  | 1.49        | 1.40     |
| 8   | 7     | 2552 | OMU  | C4-N3 | 4.54  | 1.46        | 1.38     |
| 8   | 7     | 1962 | 5MC  | C2-N1 | 4.54  | 1.49        | 1.40     |
| 33  | X     | 55   | 5MU  | C2-N1 | 4.52  | 1.45        | 1.38     |
| 8   | 7     | 2552 | OMU  | O4-C4 | -4.43 | 1.15        | 1.24     |
| 32  | W     | 54   | 5MU  | C2-N3 | 4.42  | 1.45        | 1.38     |
| 33  | X     | 55   | 5MU  | C2-N3 | 4.42  | 1.45        | 1.38     |
| 33  | X     | 56   | PSU  | C4-N3 | 4.39  | 1.47        | 1.38     |
| 8   | 7     | 2605 | PSU  | C4-N3 | 4.38  | 1.47        | 1.38     |
| 32  | W     | 32   | PSU  | C4-N3 | 4.37  | 1.46        | 1.38     |
| 8   | 7     | 746  | PSU  | C4-N3 | 4.36  | 1.46        | 1.38     |
| 32  | W     | 55   | PSU  | C4-N3 | 4.36  | 1.46        | 1.38     |
| 34  | Y     | 55   | PSU  | C4-N3 | 4.32  | 1.46        | 1.38     |
| 32  | W     | 46   | G7M  | C5-N7 | -4.32 | 1.34        | 1.39     |
| 8   | 7     | 2504 | PSU  | C4-N3 | 4.32  | 1.46        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 8   | 7     | 955  | PSU  | C4-N3 | 4.30  | 1.46        | 1.38     |
| 8   | 7     | 2498 | OMC  | C2-N1 | 4.28  | 1.49        | 1.40     |
| 8   | 7     | 2604 | PSU  | C4-N3 | 4.27  | 1.46        | 1.38     |
| 8   | 7     | 2580 | PSU  | C4-N3 | 4.26  | 1.46        | 1.38     |
| 8   | 7     | 2069 | G7M  | C5-N7 | -4.26 | 1.34        | 1.39     |
| 10  | A     | 1402 | 4OC  | C2-N1 | 4.26  | 1.49        | 1.40     |
| 8   | 7     | 2457 | PSU  | C4-N3 | 4.25  | 1.46        | 1.38     |
| 8   | 7     | 1915 | 3TD  | C2-N3 | 4.21  | 1.47        | 1.38     |
| 8   | 7     | 2498 | OMC  | O2-C2 | -4.19 | 1.16        | 1.23     |
| 10  | A     | 527  | G7M  | C5-N7 | -4.18 | 1.34        | 1.39     |
| 33  | X     | 47   | G7M  | C5-N7 | -4.13 | 1.34        | 1.39     |
| 34  | Y     | 46   | G7M  | C5-N7 | -4.06 | 1.34        | 1.39     |
| 33  | X     | 47   | G7M  | C5-C6 | 3.98  | 1.54        | 1.43     |
| 34  | Y     | 46   | G7M  | C5-C6 | 3.95  | 1.54        | 1.43     |
| 32  | W     | 46   | G7M  | C5-C6 | 3.95  | 1.54        | 1.43     |
| 10  | A     | 1402 | 4OC  | C5-C4 | 3.91  | 1.49        | 1.40     |
| 10  | A     | 527  | G7M  | C5-C6 | 3.89  | 1.54        | 1.43     |
| 10  | A     | 1518 | MA6  | C6-N6 | 3.87  | 1.48        | 1.36     |
| 8   | 7     | 2069 | G7M  | C5-C6 | 3.86  | 1.54        | 1.43     |
| 10  | A     | 1519 | MA6  | C6-N6 | 3.81  | 1.48        | 1.36     |
| 8   | 7     | 2498 | OMC  | C6-N1 | 3.76  | 1.47        | 1.38     |
| 8   | 7     | 2552 | OMU  | C6-N1 | 3.73  | 1.47        | 1.38     |
| 33  | X     | 38   | 2MA  | C5-N7 | -3.61 | 1.32        | 1.39     |
| 33  | X     | 48   | 3AU  | C4-N3 | 3.61  | 1.46        | 1.40     |
| 8   | 7     | 2552 | OMU  | O2-C2 | -3.61 | 1.16        | 1.23     |
| 33  | X     | 33   | RSP  | C5-C4 | 3.59  | 1.51        | 1.42     |
| 32  | W     | 8    | 4SU  | C5-C4 | 3.53  | 1.47        | 1.42     |
| 8   | 7     | 2503 | 2MA  | C8-N7 | 3.53  | 1.38        | 1.31     |
| 8   | 7     | 2503 | 2MA  | C5-N7 | -3.51 | 1.32        | 1.39     |
| 33  | X     | 8    | 4SU  | C5-C4 | 3.48  | 1.47        | 1.42     |
| 8   | 7     | 745  | 1MG  | C5-C6 | 3.46  | 1.54        | 1.45     |
| 32  | W     | 8    | 4SU  | C6-N1 | 3.40  | 1.46        | 1.38     |
| 33  | X     | 8    | 4SU  | C6-N1 | 3.39  | 1.46        | 1.38     |
| 33  | X     | 38   | 2MA  | C8-N7 | 3.34  | 1.37        | 1.31     |
| 10  | A     | 1402 | 4OC  | C6-N1 | 3.31  | 1.46        | 1.38     |
| 33  | X     | 48   | 3AU  | C6-N1 | 3.30  | 1.46        | 1.38     |
| 8   | 7     | 2251 | OMG  | C2-N1 | 3.29  | 1.45        | 1.37     |
| 8   | 7     | 2605 | PSU  | O4-C4 | -3.23 | 1.17        | 1.23     |
| 8   | 7     | 2604 | PSU  | O4-C4 | -3.18 | 1.17        | 1.23     |
| 8   | 7     | 2504 | PSU  | O4-C4 | -3.17 | 1.17        | 1.23     |
| 8   | 7     | 2580 | PSU  | O4-C4 | -3.17 | 1.17        | 1.23     |
| 8   | 7     | 955  | PSU  | O4-C4 | -3.17 | 1.17        | 1.23     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 33  | X     | 33   | RSP  | C2-S2   | -3.17 | 1.59        | 1.67     |
| 8   | 7     | 746  | PSU  | O4-C4   | -3.16 | 1.17        | 1.23     |
| 34  | Y     | 55   | PSU  | O4-C4   | -3.16 | 1.17        | 1.23     |
| 8   | 7     | 2457 | PSU  | O4-C4   | -3.15 | 1.17        | 1.23     |
| 32  | W     | 55   | PSU  | O4-C4   | -3.14 | 1.17        | 1.23     |
| 33  | X     | 33   | RSP  | C6-N1   | 3.14  | 1.45        | 1.38     |
| 32  | W     | 32   | PSU  | O4-C4   | -3.13 | 1.17        | 1.23     |
| 33  | X     | 56   | PSU  | O4-C4   | -3.13 | 1.17        | 1.23     |
| 34  | Y     | 46   | G7M  | C2-N1   | 3.07  | 1.45        | 1.37     |
| 10  | A     | 1498 | UR3  | C6-N1   | 3.07  | 1.45        | 1.38     |
| 34  | Y     | 46   | G7M  | C6-N1   | 3.06  | 1.44        | 1.38     |
| 10  | A     | 527  | G7M  | C2-N1   | 3.04  | 1.45        | 1.37     |
| 33  | X     | 48   | 3AU  | C11-C10 | 3.03  | 1.59        | 1.52     |
| 33  | X     | 47   | G7M  | C6-N1   | 3.02  | 1.44        | 1.38     |
| 8   | 7     | 2069 | G7M  | C2-N1   | 3.01  | 1.45        | 1.37     |
| 10  | A     | 527  | G7M  | C6-N1   | 3.00  | 1.44        | 1.38     |
| 32  | W     | 46   | G7M  | C2-N1   | 3.00  | 1.45        | 1.37     |
| 33  | X     | 47   | G7M  | C2-N1   | 2.99  | 1.45        | 1.37     |
| 32  | W     | 46   | G7M  | C6-N1   | 2.97  | 1.44        | 1.38     |
| 8   | 7     | 2069 | G7M  | C6-N1   | 2.94  | 1.44        | 1.38     |
| 10  | A     | 1207 | 2MG  | C5-C6   | 2.94  | 1.55        | 1.44     |
| 10  | A     | 966  | 2MG  | C5-C6   | 2.92  | 1.55        | 1.44     |
| 10  | A     | 1516 | 2MG  | C5-C6   | 2.89  | 1.55        | 1.44     |
| 8   | 7     | 2445 | 2MG  | C5-N7   | -2.88 | 1.33        | 1.39     |
| 8   | 7     | 2445 | 2MG  | C5-C6   | 2.88  | 1.55        | 1.44     |
| 8   | 7     | 2605 | PSU  | C1'-C5  | 2.85  | 1.56        | 1.50     |
| 33  | X     | 56   | PSU  | C1'-C5  | 2.84  | 1.56        | 1.50     |
| 10  | A     | 1207 | 2MG  | C6-N1   | 2.78  | 1.44        | 1.38     |
| 10  | A     | 966  | 2MG  | C5-N7   | -2.77 | 1.33        | 1.39     |
| 10  | A     | 1516 | 2MG  | C5-N7   | -2.76 | 1.33        | 1.39     |
| 8   | 7     | 2498 | OMC  | C5-C4   | 2.76  | 1.49        | 1.42     |
| 10  | A     | 1516 | 2MG  | C6-N1   | 2.76  | 1.44        | 1.38     |
| 8   | 7     | 2504 | PSU  | C1'-C5  | 2.76  | 1.56        | 1.50     |
| 8   | 7     | 2604 | PSU  | C1'-C5  | 2.75  | 1.56        | 1.50     |
| 10  | A     | 1402 | 4OC  | O2-C2   | -2.74 | 1.18        | 1.23     |
| 32  | W     | 55   | PSU  | C1'-C5  | 2.73  | 1.56        | 1.50     |
| 10  | A     | 966  | 2MG  | C6-N1   | 2.72  | 1.43        | 1.38     |
| 8   | 7     | 2580 | PSU  | C1'-C5  | 2.72  | 1.56        | 1.50     |
| 8   | 7     | 746  | PSU  | C1'-C5  | 2.72  | 1.56        | 1.50     |
| 10  | A     | 1207 | 2MG  | C5-N7   | -2.72 | 1.33        | 1.39     |
| 8   | 7     | 955  | PSU  | C1'-C5  | 2.71  | 1.56        | 1.50     |
| 32  | W     | 32   | PSU  | C1'-C5  | 2.70  | 1.56        | 1.50     |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 8   | 7     | 745  | 1MG  | C5-N7  | -2.69 | 1.33        | 1.39     |
| 34  | Y     | 55   | PSU  | C1'-C5 | 2.69  | 1.56        | 1.50     |
| 33  | X     | 48   | 3AU  | C5-C4  | 2.69  | 1.50        | 1.43     |
| 8   | 7     | 2457 | PSU  | C1'-C5 | 2.64  | 1.56        | 1.50     |
| 8   | 7     | 2445 | 2MG  | C6-N1  | 2.64  | 1.43        | 1.38     |
| 8   | 7     | 955  | PSU  | O2-C2  | -2.63 | 1.17        | 1.23     |
| 8   | 7     | 2504 | PSU  | O2-C2  | -2.63 | 1.17        | 1.23     |
| 32  | W     | 54   | 5MU  | O4-C4  | -2.62 | 1.18        | 1.23     |
| 8   | 7     | 1618 | 6MZ  | C5-N7  | -2.61 | 1.34        | 1.39     |
| 8   | 7     | 2605 | PSU  | O2-C2  | -2.60 | 1.17        | 1.23     |
| 33  | X     | 56   | PSU  | O2-C2  | -2.60 | 1.17        | 1.23     |
| 8   | 7     | 1915 | 3TD  | C4-N3  | 2.59  | 1.46        | 1.40     |
| 34  | Y     | 55   | PSU  | O2-C2  | -2.59 | 1.18        | 1.23     |
| 8   | 7     | 2457 | PSU  | O2-C2  | -2.59 | 1.18        | 1.23     |
| 8   | 7     | 2030 | 6MZ  | C5-N7  | -2.59 | 1.34        | 1.39     |
| 8   | 7     | 2580 | PSU  | O2-C2  | -2.58 | 1.18        | 1.23     |
| 8   | 7     | 746  | PSU  | O2-C2  | -2.58 | 1.18        | 1.23     |
| 32  | W     | 37   | MIA  | C5-N7  | -2.57 | 1.34        | 1.39     |
| 32  | W     | 32   | PSU  | O2-C2  | -2.56 | 1.18        | 1.23     |
| 8   | 7     | 1915 | 3TD  | C1'-C5 | 2.56  | 1.56        | 1.50     |
| 8   | 7     | 2604 | PSU  | O2-C2  | -2.54 | 1.18        | 1.23     |
| 33  | X     | 55   | 5MU  | O4-C4  | -2.54 | 1.18        | 1.23     |
| 32  | W     | 55   | PSU  | O2-C2  | -2.52 | 1.18        | 1.23     |
| 33  | X     | 47   | G7M  | O6-C6  | -2.50 | 1.18        | 1.23     |
| 32  | W     | 37   | MIA  | C5-C4  | -2.44 | 1.34        | 1.39     |
| 32  | W     | 46   | G7M  | O6-C6  | -2.44 | 1.18        | 1.23     |
| 10  | A     | 527  | G7M  | O6-C6  | -2.44 | 1.18        | 1.23     |
| 8   | 7     | 2069 | G7M  | O6-C6  | -2.43 | 1.19        | 1.23     |
| 34  | Y     | 46   | G7M  | O6-C6  | -2.39 | 1.19        | 1.23     |
| 8   | 7     | 2251 | OMG  | C5-C6  | 2.37  | 1.53        | 1.44     |
| 10  | A     | 1519 | MA6  | C5-C4  | -2.36 | 1.34        | 1.39     |
| 10  | A     | 1207 | 2MG  | O6-C6  | -2.36 | 1.19        | 1.23     |
| 8   | 7     | 2445 | 2MG  | O6-C6  | -2.34 | 1.19        | 1.23     |
| 10  | A     | 1516 | 2MG  | O6-C6  | -2.31 | 1.19        | 1.23     |
| 10  | A     | 966  | 2MG  | O6-C6  | -2.31 | 1.19        | 1.23     |
| 8   | 7     | 2552 | OMU  | C5-C4  | 2.30  | 1.48        | 1.43     |
| 8   | 7     | 1915 | 3TD  | O4-C4  | -2.30 | 1.18        | 1.23     |
| 32  | W     | 16   | H2U  | O2-C2  | -2.28 | 1.18        | 1.23     |
| 10  | A     | 1518 | MA6  | C5-N7  | -2.27 | 1.34        | 1.39     |
| 10  | A     | 1407 | 5MC  | O2-C2  | -2.27 | 1.19        | 1.23     |
| 8   | 7     | 2449 | H2U  | O2-C2  | -2.27 | 1.18        | 1.23     |
| 10  | A     | 1498 | UR3  | C5-C4  | 2.26  | 1.49        | 1.43     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 10  | A     | 967  | 5MC  | O2-C2   | -2.26 | 1.19        | 1.23     |
| 34  | Y     | 17   | H2U  | O2-C2   | -2.25 | 1.18        | 1.23     |
| 33  | X     | 17   | H2U  | O2-C2   | -2.25 | 1.18        | 1.23     |
| 32  | W     | 20   | H2U  | O2-C2   | -2.24 | 1.18        | 1.23     |
| 33  | X     | 21   | H2U  | O2-C2   | -2.24 | 1.19        | 1.23     |
| 10  | A     | 1518 | MA6  | C5-C4   | -2.24 | 1.34        | 1.39     |
| 8   | 7     | 1618 | 6MZ  | C6-N1   | -2.23 | 1.31        | 1.35     |
| 32  | W     | 17   | H2U  | O2-C2   | -2.22 | 1.19        | 1.23     |
| 8   | 7     | 1962 | 5MC  | O2-C2   | -2.19 | 1.19        | 1.23     |
| 8   | 7     | 2030 | 6MZ  | C5-C4   | -2.18 | 1.34        | 1.39     |
| 10  | A     | 1498 | UR3  | C4-N3   | 2.18  | 1.45        | 1.40     |
| 10  | A     | 1519 | MA6  | C5-N7   | -2.17 | 1.34        | 1.39     |
| 34  | Y     | 17   | H2U  | O4-C4   | -2.17 | 1.18        | 1.23     |
| 32  | W     | 20   | H2U  | O4-C4   | -2.17 | 1.18        | 1.23     |
| 34  | Y     | 46   | G7M  | C8-N7   | 2.16  | 1.36        | 1.33     |
| 8   | 7     | 2449 | H2U  | O4-C4   | -2.16 | 1.18        | 1.23     |
| 10  | A     | 527  | G7M  | C8-N7   | 2.15  | 1.36        | 1.33     |
| 8   | 7     | 2503 | 2MA  | C6-N6   | -2.14 | 1.28        | 1.34     |
| 33  | X     | 38   | 2MA  | C6-N6   | -2.14 | 1.28        | 1.34     |
| 33  | X     | 21   | H2U  | O4-C4   | -2.13 | 1.18        | 1.23     |
| 10  | A     | 1498 | UR3  | O4-C4   | -2.12 | 1.19        | 1.23     |
| 33  | X     | 17   | H2U  | O4-C4   | -2.12 | 1.19        | 1.23     |
| 8   | 7     | 2030 | 6MZ  | C6-N1   | -2.12 | 1.31        | 1.35     |
| 32  | W     | 17   | H2U  | O4-C4   | -2.11 | 1.19        | 1.23     |
| 32  | W     | 16   | H2U  | O4-C4   | -2.11 | 1.19        | 1.23     |
| 10  | A     | 1498 | UR3  | O2-C2   | -2.11 | 1.18        | 1.22     |
| 8   | 7     | 2580 | PSU  | O4'-C1' | -2.11 | 1.40        | 1.43     |
| 8   | 7     | 746  | PSU  | O4'-C1' | -2.10 | 1.40        | 1.43     |
| 8   | 7     | 1618 | 6MZ  | C5-C4   | -2.09 | 1.35        | 1.39     |
| 8   | 7     | 2069 | G7M  | C8-N7   | 2.08  | 1.36        | 1.33     |
| 10  | A     | 1519 | MA6  | C8-N7   | 2.08  | 1.35        | 1.31     |
| 32  | W     | 37   | MIA  | C8-N9   | -2.05 | 1.33        | 1.37     |
| 8   | 7     | 2251 | OMG  | C5-N7   | -2.04 | 1.35        | 1.39     |
| 8   | 7     | 2251 | OMG  | C8-N7   | 2.01  | 1.38        | 1.32     |
| 8   | 7     | 2030 | 6MZ  | C2-N1   | 2.01  | 1.37        | 1.33     |
| 32  | W     | 46   | G7M  | C8-N7   | 2.00  | 1.36        | 1.33     |

All (325) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|--------|-------------|----------|
| 33  | X     | 38   | 2MA  | C1'-N9-C8 | -12.89 | 98.03       | 127.14   |
| 10  | A     | 1519 | MA6  | N1-C6-N6  | -12.29 | 103.65      | 117.08   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 8   | 7     | 2503 | 2MA  | C1'-N9-C8  | -12.05 | 99.93       | 127.14   |
| 10  | A     | 1518 | MA6  | N1-C6-N6   | -11.81 | 104.17      | 117.08   |
| 33  | X     | 38   | 2MA  | C4-N9-C1'  | 11.55  | 154.12      | 126.59   |
| 8   | 7     | 2503 | 2MA  | C4-N9-C1'  | 10.46  | 151.52      | 126.59   |
| 32  | W     | 54   | 5MU  | C5-C4-N3   | 10.12  | 123.95      | 115.31   |
| 33  | X     | 55   | 5MU  | C5-C4-N3   | 10.08  | 123.91      | 115.31   |
| 32  | W     | 37   | MIA  | C11-S10-C2 | 9.45   | 109.32      | 102.27   |
| 32  | W     | 8    | 4SU  | C4-N3-C2   | -7.93  | 119.64      | 127.34   |
| 33  | X     | 8    | 4SU  | C4-N3-C2   | -7.89  | 119.68      | 127.34   |
| 33  | X     | 55   | 5MU  | C5-C6-N1   | -7.69  | 115.42      | 123.34   |
| 32  | W     | 54   | 5MU  | C5-C6-N1   | -7.32  | 115.80      | 123.34   |
| 8   | 7     | 2449 | H2U  | C4-N3-C2   | -7.17  | 119.84      | 125.79   |
| 8   | 7     | 2251 | OMG  | C1'-N9-C8  | -7.06  | 106.59      | 126.70   |
| 34  | Y     | 17   | H2U  | C4-N3-C2   | -7.02  | 119.97      | 125.79   |
| 32  | W     | 20   | H2U  | C4-N3-C2   | -6.96  | 120.02      | 125.79   |
| 33  | X     | 21   | H2U  | C4-N3-C2   | -6.94  | 120.03      | 125.79   |
| 32  | W     | 17   | H2U  | C4-N3-C2   | -6.93  | 120.04      | 125.79   |
| 8   | 7     | 2445 | 2MG  | C2-N3-C4   | 6.89   | 120.58      | 112.04   |
| 10  | A     | 966  | 2MG  | C2-N3-C4   | 6.87   | 120.56      | 112.04   |
| 33  | X     | 55   | 5MU  | C4-N3-C2   | -6.76  | 118.60      | 127.35   |
| 33  | X     | 17   | H2U  | C4-N3-C2   | -6.70  | 120.24      | 125.79   |
| 32  | W     | 54   | 5MU  | C4-N3-C2   | -6.64  | 118.75      | 127.35   |
| 10  | A     | 1516 | 2MG  | C2-N3-C4   | 6.56   | 120.17      | 112.04   |
| 32  | W     | 16   | H2U  | C4-N3-C2   | -6.55  | 120.36      | 125.79   |
| 10  | A     | 1207 | 2MG  | C2-N3-C4   | 6.52   | 120.12      | 112.04   |
| 33  | X     | 38   | 2MA  | C5-C4-N3   | -6.51  | 119.86      | 127.19   |
| 32  | W     | 37   | MIA  | C5-C4-N3   | -6.51  | 119.86      | 127.19   |
| 8   | 7     | 745  | 1MG  | C1'-N9-C4  | -6.51  | 107.17      | 126.50   |
| 10  | A     | 1519 | MA6  | C5-C6-N6   | 6.41   | 136.47      | 125.30   |
| 10  | A     | 1518 | MA6  | C5-C6-N6   | 6.22   | 136.13      | 125.30   |
| 8   | 7     | 745  | 1MG  | C1'-N9-C8  | 6.13   | 144.16      | 126.70   |
| 8   | 7     | 2251 | OMG  | C1'-N9-C4  | 5.84   | 143.85      | 126.50   |
| 8   | 7     | 1618 | 6MZ  | C5-C4-N3   | -5.80  | 119.18      | 126.75   |
| 8   | 7     | 2445 | 2MG  | C5-C4-N3   | -5.75  | 119.13      | 128.46   |
| 33  | X     | 8    | 4SU  | C5-C4-N3   | 5.67   | 119.95      | 114.69   |
| 10  | A     | 966  | 2MG  | C5-C4-N3   | -5.64  | 119.32      | 128.46   |
| 8   | 7     | 2503 | 2MA  | C5-C4-N3   | -5.54  | 120.96      | 127.19   |
| 10  | A     | 1207 | 2MG  | C1'-N9-C4  | -5.53  | 110.08      | 126.50   |
| 32  | W     | 8    | 4SU  | C5-C4-N3   | 5.51   | 119.80      | 114.69   |
| 10  | A     | 1519 | MA6  | N1-C2-N3   | -5.44  | 120.09      | 128.60   |
| 10  | A     | 1518 | MA6  | N1-C2-N3   | -5.43  | 120.10      | 128.60   |
| 8   | 7     | 1618 | 6MZ  | N1-C2-N3   | -5.40  | 120.16      | 128.60   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 8   | 7     | 1915 | 3TD  | N1-C2-N3  | 5.38  | 120.38      | 116.14   |
| 10  | A     | 1207 | 2MG  | C1'-N9-C8 | 5.38  | 142.00      | 126.70   |
| 8   | 7     | 745  | 1MG  | C5-C4-N3  | -5.36 | 119.76      | 128.46   |
| 8   | 7     | 2030 | 6MZ  | C5-C4-N3  | -5.35 | 119.77      | 126.75   |
| 10  | A     | 1516 | 2MG  | C5-C4-N3  | -5.34 | 119.81      | 128.46   |
| 8   | 7     | 2030 | 6MZ  | N1-C2-N3  | -5.34 | 120.26      | 128.60   |
| 10  | A     | 1518 | MA6  | C1'-N9-C8 | -5.29 | 115.20      | 127.14   |
| 10  | A     | 1516 | 2MG  | C1'-N9-C4 | -5.19 | 111.10      | 126.50   |
| 10  | A     | 1207 | 2MG  | C5-C4-N3  | -5.17 | 120.07      | 128.46   |
| 8   | 7     | 2552 | OMU  | C4-N3-C2  | -5.13 | 119.81      | 126.58   |
| 10  | A     | 1516 | 2MG  | C1'-N9-C8 | 5.01  | 140.97      | 126.70   |
| 32  | W     | 46   | G7M  | C2-N3-C4  | 4.98  | 121.17      | 112.30   |
| 33  | X     | 47   | G7M  | C2-N3-C4  | 4.91  | 121.05      | 112.30   |
| 10  | A     | 1518 | MA6  | C5-C4-N3  | -4.91 | 120.34      | 126.75   |
| 10  | A     | 1519 | MA6  | C5-C4-N3  | -4.86 | 120.41      | 126.75   |
| 10  | A     | 966  | 2MG  | C1'-N9-C4 | -4.86 | 112.07      | 126.50   |
| 32  | W     | 54   | 5MU  | C5M-C5-C6 | -4.86 | 116.36      | 122.85   |
| 33  | X     | 55   | 5MU  | C5M-C5-C6 | -4.84 | 116.38      | 122.85   |
| 8   | 7     | 2503 | 2MA  | N9-C8-N7  | -4.84 | 107.30      | 113.91   |
| 10  | A     | 1519 | MA6  | C1'-N9-C8 | -4.76 | 116.38      | 127.14   |
| 8   | 7     | 2457 | PSU  | C4-N3-C2  | -4.76 | 119.48      | 126.34   |
| 8   | 7     | 2251 | OMG  | C5-C4-N3  | -4.74 | 120.77      | 128.46   |
| 32  | W     | 46   | G7M  | C5-C4-N3  | -4.73 | 119.08      | 128.15   |
| 10  | A     | 966  | 2MG  | C1'-N9-C8 | 4.72  | 140.15      | 126.70   |
| 33  | X     | 55   | 5MU  | N3-C2-N1  | 4.71  | 121.15      | 114.89   |
| 10  | A     | 1519 | MA6  | N9-C8-N7  | -4.68 | 107.51      | 113.91   |
| 8   | 7     | 2445 | 2MG  | C2-N1-C6  | -4.66 | 119.12      | 124.48   |
| 8   | 7     | 2604 | PSU  | C4-N3-C2  | -4.64 | 119.66      | 126.34   |
| 32  | W     | 32   | PSU  | C4-N3-C2  | -4.63 | 119.67      | 126.34   |
| 34  | Y     | 55   | PSU  | C4-N3-C2  | -4.63 | 119.67      | 126.34   |
| 10  | A     | 1498 | UR3  | C4-N3-C2  | -4.62 | 120.21      | 124.56   |
| 8   | 7     | 2504 | PSU  | C4-N3-C2  | -4.62 | 119.69      | 126.34   |
| 32  | W     | 54   | 5MU  | N3-C2-N1  | 4.62  | 121.02      | 114.89   |
| 32  | W     | 55   | PSU  | C4-N3-C2  | -4.61 | 119.70      | 126.34   |
| 8   | 7     | 2605 | PSU  | C4-N3-C2  | -4.61 | 119.70      | 126.34   |
| 33  | X     | 47   | G7M  | C5-C4-N3  | -4.59 | 119.34      | 128.15   |
| 8   | 7     | 955  | PSU  | C4-N3-C2  | -4.58 | 119.74      | 126.34   |
| 8   | 7     | 746  | PSU  | C4-N3-C2  | -4.57 | 119.76      | 126.34   |
| 10  | A     | 1518 | MA6  | N9-C8-N7  | -4.56 | 107.68      | 113.91   |
| 8   | 7     | 2580 | PSU  | C4-N3-C2  | -4.54 | 119.80      | 126.34   |
| 8   | 7     | 2445 | 2MG  | C1'-N9-C4 | -4.54 | 113.02      | 126.50   |
| 8   | 7     | 2030 | 6MZ  | C4-C5-C6  | 4.54  | 120.33      | 116.81   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 33  | X     | 56   | PSU  | C4-N3-C2  | -4.50 | 119.86      | 126.34   |
| 10  | A     | 966  | 2MG  | C2-N1-C6  | -4.48 | 119.33      | 124.48   |
| 8   | 7     | 2445 | 2MG  | C1'-N9-C8 | 4.46  | 139.40      | 126.70   |
| 8   | 7     | 1618 | 6MZ  | C4-C5-C6  | 4.44  | 120.25      | 116.81   |
| 10  | A     | 1516 | 2MG  | C2-N1-C6  | -4.42 | 119.39      | 124.48   |
| 10  | A     | 527  | G7M  | C2-N3-C4  | 4.42  | 120.18      | 112.30   |
| 10  | A     | 1207 | 2MG  | C2-N1-C6  | -4.39 | 119.43      | 124.48   |
| 34  | Y     | 46   | G7M  | C2-N3-C4  | 4.38  | 120.11      | 112.30   |
| 8   | 7     | 2457 | PSU  | N1-C2-N3  | 4.34  | 120.04      | 115.13   |
| 8   | 7     | 2069 | G7M  | C2-N3-C4  | 4.33  | 120.01      | 112.30   |
| 8   | 7     | 2030 | 6MZ  | N9-C8-N7  | -4.32 | 108.01      | 113.91   |
| 32  | W     | 37   | MIA  | N9-C8-N7  | -4.29 | 108.05      | 113.91   |
| 8   | 7     | 2580 | PSU  | N1-C2-N3  | 4.25  | 119.95      | 115.13   |
| 8   | 7     | 2251 | OMG  | C2-N3-C4  | 4.25  | 119.86      | 112.30   |
| 32  | W     | 54   | 5MU  | C5M-C5-C4 | 4.23  | 123.42      | 118.77   |
| 32  | W     | 37   | MIA  | C4-C5-C6  | 4.22  | 120.08      | 116.81   |
| 8   | 7     | 955  | PSU  | N1-C2-N3  | 4.21  | 119.90      | 115.13   |
| 33  | X     | 38   | 2MA  | N9-C8-N7  | -4.20 | 108.17      | 113.91   |
| 34  | Y     | 55   | PSU  | N1-C2-N3  | 4.17  | 119.85      | 115.13   |
| 32  | W     | 32   | PSU  | N1-C2-N3  | 4.17  | 119.85      | 115.13   |
| 8   | 7     | 2604 | PSU  | N1-C2-N3  | 4.15  | 119.83      | 115.13   |
| 32  | W     | 55   | PSU  | N1-C2-N3  | 4.13  | 119.81      | 115.13   |
| 33  | X     | 56   | PSU  | N1-C2-N3  | 4.12  | 119.80      | 115.13   |
| 32  | W     | 54   | 5MU  | O4-C4-C5  | -4.12 | 120.13      | 124.90   |
| 10  | A     | 1518 | MA6  | C4-N9-C1' | 4.10  | 136.37      | 126.59   |
| 32  | W     | 46   | G7M  | C5-C6-N1  | 4.10  | 120.34      | 111.79   |
| 8   | 7     | 2504 | PSU  | N1-C2-N3  | 4.09  | 119.76      | 115.13   |
| 33  | X     | 47   | G7M  | C5-C6-N1  | 4.07  | 120.29      | 111.79   |
| 33  | X     | 55   | 5MU  | C5M-C5-C4 | 4.05  | 123.22      | 118.77   |
| 10  | A     | 527  | G7M  | C5-C4-N3  | -4.05 | 120.39      | 128.15   |
| 8   | 7     | 1915 | 3TD  | C4-N3-C2  | -4.04 | 120.22      | 124.61   |
| 8   | 7     | 746  | PSU  | N1-C2-N3  | 4.03  | 119.70      | 115.13   |
| 8   | 7     | 2605 | PSU  | N1-C2-N3  | 4.02  | 119.69      | 115.13   |
| 34  | Y     | 46   | G7M  | C5-C4-N3  | -4.01 | 120.47      | 128.15   |
| 8   | 7     | 1618 | 6MZ  | C9-N6-C6  | -4.00 | 119.42      | 122.87   |
| 10  | A     | 527  | G7M  | C5-C6-N1  | 3.98  | 120.11      | 111.79   |
| 8   | 7     | 2069 | G7M  | C5-C4-N3  | -3.98 | 120.52      | 128.15   |
| 32  | W     | 46   | G7M  | N9-C4-N3  | 3.96  | 133.89      | 125.94   |
| 8   | 7     | 1618 | 6MZ  | N9-C8-N7  | -3.96 | 108.50      | 113.91   |
| 34  | Y     | 46   | G7M  | C5-C6-N1  | 3.93  | 120.00      | 111.79   |
| 8   | 7     | 2069 | G7M  | C5-C6-N1  | 3.93  | 119.99      | 111.79   |
| 32  | W     | 8    | 4SU  | N3-C2-N1  | 3.91  | 120.08      | 114.89   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 8   | 7     | 2552 | OMU  | N3-C2-N1    | 3.86  | 120.02      | 114.89   |
| 8   | 7     | 2030 | 6MZ  | C4-N9-C1'   | -3.85 | 117.41      | 126.59   |
| 33  | X     | 55   | 5MU  | O4-C4-C5    | -3.82 | 120.47      | 124.90   |
| 33  | X     | 47   | G7M  | N9-C4-N3    | 3.80  | 133.58      | 125.94   |
| 33  | X     | 8    | 4SU  | N3-C2-N1    | 3.80  | 119.94      | 114.89   |
| 32  | W     | 37   | MIA  | N3-C2-N1    | -3.76 | 120.06      | 126.95   |
| 8   | 7     | 745  | 1MG  | C2-N3-C4    | 3.76  | 120.42      | 111.98   |
| 33  | X     | 48   | 3AU  | C4-N3-C2    | -3.74 | 119.93      | 124.63   |
| 8   | 7     | 1618 | 6MZ  | N3-C4-N9    | 3.71  | 133.20      | 127.08   |
| 8   | 7     | 1618 | 6MZ  | C2-N3-C4    | 3.68  | 120.45      | 111.75   |
| 8   | 7     | 2445 | 2MG  | N9-C4-N3    | 3.66  | 133.29      | 125.94   |
| 33  | X     | 38   | 2MA  | N3-C4-N9    | 3.66  | 132.06      | 126.99   |
| 32  | W     | 37   | MIA  | N3-C4-N9    | 3.64  | 132.05      | 126.99   |
| 10  | A     | 1519 | MA6  | C4-N9-C1'   | 3.61  | 135.20      | 126.59   |
| 10  | A     | 1518 | MA6  | C2-N1-C6    | 3.55  | 120.14      | 111.75   |
| 10  | A     | 966  | 2MG  | N9-C4-N3    | 3.55  | 133.07      | 125.94   |
| 8   | 7     | 2251 | OMG  | N9-C8-N7    | -3.54 | 106.73      | 113.39   |
| 10  | A     | 1518 | MA6  | C4-C5-C6    | 3.52  | 119.82      | 115.88   |
| 10  | A     | 1519 | MA6  | C2-N1-C6    | 3.52  | 120.06      | 111.75   |
| 32  | W     | 37   | MIA  | C4-N9-C1'   | -3.52 | 118.22      | 126.59   |
| 32  | W     | 8    | 4SU  | C5-C4-S4    | -3.49 | 119.97      | 124.47   |
| 32  | W     | 37   | MIA  | C12-C13-C14 | -3.49 | 120.35      | 127.14   |
| 8   | 7     | 2457 | PSU  | C6-C5-C4    | 3.47  | 120.63      | 118.20   |
| 10  | A     | 1519 | MA6  | C2-N3-C4    | 3.46  | 119.91      | 111.75   |
| 10  | A     | 1518 | MA6  | C2-N3-C4    | 3.45  | 119.90      | 111.75   |
| 8   | 7     | 2030 | 6MZ  | C2-N3-C4    | 3.44  | 119.88      | 111.75   |
| 32  | W     | 46   | G7M  | O6-C6-C5    | -3.44 | 120.31      | 128.06   |
| 8   | 7     | 2069 | G7M  | O6-C6-C5    | -3.42 | 120.36      | 128.06   |
| 10  | A     | 527  | G7M  | O6-C6-C5    | -3.41 | 120.36      | 128.06   |
| 8   | 7     | 745  | 1MG  | N9-C4-N3    | 3.40  | 132.77      | 125.94   |
| 34  | Y     | 46   | G7M  | O6-C6-C5    | -3.39 | 120.41      | 128.06   |
| 33  | X     | 8    | 4SU  | C5-C4-S4    | -3.39 | 120.10      | 124.47   |
| 33  | X     | 47   | G7M  | O6-C6-C5    | -3.38 | 120.43      | 128.06   |
| 10  | A     | 967  | 5MC  | C5-C6-N1    | -3.38 | 119.87      | 123.34   |
| 10  | A     | 1519 | MA6  | C4-C5-C6    | 3.37  | 119.65      | 115.88   |
| 33  | X     | 48   | 3AU  | C5-C4-N3    | 3.33  | 119.89      | 115.50   |
| 34  | Y     | 17   | H2U  | N3-C2-N1    | 3.32  | 120.16      | 116.65   |
| 8   | 7     | 2552 | OMU  | C5-C4-N3    | 3.31  | 119.80      | 114.84   |
| 34  | Y     | 55   | PSU  | C6-C5-C4    | 3.31  | 120.51      | 118.20   |
| 8   | 7     | 2503 | 2MA  | C5-N7-C8    | 3.31  | 108.21      | 103.51   |
| 10  | A     | 1519 | MA6  | C5-N7-C8    | 3.29  | 108.19      | 103.51   |
| 10  | A     | 1516 | 2MG  | N9-C4-N3    | 3.27  | 132.50      | 125.94   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 8   | 7     | 2030 | 6MZ  | N3-C4-N9  | 3.26  | 132.46      | 127.08   |
| 32  | W     | 32   | PSU  | C6-C5-C4  | 3.25  | 120.47      | 118.20   |
| 32  | W     | 37   | MIA  | C5-N7-C8  | 3.25  | 108.12      | 103.51   |
| 10  | A     | 1518 | MA6  | C5-N7-C8  | 3.24  | 108.11      | 103.51   |
| 33  | X     | 17   | H2U  | N3-C2-N1  | 3.24  | 120.08      | 116.65   |
| 8   | 7     | 955  | PSU  | C6-C5-C4  | 3.22  | 120.45      | 118.20   |
| 8   | 7     | 2580 | PSU  | C6-C5-C4  | 3.22  | 120.45      | 118.20   |
| 32  | W     | 17   | H2U  | N3-C2-N1  | 3.21  | 120.05      | 116.65   |
| 8   | 7     | 1962 | 5MC  | C5-C6-N1  | -3.21 | 120.04      | 123.34   |
| 8   | 7     | 2030 | 6MZ  | C1'-N9-C8 | 3.20  | 134.36      | 127.14   |
| 8   | 7     | 2449 | H2U  | N3-C2-N1  | 3.17  | 120.00      | 116.65   |
| 32  | W     | 37   | MIA  | N6-C6-N1  | -3.16 | 114.47      | 118.50   |
| 32  | W     | 46   | G7M  | C2-N1-C6  | -3.15 | 119.35      | 125.10   |
| 8   | 7     | 2604 | PSU  | C6-C5-C4  | 3.15  | 120.40      | 118.20   |
| 33  | X     | 21   | H2U  | N3-C2-N1  | 3.14  | 119.97      | 116.65   |
| 8   | 7     | 2069 | G7M  | N9-C4-N3  | 3.13  | 132.22      | 125.94   |
| 33  | X     | 38   | 2MA  | C5-N7-C8  | 3.12  | 107.94      | 103.51   |
| 34  | Y     | 46   | G7M  | N9-C4-N3  | 3.12  | 132.20      | 125.94   |
| 32  | W     | 20   | H2U  | N3-C2-N1  | 3.12  | 119.95      | 116.65   |
| 8   | 7     | 2030 | 6MZ  | C5-N7-C8  | 3.12  | 107.94      | 103.51   |
| 8   | 7     | 2504 | PSU  | C6-C5-C4  | 3.11  | 120.37      | 118.20   |
| 10  | A     | 527  | G7M  | N9-C4-N3  | 3.11  | 132.18      | 125.94   |
| 8   | 7     | 2503 | 2MA  | N3-C2-N1  | -3.10 | 120.01      | 125.72   |
| 8   | 7     | 745  | 1MG  | N9-C8-N7  | -3.10 | 107.55      | 113.39   |
| 33  | X     | 47   | G7M  | C2-N1-C6  | -3.07 | 119.49      | 125.10   |
| 10  | A     | 1207 | 2MG  | N9-C4-N3  | 3.06  | 132.08      | 125.94   |
| 8   | 7     | 2580 | PSU  | C6-N1-C2  | -3.04 | 119.57      | 122.68   |
| 33  | X     | 38   | 2MA  | N3-C2-N1  | -3.03 | 120.15      | 125.72   |
| 32  | W     | 16   | H2U  | N3-C2-N1  | 3.01  | 119.84      | 116.65   |
| 10  | A     | 527  | G7M  | C2-N1-C6  | -3.01 | 119.61      | 125.10   |
| 8   | 7     | 2069 | G7M  | C2-N1-C6  | -2.98 | 119.66      | 125.10   |
| 32  | W     | 37   | MIA  | C1'-N9-C8 | 2.98  | 133.87      | 127.14   |
| 32  | W     | 55   | PSU  | C6-C5-C4  | 2.98  | 120.28      | 118.20   |
| 8   | 7     | 955  | PSU  | C6-N1-C2  | -2.98 | 119.64      | 122.68   |
| 34  | Y     | 46   | G7M  | C2-N1-C6  | -2.97 | 119.68      | 125.10   |
| 33  | X     | 56   | PSU  | C6-N1-C2  | -2.96 | 119.66      | 122.68   |
| 8   | 7     | 746  | PSU  | C6-C5-C4  | 2.95  | 120.26      | 118.20   |
| 8   | 7     | 1618 | 6MZ  | C4-N9-C1' | -2.94 | 119.58      | 126.59   |
| 8   | 7     | 2251 | OMG  | C2-N1-C6  | -2.94 | 119.73      | 125.10   |
| 8   | 7     | 2251 | OMG  | N9-C4-N3  | 2.94  | 131.85      | 125.94   |
| 32  | W     | 37   | MIA  | C2-N3-C4  | 2.94  | 120.09      | 112.35   |
| 8   | 7     | 1618 | 6MZ  | C5-N7-C8  | 2.93  | 107.67      | 103.51   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 8   | 7     | 2449 | H2U  | C5-C4-N3  | 2.92  | 119.93      | 116.65   |
| 10  | A     | 1407 | 5MC  | C5-C6-N1  | -2.90 | 120.36      | 123.34   |
| 10  | A     | 1518 | MA6  | N3-C4-N9  | 2.88  | 131.83      | 127.08   |
| 8   | 7     | 2552 | OMU  | O4-C4-C5  | -2.87 | 120.12      | 125.16   |
| 32  | W     | 37   | MIA  | S10-C2-N3 | 2.85  | 125.88      | 116.01   |
| 32  | W     | 16   | H2U  | C5-C6-N1  | 2.83  | 120.95      | 111.61   |
| 33  | X     | 55   | 5MU  | C6-C5-C4  | 2.83  | 120.40      | 118.03   |
| 34  | Y     | 55   | PSU  | C6-N1-C2  | -2.82 | 119.80      | 122.68   |
| 8   | 7     | 2457 | PSU  | C6-N1-C2  | -2.82 | 119.80      | 122.68   |
| 32  | W     | 55   | PSU  | C6-N1-C2  | -2.82 | 119.80      | 122.68   |
| 32  | W     | 20   | H2U  | C5-C4-N3  | 2.81  | 119.81      | 116.65   |
| 32  | W     | 32   | PSU  | C6-N1-C2  | -2.80 | 119.82      | 122.68   |
| 8   | 7     | 2605 | PSU  | C6-N1-C2  | -2.80 | 119.82      | 122.68   |
| 8   | 7     | 746  | PSU  | C6-N1-C2  | -2.80 | 119.82      | 122.68   |
| 8   | 7     | 2604 | PSU  | C6-N1-C2  | -2.80 | 119.83      | 122.68   |
| 8   | 7     | 2504 | PSU  | C6-N1-C2  | -2.79 | 119.83      | 122.68   |
| 10  | A     | 1207 | 2MG  | N9-C8-N7  | -2.77 | 108.17      | 113.39   |
| 8   | 7     | 2445 | 2MG  | C5-C6-N1  | 2.77  | 120.23      | 113.19   |
| 10  | A     | 966  | 2MG  | C5-C6-N1  | 2.77  | 120.23      | 113.19   |
| 10  | A     | 1516 | 2MG  | N9-C8-N7  | -2.76 | 108.19      | 113.39   |
| 32  | W     | 46   | G7M  | CN7-N7-C5 | 2.75  | 130.19      | 126.77   |
| 34  | Y     | 17   | H2U  | C5-C4-N3  | 2.75  | 119.74      | 116.65   |
| 32  | W     | 16   | H2U  | C5-C4-N3  | 2.75  | 119.74      | 116.65   |
| 33  | X     | 21   | H2U  | C5-C4-N3  | 2.75  | 119.73      | 116.65   |
| 33  | X     | 17   | H2U  | C5-C6-N1  | 2.74  | 120.63      | 111.61   |
| 32  | W     | 17   | H2U  | C5-C4-N3  | 2.73  | 119.71      | 116.65   |
| 33  | X     | 56   | PSU  | C6-C5-C4  | 2.72  | 120.10      | 118.20   |
| 32  | W     | 17   | H2U  | C5-C6-N1  | 2.71  | 120.54      | 111.61   |
| 33  | X     | 47   | G7M  | CN7-N7-C5 | 2.71  | 130.13      | 126.77   |
| 8   | 7     | 745  | 1MG  | C5-C6-N1  | 2.70  | 120.12      | 114.91   |
| 10  | A     | 1516 | 2MG  | C5-C6-N1  | 2.70  | 120.04      | 113.19   |
| 10  | A     | 1207 | 2MG  | C5-C6-N1  | 2.69  | 120.03      | 113.19   |
| 10  | A     | 1519 | MA6  | N3-C4-N9  | 2.69  | 131.51      | 127.08   |
| 34  | Y     | 17   | H2U  | C5-C6-N1  | 2.68  | 120.44      | 111.61   |
| 33  | X     | 21   | H2U  | C5-C6-N1  | 2.67  | 120.42      | 111.61   |
| 10  | A     | 966  | 2MG  | N9-C8-N7  | -2.66 | 108.38      | 113.39   |
| 8   | 7     | 2251 | OMG  | C5-C6-N1  | 2.65  | 119.91      | 113.19   |
| 32  | W     | 20   | H2U  | C5-C6-N1  | 2.64  | 120.32      | 111.61   |
| 8   | 7     | 2503 | 2MA  | N3-C4-N9  | 2.64  | 130.65      | 126.99   |
| 32  | W     | 54   | 5MU  | C6-C5-C4  | 2.61  | 120.21      | 118.03   |
| 8   | 7     | 2449 | H2U  | C5-C6-N1  | 2.60  | 120.18      | 111.61   |
| 8   | 7     | 2503 | 2MA  | C4-N9-C8  | 2.60  | 108.54      | 105.73   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 33  | X     | 17   | H2U  | C5-C4-N3    | 2.59  | 119.56      | 116.65   |
| 10  | A     | 527  | G7M  | CN7-N7-C5   | 2.58  | 129.97      | 126.77   |
| 8   | 7     | 2445 | 2MG  | O6-C6-C5    | -2.57 | 119.79      | 126.60   |
| 8   | 7     | 955  | PSU  | O2-C2-N1    | -2.56 | 119.97      | 122.79   |
| 10  | A     | 966  | 2MG  | N1-C2-N3    | -2.55 | 120.01      | 123.95   |
| 8   | 7     | 2445 | 2MG  | N9-C8-N7    | -2.54 | 108.61      | 113.39   |
| 10  | A     | 1516 | 2MG  | O6-C6-C5    | -2.53 | 119.89      | 126.60   |
| 8   | 7     | 2457 | PSU  | O2-C2-N1    | -2.52 | 120.02      | 122.79   |
| 34  | Y     | 17   | H2U  | O2-C2-N1    | -2.52 | 119.94      | 123.11   |
| 10  | A     | 966  | 2MG  | O6-C6-C5    | -2.52 | 119.92      | 126.60   |
| 32  | W     | 37   | MIA  | C5-C6-N6    | 2.51  | 126.00      | 121.76   |
| 8   | 7     | 2503 | 2MA  | C4-C5-N7    | -2.51 | 107.56      | 110.62   |
| 10  | A     | 1518 | MA6  | C4-N9-C8    | 2.50  | 108.43      | 105.73   |
| 34  | Y     | 46   | G7M  | CN7-N7-C5   | 2.49  | 129.86      | 126.77   |
| 10  | A     | 1207 | 2MG  | O6-C6-C5    | -2.48 | 120.02      | 126.60   |
| 8   | 7     | 2251 | OMG  | O6-C6-C5    | -2.48 | 120.03      | 126.60   |
| 10  | A     | 1519 | MA6  | C4-N9-C8    | 2.47  | 108.41      | 105.73   |
| 32  | W     | 17   | H2U  | O2-C2-N1    | -2.47 | 120.01      | 123.11   |
| 8   | 7     | 2449 | H2U  | O2-C2-N1    | -2.47 | 120.01      | 123.11   |
| 8   | 7     | 2604 | PSU  | O2-C2-N1    | -2.46 | 120.08      | 122.79   |
| 10  | A     | 1207 | 2MG  | N1-C2-N3    | -2.45 | 120.16      | 123.95   |
| 10  | A     | 1516 | 2MG  | N1-C2-N3    | -2.45 | 120.17      | 123.95   |
| 8   | 7     | 2580 | PSU  | O2-C2-N1    | -2.45 | 120.10      | 122.79   |
| 8   | 7     | 2605 | PSU  | C6-C5-C4    | 2.44  | 119.90      | 118.20   |
| 8   | 7     | 2069 | G7M  | CN7-N7-C5   | 2.44  | 129.79      | 126.77   |
| 8   | 7     | 1618 | 6MZ  | C1'-N9-C8   | 2.43  | 132.63      | 127.14   |
| 8   | 7     | 2503 | 2MA  | CM2-C2-N1   | 2.43  | 120.94      | 117.15   |
| 8   | 7     | 746  | PSU  | O2-C2-N1    | -2.43 | 120.12      | 122.79   |
| 32  | W     | 55   | PSU  | O2-C2-N1    | -2.42 | 120.12      | 122.79   |
| 32  | W     | 20   | H2U  | O2-C2-N1    | -2.41 | 120.08      | 123.11   |
| 8   | 7     | 2445 | 2MG  | N1-C2-N3    | -2.41 | 120.23      | 123.95   |
| 10  | A     | 1402 | 4OC  | C6-C5-C4    | 2.39  | 119.89      | 116.96   |
| 33  | X     | 56   | PSU  | O2-C2-N1    | -2.39 | 120.16      | 122.79   |
| 32  | W     | 32   | PSU  | O2-C2-N1    | -2.39 | 120.16      | 122.79   |
| 8   | 7     | 2251 | OMG  | C8-N7-C5    | 2.38  | 108.55      | 104.24   |
| 34  | Y     | 55   | PSU  | O2-C2-N1    | -2.37 | 120.18      | 122.79   |
| 32  | W     | 37   | MIA  | C16-C14-C15 | 2.37  | 119.84      | 114.60   |
| 32  | W     | 16   | H2U  | O2-C2-N1    | -2.37 | 120.13      | 123.11   |
| 33  | X     | 55   | 5MU  | O4-C4-N3    | -2.35 | 115.62      | 120.12   |
| 10  | A     | 1498 | UR3  | C1'-N1-C2   | 2.34  | 120.95      | 116.99   |
| 8   | 7     | 2504 | PSU  | O2-C2-N1    | -2.33 | 120.23      | 122.79   |
| 8   | 7     | 2605 | PSU  | O2-C2-N1    | -2.32 | 120.24      | 122.79   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 33  | X     | 21   | H2U  | O2-C2-N1    | -2.31 | 120.21      | 123.11   |
| 10  | A     | 1519 | MA6  | C4-C5-N7    | -2.31 | 107.81      | 110.62   |
| 8   | 7     | 2030 | 6MZ  | C4-N9-C8    | 2.30  | 108.22      | 105.73   |
| 32  | W     | 37   | MIA  | C4-C5-N7    | -2.30 | 107.82      | 110.62   |
| 8   | 7     | 745  | 1MG  | C8-N7-C5    | 2.25  | 108.31      | 104.24   |
| 8   | 7     | 2503 | 2MA  | C5-C4-N9    | 2.24  | 108.39      | 105.78   |
| 10  | A     | 1518 | MA6  | C4-C5-N7    | -2.20 | 107.94      | 110.62   |
| 32  | W     | 54   | 5MU  | O4-C4-N3    | -2.19 | 115.92      | 120.12   |
| 33  | X     | 38   | 2MA  | C4-C5-N7    | -2.18 | 107.97      | 110.62   |
| 33  | X     | 38   | 2MA  | C6-C5-C4    | 2.16  | 120.09      | 117.18   |
| 8   | 7     | 2580 | PSU  | O4'-C1'-C2' | 2.15  | 108.18      | 105.14   |
| 32  | W     | 8    | 4SU  | O2-C2-N1    | -2.12 | 119.97      | 122.79   |
| 33  | X     | 47   | G7M  | CN7-N7-C8   | -2.11 | 121.58      | 124.84   |
| 8   | 7     | 2030 | 6MZ  | C4-C5-N7    | -2.11 | 108.05      | 110.62   |
| 8   | 7     | 2503 | 2MA  | N6-C6-N1    | 2.11  | 120.01      | 117.03   |
| 10  | A     | 967  | 5MC  | CM5-C5-C6   | -2.10 | 120.05      | 122.85   |
| 8   | 7     | 1962 | 5MC  | CM5-C5-C6   | -2.09 | 120.06      | 122.85   |
| 10  | A     | 527  | G7M  | CN7-N7-C8   | -2.07 | 121.64      | 124.84   |
| 10  | A     | 1516 | 2MG  | C8-N7-C5    | 2.06  | 107.98      | 104.24   |
| 8   | 7     | 2445 | 2MG  | CM2-N2-C2   | -2.06 | 119.31      | 123.86   |
| 33  | X     | 55   | 5MU  | O2-C2-N1    | -2.06 | 120.05      | 122.79   |
| 10  | A     | 1407 | 5MC  | CM5-C5-C6   | -2.04 | 120.12      | 122.85   |
| 10  | A     | 1207 | 2MG  | C8-N7-C5    | 2.04  | 107.93      | 104.24   |
| 10  | A     | 966  | 2MG  | C8-N7-C5    | 2.04  | 107.93      | 104.24   |
| 32  | W     | 46   | G7M  | CN7-N7-C8   | -2.03 | 121.70      | 124.84   |
| 8   | 7     | 2552 | OMU  | O2-C2-N1    | -2.03 | 120.08      | 122.79   |
| 33  | X     | 48   | 3AU  | C6-N1-C2    | -2.02 | 119.98      | 121.79   |
| 32  | W     | 37   | MIA  | C4-N9-C8    | 2.02  | 107.91      | 105.73   |
| 33  | X     | 38   | 2MA  | N6-C6-N1    | 2.01  | 119.87      | 117.03   |

There are no chirality outliers.

All (80) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 10  | A     | 527  | G7M  | O4'-C4'-C5'-O5' |
| 10  | A     | 527  | G7M  | C3'-C4'-C5'-O5' |
| 34  | Y     | 17   | H2U  | O4'-C4'-C5'-O5' |
| 34  | Y     | 17   | H2U  | C3'-C4'-C5'-O5' |
| 34  | Y     | 17   | H2U  | O4'-C1'-N1-C6   |
| 34  | Y     | 17   | H2U  | C2'-C1'-N1-C2   |
| 34  | Y     | 17   | H2U  | C2'-C1'-N1-C6   |
| 8   | 7     | 1618 | 6MZ  | C5-C6-N6-C9     |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 8   | 7     | 1618 | 6MZ  | N1-C6-N6-C9     |
| 8   | 7     | 1618 | 6MZ  | O4'-C4'-C5'-O5' |
| 8   | 7     | 1618 | 6MZ  | C3'-C4'-C5'-O5' |
| 8   | 7     | 2030 | 6MZ  | C5-C6-N6-C9     |
| 8   | 7     | 2030 | 6MZ  | N1-C6-N6-C9     |
| 8   | 7     | 2251 | OMG  | O4'-C4'-C5'-O5' |
| 8   | 7     | 2251 | OMG  | C1'-C2'-O2'-CM2 |
| 32  | W     | 54   | 5MU  | C3'-C4'-C5'-O5' |
| 32  | W     | 54   | 5MU  | O4'-C4'-C5'-O5' |
| 33  | X     | 8    | 4SU  | C3'-C4'-C5'-O5' |
| 33  | X     | 8    | 4SU  | O4'-C4'-C5'-O5' |
| 33  | X     | 17   | H2U  | O4'-C1'-N1-C6   |
| 33  | X     | 33   | RSP  | C4'-C5'-O5'-P   |
| 33  | X     | 38   | 2MA  | O4'-C1'-N9-C8   |
| 33  | X     | 38   | 2MA  | O4'-C1'-N9-C4   |
| 33  | X     | 47   | G7M  | O4'-C4'-C5'-O5' |
| 33  | X     | 47   | G7M  | C3'-C4'-C5'-O5' |
| 33  | X     | 55   | 5MU  | C3'-C4'-C5'-O5' |
| 33  | X     | 55   | 5MU  | O4'-C4'-C5'-O5' |
| 33  | X     | 47   | G7M  | C4'-C5'-O5'-P   |
| 10  | A     | 1519 | MA6  | O4'-C4'-C5'-O5' |
| 34  | Y     | 46   | G7M  | C3'-C4'-C5'-O5' |
| 34  | Y     | 54   | 5MU  | C3'-C4'-C5'-O5' |
| 34  | Y     | 54   | 5MU  | O4'-C4'-C5'-O5' |
| 8   | 7     | 2251 | OMG  | C3'-C4'-C5'-O5' |
| 8   | 7     | 2498 | OMC  | O4'-C4'-C5'-O5' |
| 32  | W     | 8    | 4SU  | C3'-C4'-C5'-O5' |
| 32  | W     | 8    | 4SU  | O4'-C4'-C5'-O5' |
| 10  | A     | 1519 | MA6  | C3'-C4'-C5'-O5' |
| 8   | 7     | 2498 | OMC  | C3'-C4'-C5'-O5' |
| 33  | X     | 38   | 2MA  | O4'-C4'-C5'-O5' |
| 10  | A     | 1498 | UR3  | O4'-C4'-C5'-O5' |
| 33  | X     | 38   | 2MA  | C3'-C4'-C5'-O5' |
| 10  | A     | 1498 | UR3  | C3'-C4'-C5'-O5' |
| 33  | X     | 17   | H2U  | C4'-C5'-O5'-P   |
| 33  | X     | 38   | 2MA  | C4'-C5'-O5'-P   |
| 8   | 7     | 1915 | 3TD  | O4'-C4'-C5'-O5' |
| 33  | X     | 48   | 3AU  | O4'-C4'-C5'-O5' |
| 32  | W     | 46   | G7M  | C2'-C1'-N9-C4   |
| 10  | A     | 1519 | MA6  | C5-C6-N6-C10    |
| 34  | Y     | 46   | G7M  | O4'-C4'-C5'-O5' |
| 33  | X     | 48   | 3AU  | C10-C11-C12-N40 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 32  | W     | 46   | G7M  | C4'-C5'-O5'-P   |
| 33  | X     | 21   | H2U  | C4'-C5'-O5'-P   |
| 33  | X     | 48   | 3AU  | C4'-C5'-O5'-P   |
| 8   | 7     | 2069 | G7M  | O4'-C4'-C5'-O5' |
| 32  | W     | 46   | G7M  | C2'-C1'-N9-C8   |
| 34  | Y     | 17   | H2U  | C4'-C5'-O5'-P   |
| 32  | W     | 17   | H2U  | O4'-C4'-C5'-O5' |
| 32  | W     | 46   | G7M  | O4'-C4'-C5'-O5' |
| 33  | X     | 48   | 3AU  | C3'-C4'-C5'-O5' |
| 34  | Y     | 17   | H2U  | O4'-C1'-N1-C2   |
| 8   | 7     | 2069 | G7M  | C4'-C5'-O5'-P   |
| 32  | W     | 16   | H2U  | C4'-C5'-O5'-P   |
| 32  | W     | 37   | MIA  | C5-C6-N6-C12    |
| 32  | W     | 37   | MIA  | N6-C12-C13-C14  |
| 33  | X     | 17   | H2U  | C2'-C1'-N1-C6   |
| 33  | X     | 56   | PSU  | O4'-C1'-C5-C4   |
| 8   | 7     | 747  | 5MU  | C4'-C5'-O5'-P   |
| 8   | 7     | 1915 | 3TD  | C3'-C4'-C5'-O5' |
| 8   | 7     | 2069 | G7M  | C3'-C4'-C5'-O5' |
| 8   | 7     | 2503 | 2MA  | O4'-C1'-N9-C8   |
| 8   | 7     | 746  | PSU  | O4'-C1'-C5-C6   |
| 33  | X     | 21   | H2U  | O4'-C1'-N1-C6   |
| 33  | X     | 17   | H2U  | O4'-C1'-N1-C2   |
| 32  | W     | 20   | H2U  | C4'-C5'-O5'-P   |
| 32  | W     | 37   | MIA  | N1-C6-N6-C12    |
| 8   | 7     | 2030 | 6MZ  | O4'-C4'-C5'-O5' |
| 32  | W     | 46   | G7M  | C3'-C4'-C5'-O5' |
| 33  | X     | 17   | H2U  | C2'-C1'-N1-C2   |
| 32  | W     | 17   | H2U  | C3'-C4'-C5'-O5' |
| 8   | 7     | 2457 | PSU  | C3'-C4'-C5'-O5' |

There are no ring outliers.

23 monomers are involved in 36 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 34  | Y     | 54   | 5MU  | 4       | 0            |
| 33  | X     | 55   | 5MU  | 1       | 0            |
| 34  | Y     | 55   | PSU  | 1       | 0            |
| 33  | X     | 56   | PSU  | 1       | 0            |
| 8   | 7     | 747  | 5MU  | 1       | 0            |
| 32  | W     | 46   | G7M  | 1       | 0            |
| 8   | 7     | 2251 | OMG  | 1       | 0            |

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| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 8   | 7     | 2503 | 2MA  | 3       | 0            |
| 32  | W     | 54   | 5MU  | 2       | 0            |
| 32  | W     | 37   | MIA  | 2       | 0            |
| 10  | A     | 1518 | MA6  | 1       | 0            |
| 33  | X     | 38   | 2MA  | 3       | 0            |
| 10  | A     | 1402 | 4OC  | 2       | 0            |
| 8   | 7     | 2030 | 6MZ  | 3       | 0            |
| 8   | 7     | 1915 | 3TD  | 1       | 0            |
| 33  | X     | 48   | 3AU  | 2       | 0            |
| 8   | 7     | 1939 | 5MU  | 1       | 0            |
| 8   | 7     | 2449 | H2U  | 1       | 0            |
| 32  | W     | 17   | H2U  | 1       | 0            |
| 32  | W     | 16   | H2U  | 3       | 0            |
| 8   | 7     | 2604 | PSU  | 1       | 0            |
| 34  | Y     | 46   | G7M  | 1       | 0            |
| 33  | X     | 47   | G7M  | 1       | 0            |

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 293 ligands modelled in this entry, 289 are monoatomic - leaving 4 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 | $\# Z  > 2$ |
| 62  | PUT  | 7     | 3001 | -    | 5,5,5        | 0.25 | 0           | 4,4,4       | 0.52 | 0           |
| 62  | PUT  | 7     | 3002 | -    | 5,5,5        | 0.25 | 0           | 4,4,4       | 0.54 | 0           |
| 63  | SPD  | 7     | 3003 | -    | 9,9,9        | 0.32 | 0           | 8,8,8       | 0.85 | 0           |
| 65  | ALA  | Y     | 102  | 34   | 3,4,5        | 1.17 | 1 (33%)     | 2,4,6       | 3.11 | 1 (50%)     |

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 |
|-----|------|-------|------|------|---------|----------|-------|
| 62  | PUT  | 7     | 3001 | -    | -       | 1/3/3/3  | -     |
| 62  | PUT  | 7     | 3002 | -    | -       | 0/3/3/3  | -     |
| 63  | SPD  | 7     | 3003 | -    | -       | 0/7/7/7  | -     |
| 65  | ALA  | Y     | 102  | 34   | -       | 0/0/2/4  | -     |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 65  | Y     | 102 | ALA  | O-C   | 2.01 | 1.27        | 1.19     |

All (1) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 65  | Y     | 102 | ALA  | O-C-CA | -4.39 | 110.38      | 124.28   |

There are no chirality outliers.

All (1) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       |
|-----|-------|------|------|-------------|
| 62  | 7     | 3001 | PUT  | C1-C2-C3-C4 |

There are no ring outliers.

1 monomer is involved in 2 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 63  | 7     | 3003 | SPD  | 2       | 0            |

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

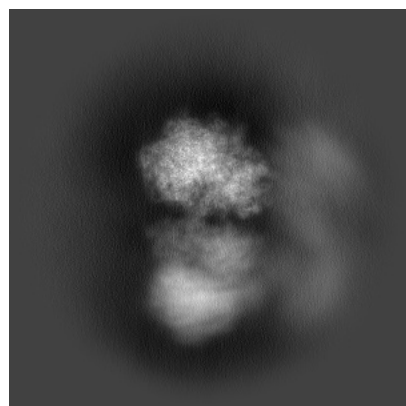
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17743. These allow visual inspection of the internal detail of the map and identification of artifacts.

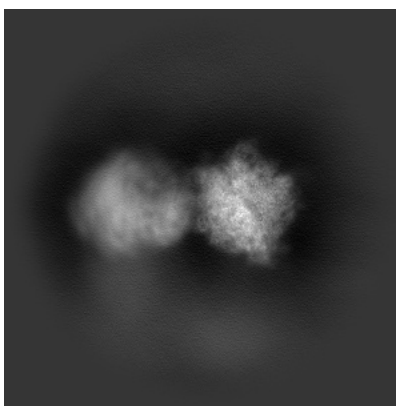
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

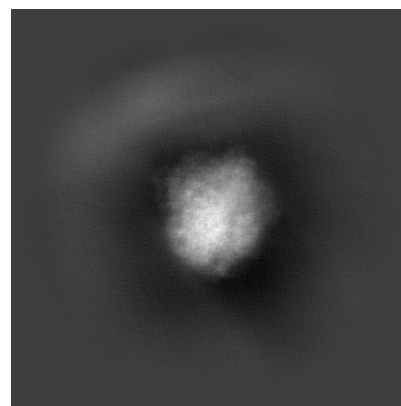
#### 6.1.1 Primary map



X

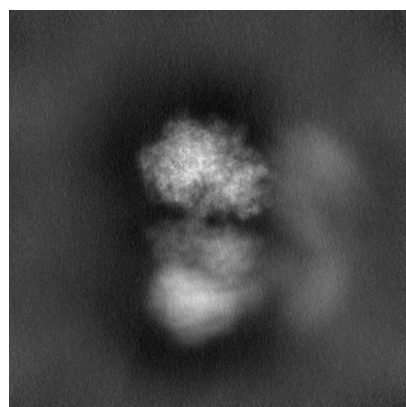


Y

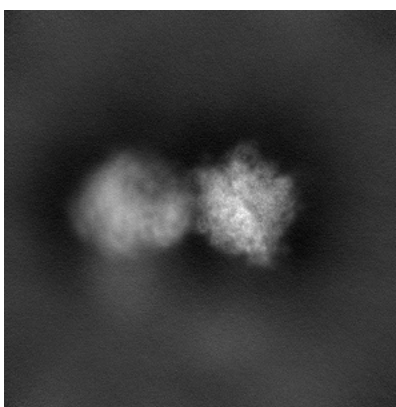


Z

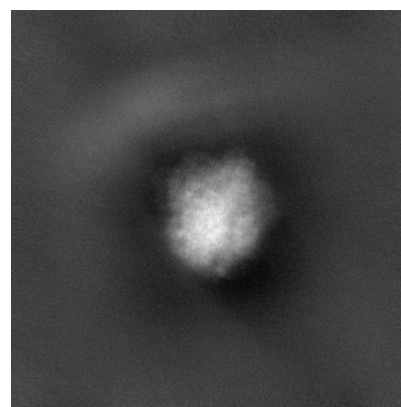
#### 6.1.2 Raw map



X



Y

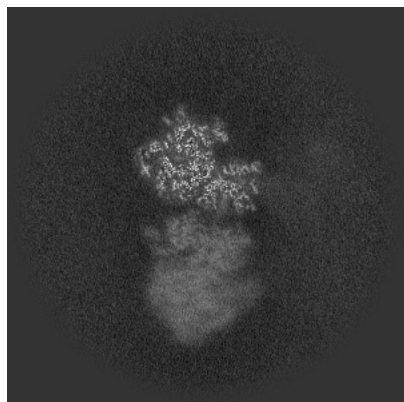


Z

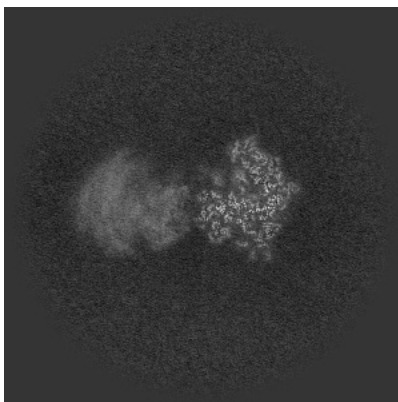
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

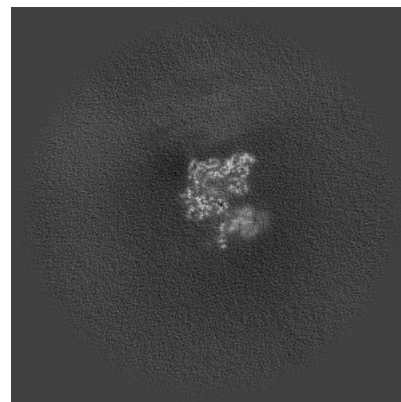
### 6.2.1 Primary map



X Index: 351

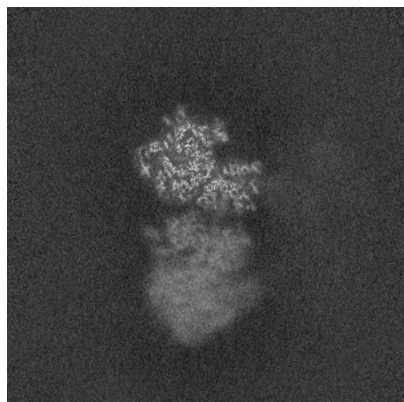


Y Index: 351

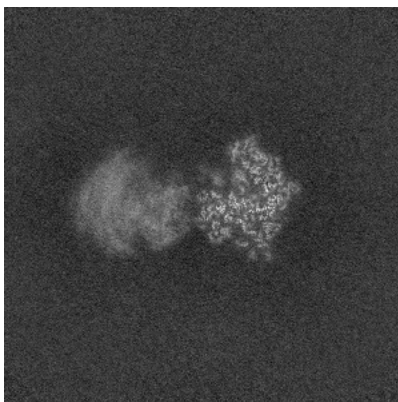


Z Index: 351

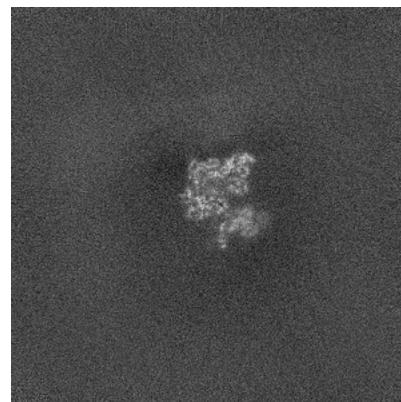
### 6.2.2 Raw map



X Index: 351



Y Index: 351

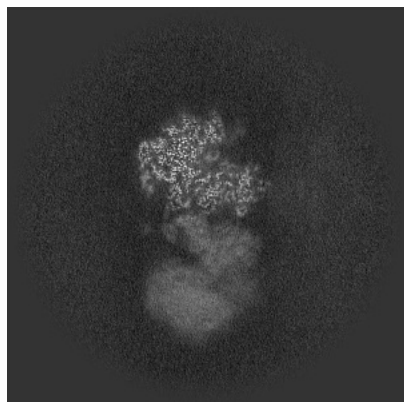


Z Index: 351

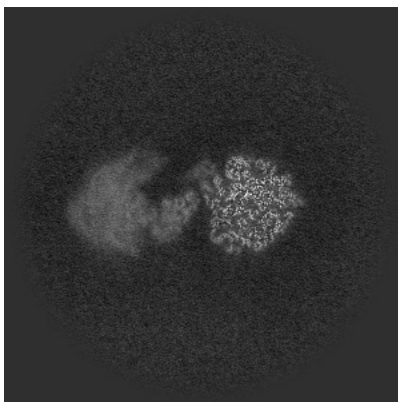
The images above show central slices of the map in three orthogonal directions.

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

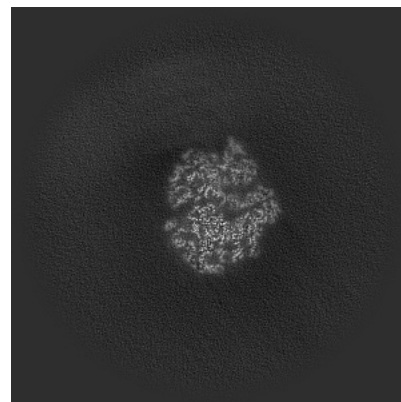
### 6.3.1 Primary map



X Index: 369

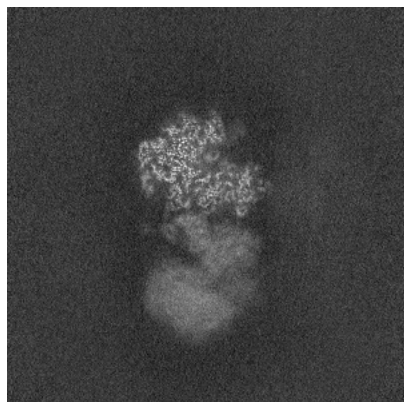


Y Index: 312

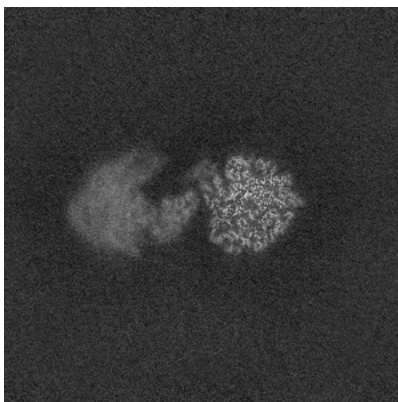


Z Index: 411

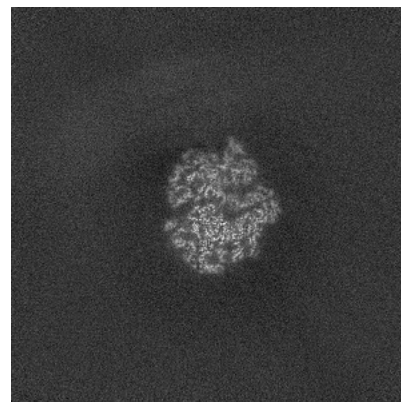
### 6.3.2 Raw map



X Index: 369



Y Index: 312

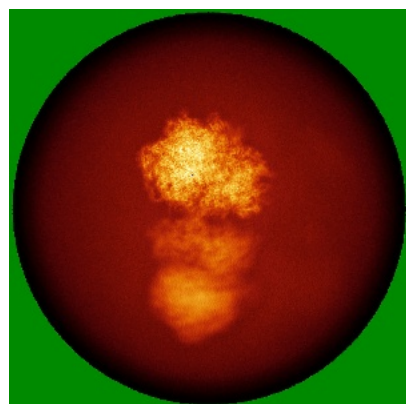


Z Index: 411

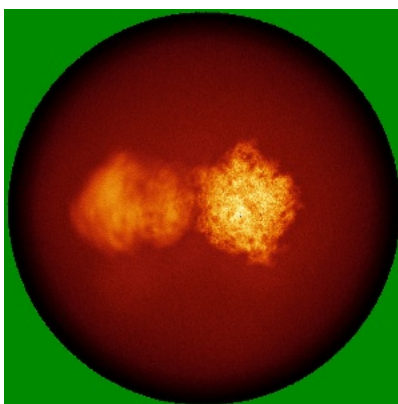
The images above show the largest variance slices of the map in three orthogonal directions.

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

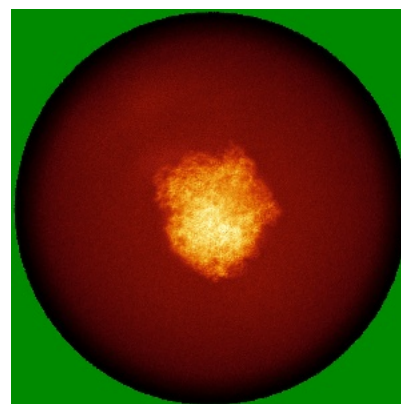
### 6.4.1 Primary map



X

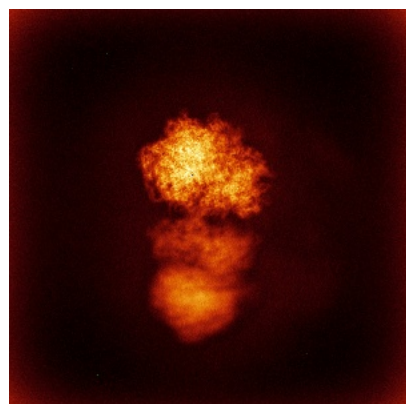


Y

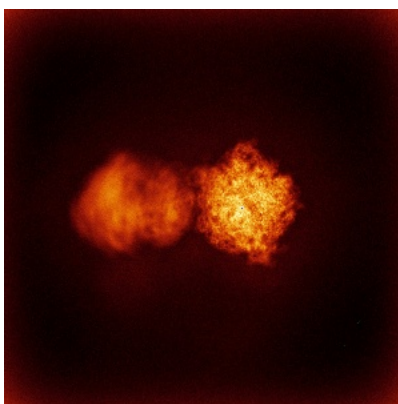


Z

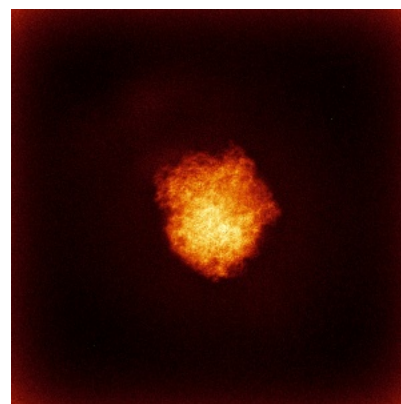
### 6.4.2 Raw map



X



Y

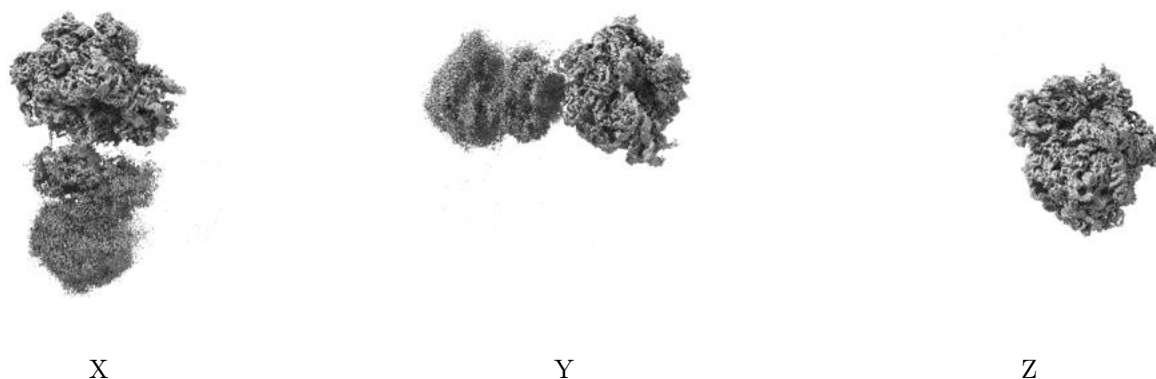


Z

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

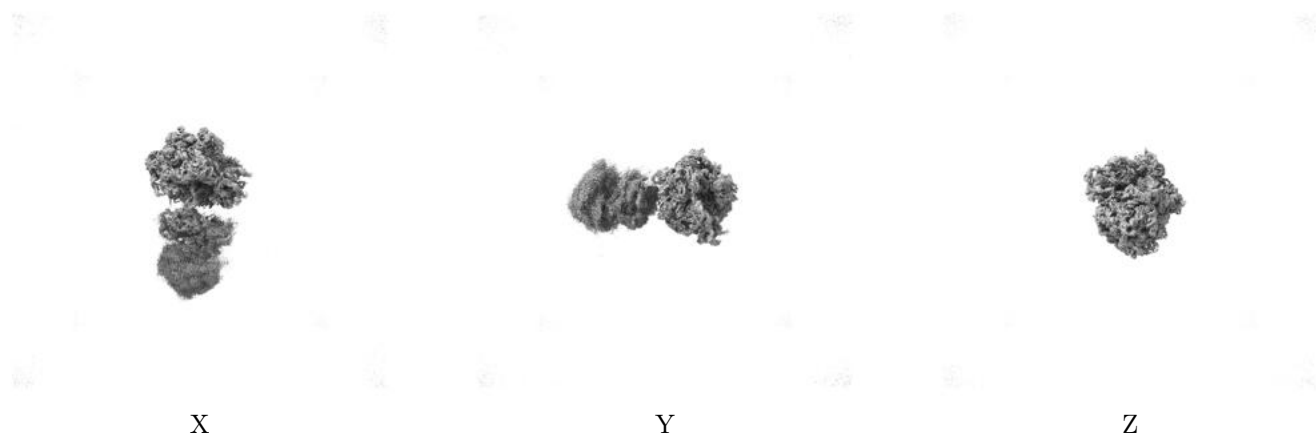
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 5.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

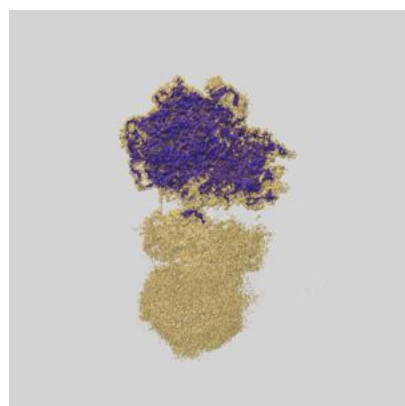
## 6.6 Mask visualisation [i](#)

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

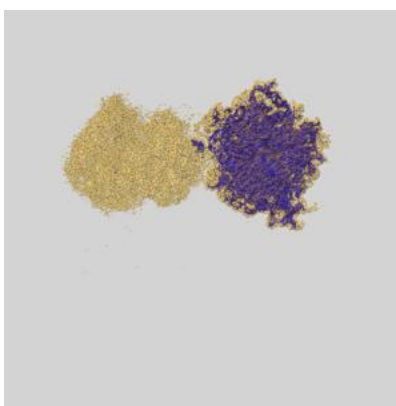
A mask typically either:

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

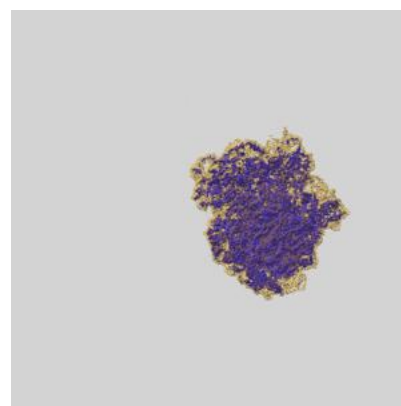
### 6.6.1 emd\_17743\_msk\_1.map [i](#)



X



Y

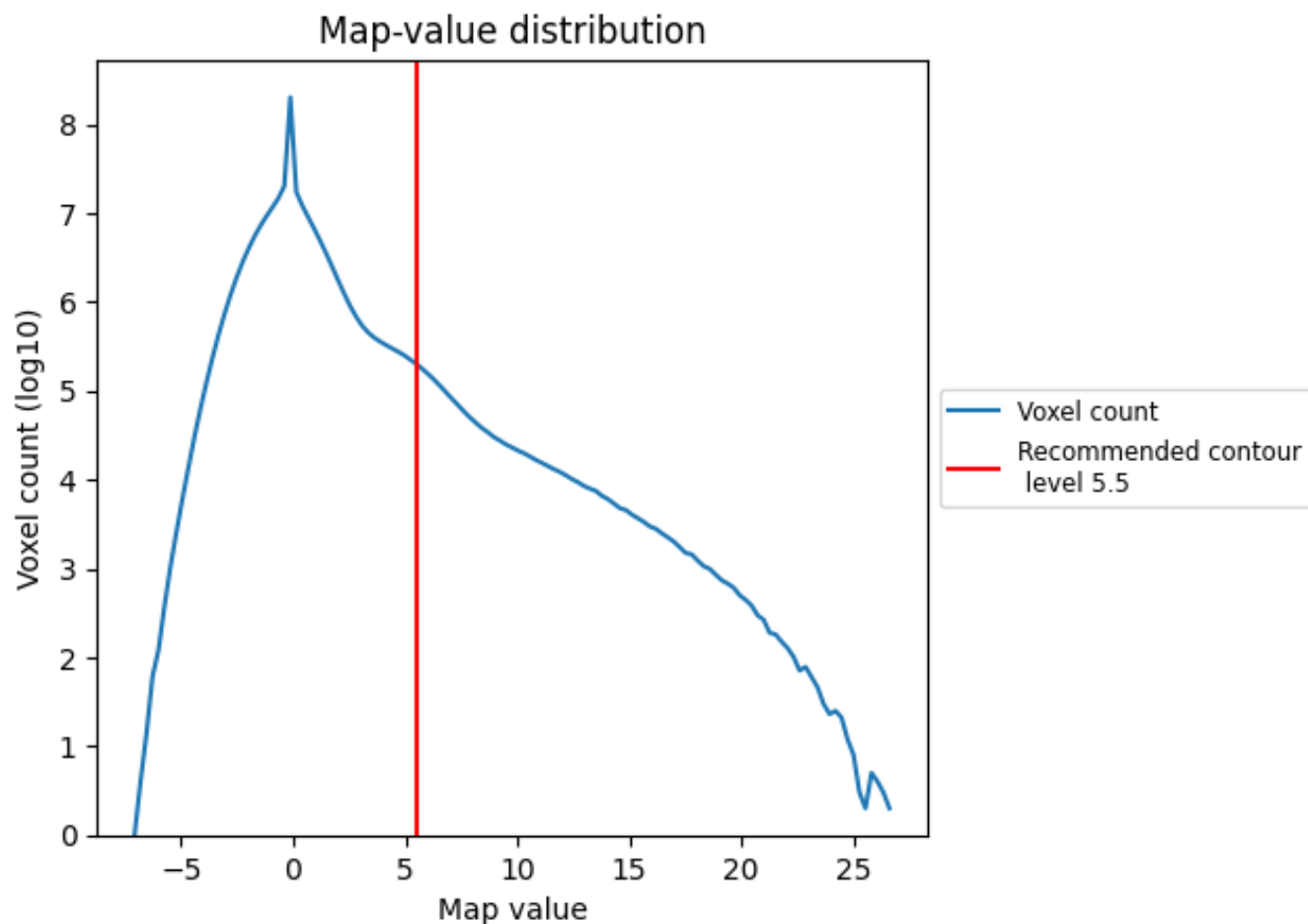


Z

## 7 Map analysis [i](#)

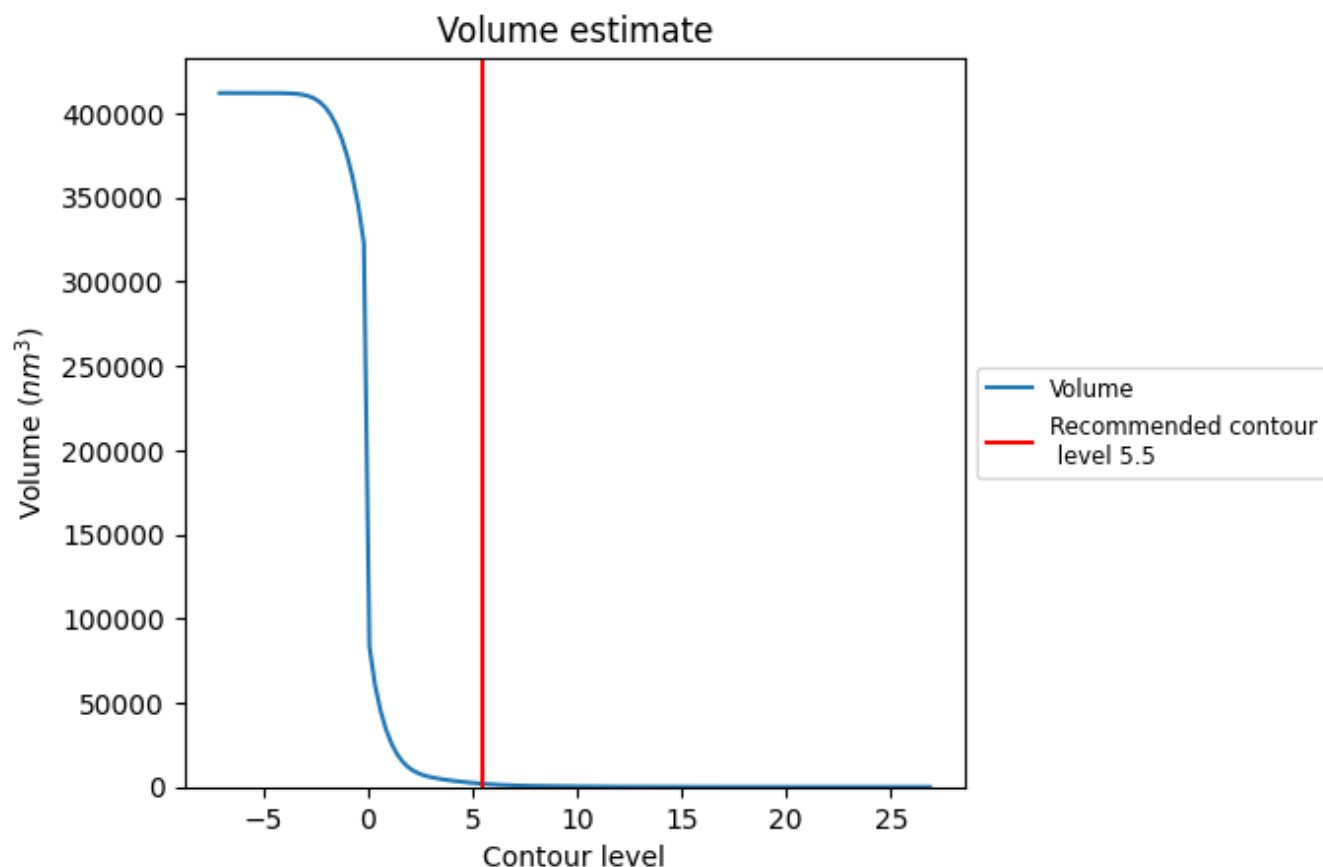
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

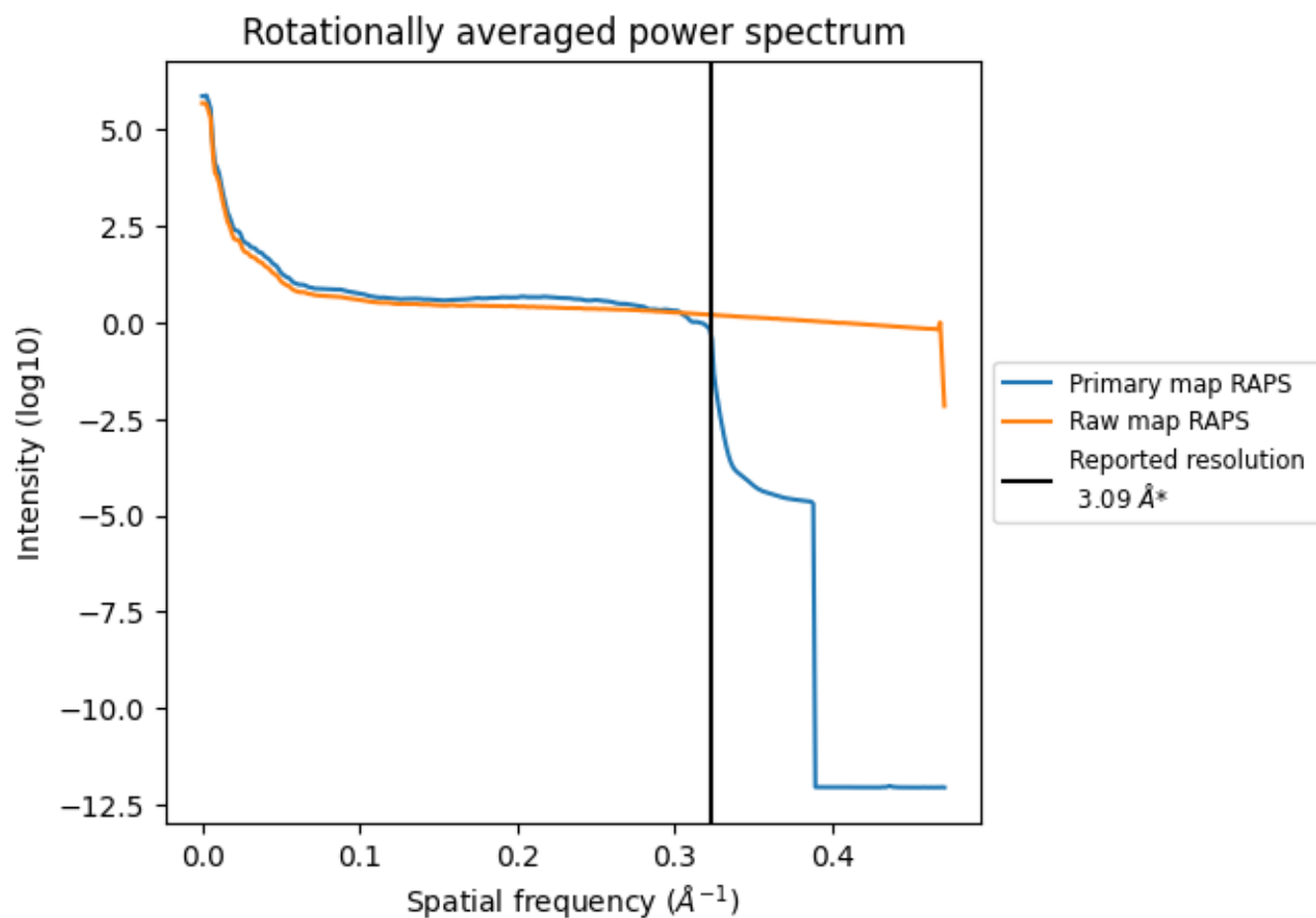
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1904  $\text{nm}^3$ ; this corresponds to an approximate mass of 1720 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ

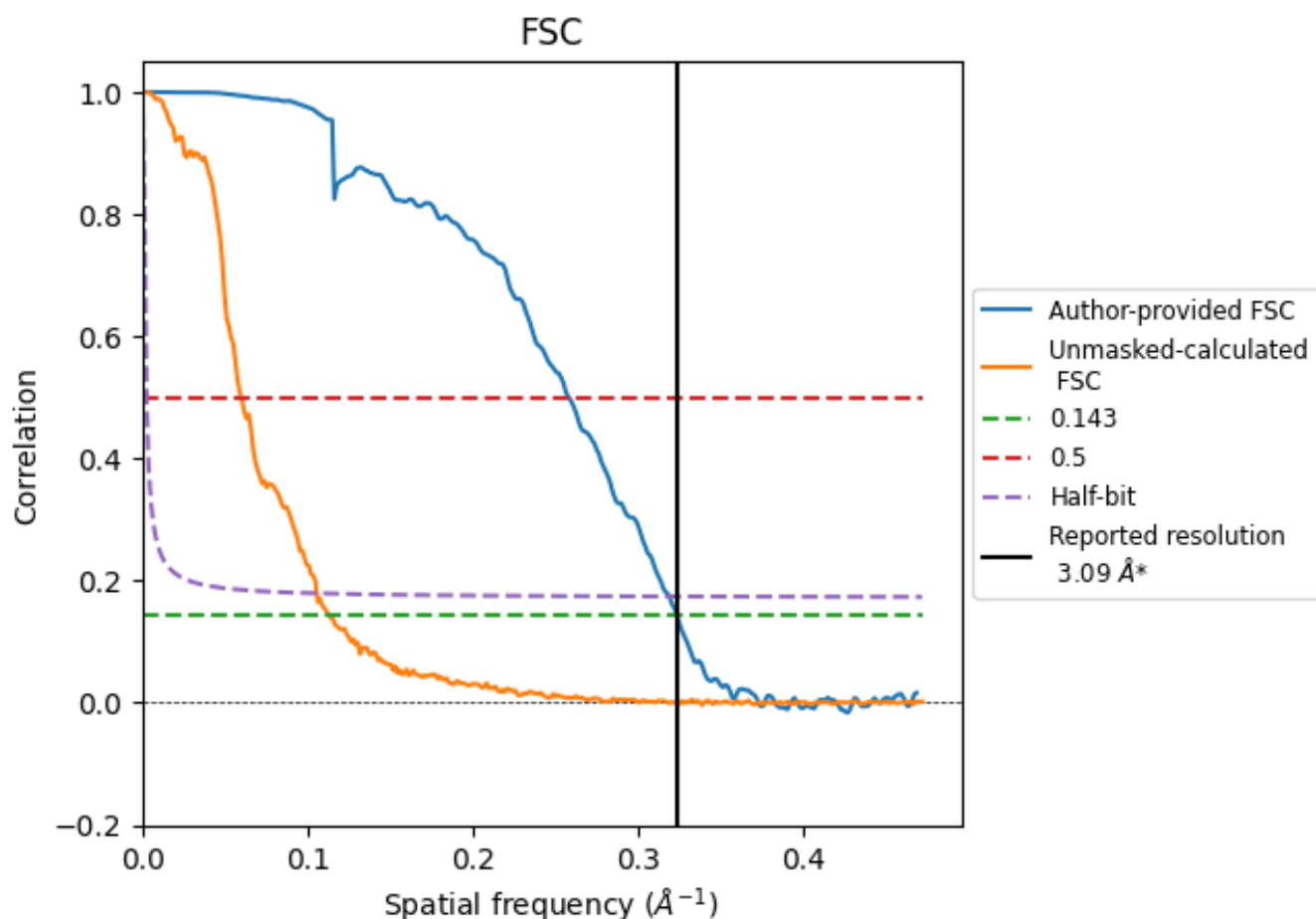


\*Reported resolution corresponds to spatial frequency of 0.324 Å<sup>-1</sup>

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.324 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

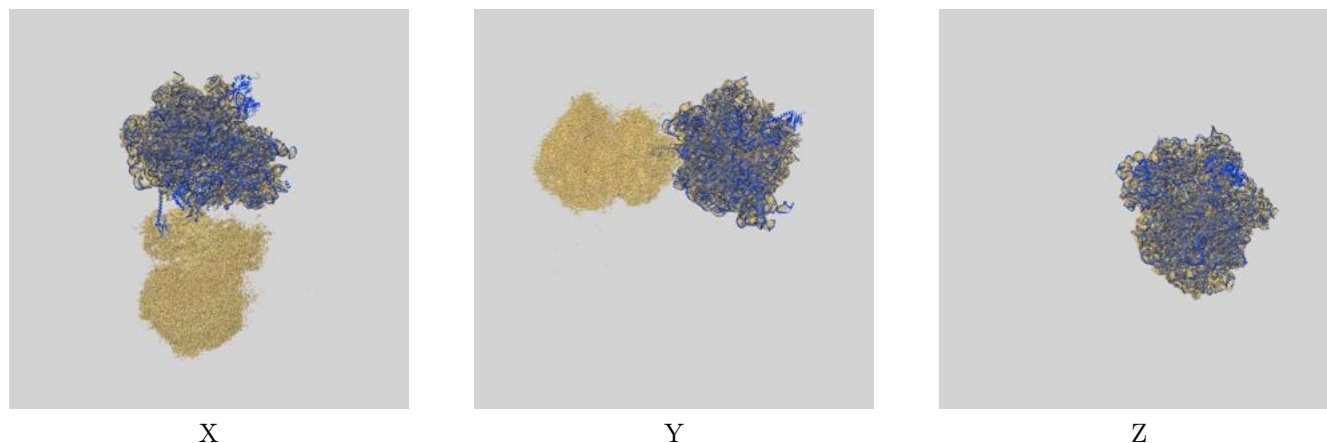
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |       |          |
|---------------------------|------------------------------------|-------|----------|
|                           | 0.143                              | 0.5   | Half-bit |
| Reported by author        | 3.09                               | -     | -        |
| Author-provided FSC curve | 3.09                               | 3.88  | 3.14     |
| Unmasked-calculated*      | 8.83                               | 16.72 | 9.47     |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.83 differs from the reported value 3.09 by more than 10 %

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

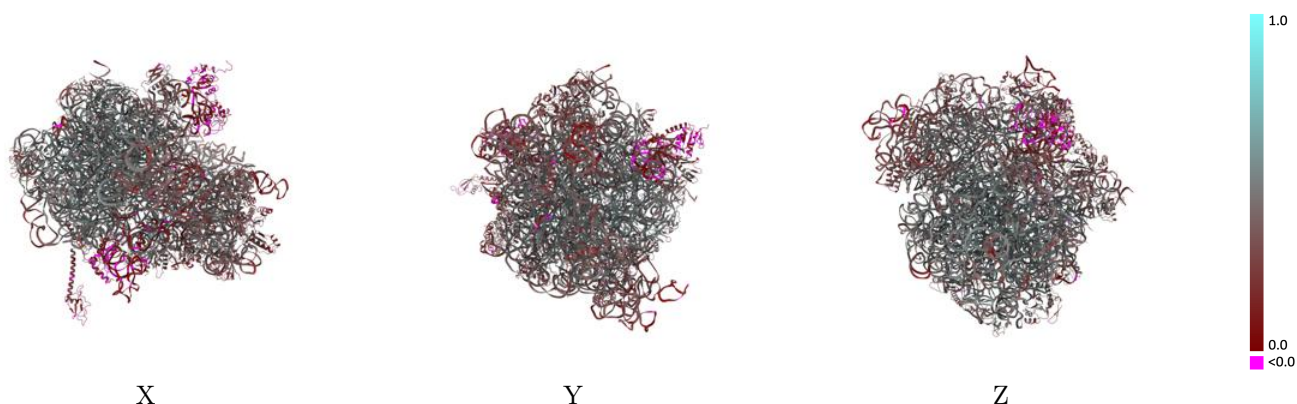
This section contains information regarding the fit between EMDB map EMD-17743 and PDB model 8PKL. Per-residue inclusion information can be found in section 3 on page 18.

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



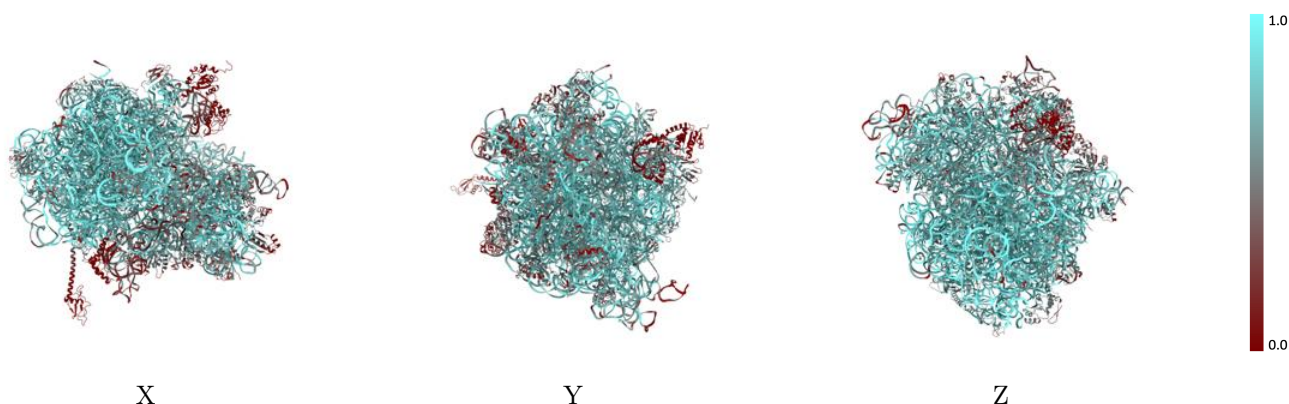
The images above show the 3D surface view of the map at the recommended contour level 5.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



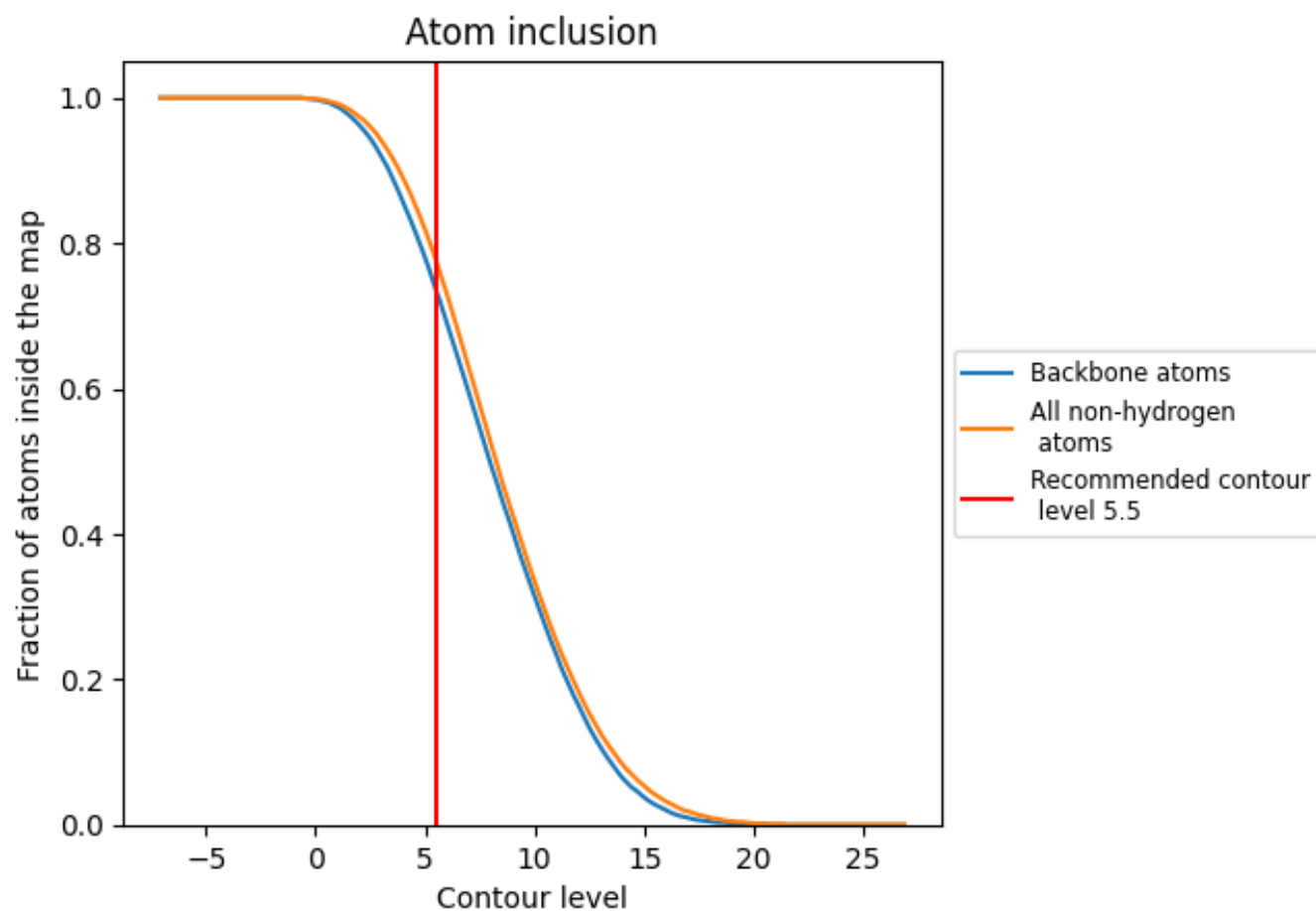
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (5.5).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 78% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (5.5) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.7760   |  0.4140   |
| 0     |  0.7850   |  0.4090   |
| 1     |  0.7440   |  0.4470   |
| 2     |  0.5860   |  0.3790   |
| 3     |  0.7050   |  0.3980   |
| 4     |  0.3520   |  0.2890   |
| 5     |  0.7500   |  0.4200   |
| 6     |  0.8390   |  0.4680   |
| 7     |  0.9070   |  0.4640   |
| 8     |  0.8620   |  0.4070   |
| A     |  0.8520   |  0.4170   |
| B     |  0.3770   |  0.3190   |
| C     |  0.5310   |  0.3430   |
| D     |  0.3880   |  0.3240   |
| E     |  0.5930  |  0.4000  |
| F     |  0.4590 |  0.3680 |
| G     |  0.5640 |  0.3560 |
| H     |  0.5330 |  0.3850 |
| I     |  0.5530 |  0.3570 |
| J     |  0.4010 |  0.2920 |
| K     |  0.6380 |  0.4070 |
| L     |  0.7040 |  0.4000 |
| M     |  0.5470 |  0.3370 |
| N     |  0.5980 |  0.3490 |
| O     |  0.5970 |  0.3590 |
| P     |  0.5090 |  0.3680 |
| Q     |  0.5540 |  0.3710 |
| R     |  0.5930 |  0.4290 |
| S     |  0.5660 |  0.3590 |
| T     |  0.5620 |  0.2880 |
| U     |  0.4910 |  0.3340 |
| V     |  0.5400 |  0.2600 |
| W     |  0.8680 |  0.3690 |
| X     |  0.3800 |  0.1560 |
| Y     |  0.6400 |  0.3290 |



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*Continued from previous page...*

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| a     |  0.0280   |  0.0810   |
| b     |  0.7870   |  0.4670   |
| c     |  0.7280   |  0.4470   |
| d     |  0.6570   |  0.4130   |
| e     |  0.5260   |  0.3060   |
| f     |  0.5230   |  0.3470   |
| g     |  0.6970   |  0.4000   |
| h     |  0.7560   |  0.4370   |
| i     |  0.1760   |  0.2140   |
| j     |  0.0040   |  0.0530   |
| k     |  0.0030   |  0.0530   |
| l     |  0.8680   |  0.4860   |
| m     |  0.7950   |  0.4450   |
| n     |  0.7080   |  0.4280   |
| o     |  0.6900   |  0.4300   |
| p     |  0.3680   |  0.2100   |
| q     |  0.7830   |  0.4440   |
| r     |  0.5830  |  0.3550  |
| s     |  0.6790 |  0.4210 |
| t     |  0.8070 |  0.4630 |
| u     |  0.6410 |  0.4170 |
| v     |  0.7520 |  0.4520 |
| w     |  0.7180 |  0.4240 |
| x     |  0.6150 |  0.3940 |
| y     |  0.6340 |  0.3780 |
| z     |  0.7770 |  0.4470 |