



## Full wwPDB EM Validation Report ⓘ

Jun 18, 2026 – 01:31 pm BST

PDB ID : 7OII / pdb\_00007oii  
EMDB ID : EMD-12930  
Title : CspA-70 cotranslational folding intermediate 2  
Authors : Agirrezabala, X.; Samatova, E.; Macher, M.; Liutkute, M.; Gil-Carton, D.;  
Novacek, J.; Valle, M.; Rodnina, M.V.  
Deposited on : 2021-05-11  
Resolution : 3.00 Å(reported)  
Based on initial model : 6ORE

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

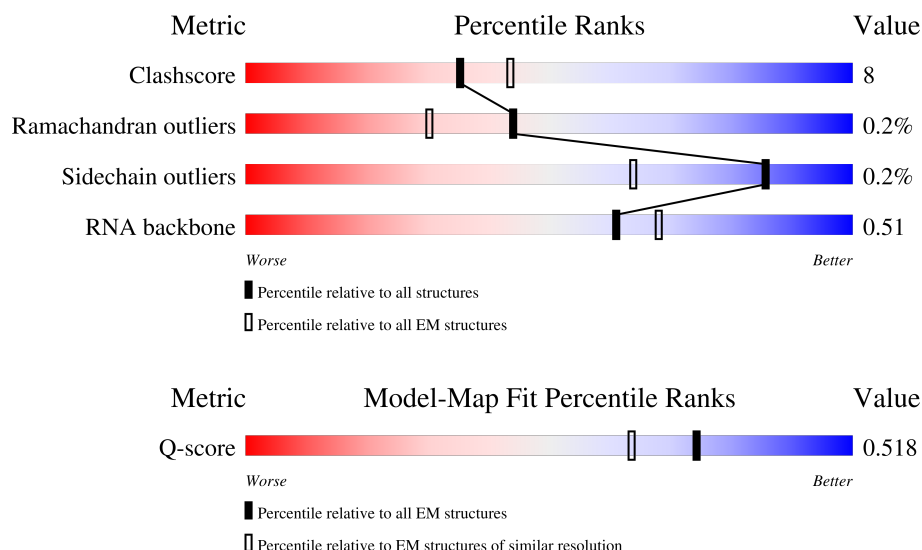
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.00 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                       | 14081 ( 2.50 - 3.50 )                                    |

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   | 1     | 2903   | <br>65% 29% 6%   |
| 2   | 2     | 1534   | <br>66% 28% 6%   |
| 3   | 3     | 120    | <br>75% 21% 4%   |

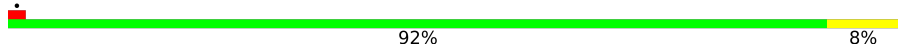
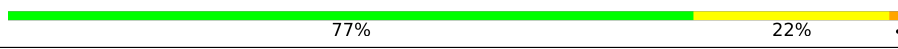
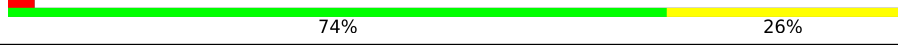
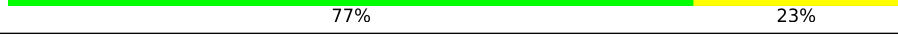
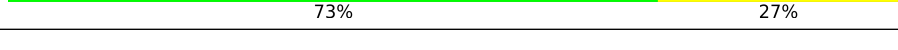
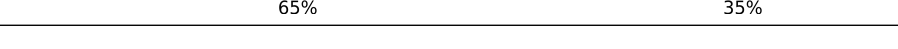
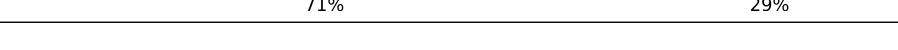
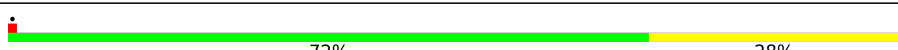
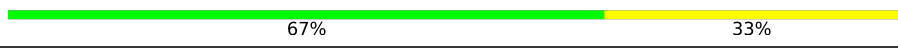
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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 4   | C     | 271    |                  |
| 5   | D     | 209    |                  |
| 6   | E     | 201    |                  |
| 7   | F     | 177    |                  |
| 8   | G     | 175    |                  |
| 9   | H     | 149    |                  |
| 10  | I     | 142    |                  |
| 11  | J     | 123    |                  |
| 12  | K     | 144    |                  |
| 13  | L     | 136    |                  |
| 14  | M     | 119    |                  |
| 15  | N     | 116    |                  |
| 16  | O     | 114    |                  |
| 17  | P     | 117    |                  |
| 18  | Q     | 103    |                  |
| 19  | R     | 110    |                  |
| 20  | S     | 94     |                  |
| 21  | T     | 103    |                  |
| 22  | U     | 94     |                  |
| 23  | V     | 84     |                  |
| 24  | W     | 77     |                  |
| 25  | X     | 62     |                  |
| 26  | Y     | 58     |                  |
| 27  | Z     | 66     |                  |
| 28  | a     | 56     |                  |

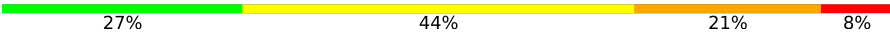
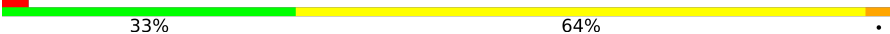
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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 29  | b     | 52     |    |
| 30  | c     | 46     |    |
| 31  | d     | 64     |    |
| 32  | e     | 38     |    |
| 33  | f     | 225    |    |
| 34  | g     | 208    |    |
| 35  | h     | 205    |    |
| 36  | i     | 156    |    |
| 37  | j     | 104    |    |
| 38  | k     | 151    |    |
| 39  | l     | 129    |    |
| 40  | m     | 127    |  |
| 41  | n     | 99     |  |
| 42  | o     | 117    |  |
| 43  | p     | 123    |  |
| 44  | q     | 116    |  |
| 45  | r     | 100    |  |
| 46  | s     | 88     |  |
| 47  | t     | 82     |  |
| 48  | u     | 80     |  |
| 49  | v     | 66     |  |
| 50  | w     | 83     |  |
| 51  | x     | 86     |  |
| 52  | y     | 70     |  |
| 53  | 4     | 6      |  |

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| Mol | Chain | Length | Quality of chain                                                                   |
|-----|-------|--------|------------------------------------------------------------------------------------|
| 54  | z     | 85     |  |
| 55  | B     | 39     |  |

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 54  | 5MU  | z     | 71  | -         | -        | X       | -                |

## 2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 145171 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 RNA chain called 23S rRNA.

| Mol | Chain | Residues | Atoms |       |       |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|-------|
| 1   | 1     | 2903     | Total | C     | N     | O     | P    | 0       | 0     |
|     |       |          | 62336 | 27816 | 11470 | 20147 | 2903 |         |       |

- Molecule 2 is a RNA chain called 16S rRNA.

| Mol | Chain | Residues | Atoms |       |      |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|-------|
| 2   | 2     | 1534     | Total | C     | N    | O     | P    | 0       | 0     |
|     |       |          | 32929 | 14693 | 6041 | 10661 | 1534 |         |       |

- Molecule 3 is a RNA chain called 5S rRNA.

| Mol | Chain | Residues | Atoms |      |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|-------|
| 3   | 3     | 120      | Total | C    | N   | O   | P   | 0       | 0     |
|     |       |          | 2569  | 1144 | 468 | 837 | 120 |         |       |

- Molecule 4 is a protein called 50S ribosomal protein L2.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 4   | C     | 271      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2082  | 1288 | 423 | 364 | 7 |         |       |

- Molecule 5 is a protein called 50S ribosomal protein L3.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 5   | D     | 209      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1565  | 979 | 288 | 294 | 4 |         |       |

- Molecule 6 is a protein called 50S ribosomal protein L4.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 6   | E     | 201      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1552  | 974 | 283 | 290 | 5 |         |       |

- Molecule 7 is a protein called 50S ribosomal protein L5.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 7   | F     | 177      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1410  | 899 | 249 | 256 | 6 |         |       |

- Molecule 8 is a protein called 50S ribosomal protein L6.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 8   | G     | 175      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1313  | 826 | 241 | 244 | 2 |         |       |

- Molecule 9 is a protein called 50S ribosomal protein L9.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 9   | H     | 149      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1111  | 699 | 197 | 214 | 1 |         |       |

- Molecule 10 is a protein called 50S ribosomal protein L13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 10  | I     | 142      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1129  | 714 | 212 | 199 | 4 |         |       |

- Molecule 11 is a protein called 50S ribosomal protein L14.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 11  | J     | 123      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 946   | 593 | 181 | 166 | 6 |         |       |

- Molecule 12 is a protein called 50S ribosomal protein L15.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 12  | K     | 144      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1053  | 654 | 207 | 190 | 2 |         |       |

- Molecule 13 is a protein called 50S ribosomal protein L16.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 13  | L     | 136      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1074  | 686 | 205 | 177 | 6 |         |       |

- Molecule 14 is a protein called 50S ribosomal protein L17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 14  | M     | 119      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 951   | 588 | 195 | 163 | 5 |         |       |

- Molecule 15 is a protein called 50S ribosomal protein L18.

| Mol | Chain | Residues | Atoms |     |     |     |  | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|-------|
| 15  | N     | 116      | Total | C   | N   | O   |  | 0       | 0     |
|     |       |          | 892   | 552 | 178 | 162 |  |         |       |

- Molecule 16 is a protein called 50S ribosomal protein L19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 16  | O     | 114      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 917   | 574 | 179 | 163 | 1 |         |       |

- Molecule 17 is a protein called 50S ribosomal protein L20.

| Mol | Chain | Residues | Atoms |     |     |     |  | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|-------|
| 17  | P     | 117      | Total | C   | N   | O   |  | 0       | 0     |
|     |       |          | 947   | 604 | 192 | 151 |  |         |       |

- Molecule 18 is a protein called 50S ribosomal protein L21.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 18  | Q     | 103      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 816   | 516 | 153 | 145 | 2 |         |       |

- Molecule 19 is a protein called 50S ribosomal protein L22.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 19  | R     | 110      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 857   | 532 | 166 | 156 | 3 |         |       |

- Molecule 20 is a protein called 50S ribosomal protein L23.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 20  | S     | 94       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 746   | 470 | 140 | 134 | 2 |         |       |

- Molecule 21 is a protein called 50S ribosomal protein L24.



| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 21  | T     | 103      | Total | C   | N   | O   |         |       |
|     |       |          | 788   | 498 | 148 | 142 | 0       | 0     |

- Molecule 22 is a protein called 50S ribosomal protein L25.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 22  | U     | 94       | Total | C   | N   | O   | S |         |       |
|     |       |          | 753   | 479 | 137 | 134 | 3 | 0       | 0     |

- Molecule 23 is a protein called 50S ribosomal protein L27.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 23  | V     | 84       | Total | C   | N   | O   | S |         |       |
|     |       |          | 634   | 391 | 129 | 113 | 1 | 0       | 0     |

- Molecule 24 is a protein called 50S ribosomal protein L28.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 24  | W     | 77       | Total | C   | N   | O   | S |         |       |
|     |       |          | 625   | 388 | 129 | 106 | 2 | 0       | 0     |

- Molecule 25 is a protein called 50S ribosomal protein L29.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 25  | X     | 62       | Total | C   | N  | O  | S |         |       |
|     |       |          | 501   | 308 | 98 | 94 | 1 | 0       | 0     |

- Molecule 26 is a protein called 50S ribosomal protein L30.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 26  | Y     | 58       | Total | C   | N  | O  | S |         |       |
|     |       |          | 448   | 281 | 87 | 78 | 2 | 0       | 0     |

- Molecule 27 is a protein called 50S ribosomal protein L31.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 27  | Z     | 66       | Total | C   | N  | O  | S |         |       |
|     |       |          | 522   | 323 | 99 | 94 | 6 | 0       | 0     |

- Molecule 28 is a protein called 50S ribosomal protein L32.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 28  | a     | 56       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 444   | 269 | 94 | 80 | 1 |         |       |

- Molecule 29 is a protein called 50S ribosomal protein L33.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 29  | b     | 52       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 426   | 275 | 78 | 73 |   |         |       |

- Molecule 30 is a protein called 50S ribosomal protein L34.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 30  | c     | 46       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 377   | 228 | 90 | 57 | 2 |         |       |

- Molecule 31 is a protein called 50S ribosomal protein L35.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 31  | d     | 64       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 504   | 323 | 105 | 74 | 2 |         |       |

- Molecule 32 is a protein called 50S ribosomal protein L36.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 32  | e     | 38       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 302   | 185 | 65 | 48 | 4 |         |       |

- Molecule 33 is a protein called 30S ribosomal protein S2.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 33  | f     | 225      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1760  | 1113 | 316 | 323 | 8 |         |       |

- Molecule 34 is a protein called 30S ribosomal protein S3.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 34  | g     | 208      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1636  | 1036 | 307 | 290 | 3 |         |       |

- Molecule 35 is a protein called 30S ribosomal protein S4.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 35  | h     | 205      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1643  | 1026 | 315 | 298 | 4 |         |       |

- Molecule 36 is a protein called 30S ribosomal protein S5.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 36  | i     | 156      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1152  | 717 | 217 | 212 | 6 |         |       |

- Molecule 37 is a protein called 30S ribosomal protein S6.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 37  | j     | 104      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 848   | 536 | 153 | 152 | 7 |         |       |

- Molecule 38 is a protein called 30S ribosomal protein S7.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 38  | k     | 151      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1181  | 735 | 227 | 215 | 4 |         |       |

- Molecule 39 is a protein called 30S ribosomal protein S8.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 39  | l     | 129      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 979   | 616 | 173 | 184 | 6 |         |       |

- Molecule 40 is a protein called 30S ribosomal protein S9.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 40  | m     | 127      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1022  | 634 | 206 | 179 | 3 |         |       |

- Molecule 41 is a protein called 30S ribosomal protein S10.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 41  | n     | 99       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 790   | 495 | 151 | 143 | 1 |         |       |

- Molecule 42 is a protein called 30S ribosomal protein S11.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 42  | o     | 117      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 877   | 540 | 174 | 160 | 3 |         |       |

- Molecule 43 is a protein called 30S ribosomal protein S12.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 43  | p     | 123      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 957   | 591 | 196 | 165 | 5 |         |       |

- Molecule 44 is a protein called 30S ribosomal protein S13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 44  | q     | 116      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 900   | 558 | 181 | 158 | 3 |         |       |

- Molecule 45 is a protein called 30S ribosomal protein S14.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 45  | r     | 100      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 805   | 499 | 164 | 139 | 3 |         |       |

- Molecule 46 is a protein called 30S ribosomal protein S15.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 46  | s     | 88       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 714   | 439 | 144 | 130 | 1 |         |       |

- Molecule 47 is a protein called 30S ribosomal protein S16.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 47  | t     | 82       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 649   | 406 | 128 | 114 | 1 |         |       |

- Molecule 48 is a protein called 30S ribosomal protein S17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 48  | u     | 80       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 648   | 411 | 121 | 113 | 3 |         |       |

- Molecule 49 is a protein called 30S ribosomal protein S18.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 49  | v     | 66       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 544   | 344 | 102 | 97 | 1 |         |       |

- Molecule 50 is a protein called 30S ribosomal protein S19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 50  | w     | 83       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 663   | 424 | 126 | 111 | 2 |         |       |

- Molecule 51 is a protein called 30S ribosomal protein S20.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 51  | x     | 86       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 669   | 414 | 138 | 114 | 3 |         |       |

- Molecule 52 is a protein called 30S ribosomal protein S21.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 52  | y     | 70       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 589   | 366 | 125 | 97 | 1 |         |       |

- Molecule 53 is a RNA chain called mRNA.

| Mol | Chain | Residues | Atoms |    |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---|---------|-------|
| 53  | 4     | 6        | Total | C  | N  | O  | P | 0       | 0     |
|     |       |          | 122   | 55 | 17 | 44 | 6 |         |       |

- Molecule 54 is a RNA chain called tRNA-Leu.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 54  | z     | 85       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 1830  | 822 | 328 | 595 | 85 |         |       |

- Molecule 55 is a protein called Cold-shock DNA-binding protein family.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 55  | B     | 39       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 250   | 159 | 43 | 48 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference      |
|-------|---------|----------|--------|----------|----------------|
| B     | 8       | ILE      | VAL    | conflict | UNP A0A1H2D2H5 |

- Molecule 56 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms        |           | AltConf |
|-----|-------|----------|--------------|-----------|---------|
| 56  | 1     | 282      | Total<br>282 | Mg<br>282 | 0       |
| 56  | 2     | 119      | Total<br>119 | Mg<br>119 | 0       |
| 56  | 3     | 8        | Total<br>8   | Mg<br>8   | 0       |
| 56  | C     | 1        | Total<br>1   | Mg<br>1   | 0       |
| 56  | D     | 1        | Total<br>1   | Mg<br>1   | 0       |
| 56  | M     | 1        | Total<br>1   | Mg<br>1   | 0       |
| 56  | P     | 1        | Total<br>1   | Mg<br>1   | 0       |
| 56  | a     | 2        | Total<br>2   | Mg<br>2   | 0       |
| 56  | h     | 1        | Total<br>1   | Mg<br>1   | 0       |
| 56  | q     | 1        | Total<br>1   | Mg<br>1   | 0       |
| 56  | 4     | 1        | Total<br>1   | Mg<br>1   | 0       |
| 56  | z     | 4        | Total<br>4   | Mg<br>4   | 0       |

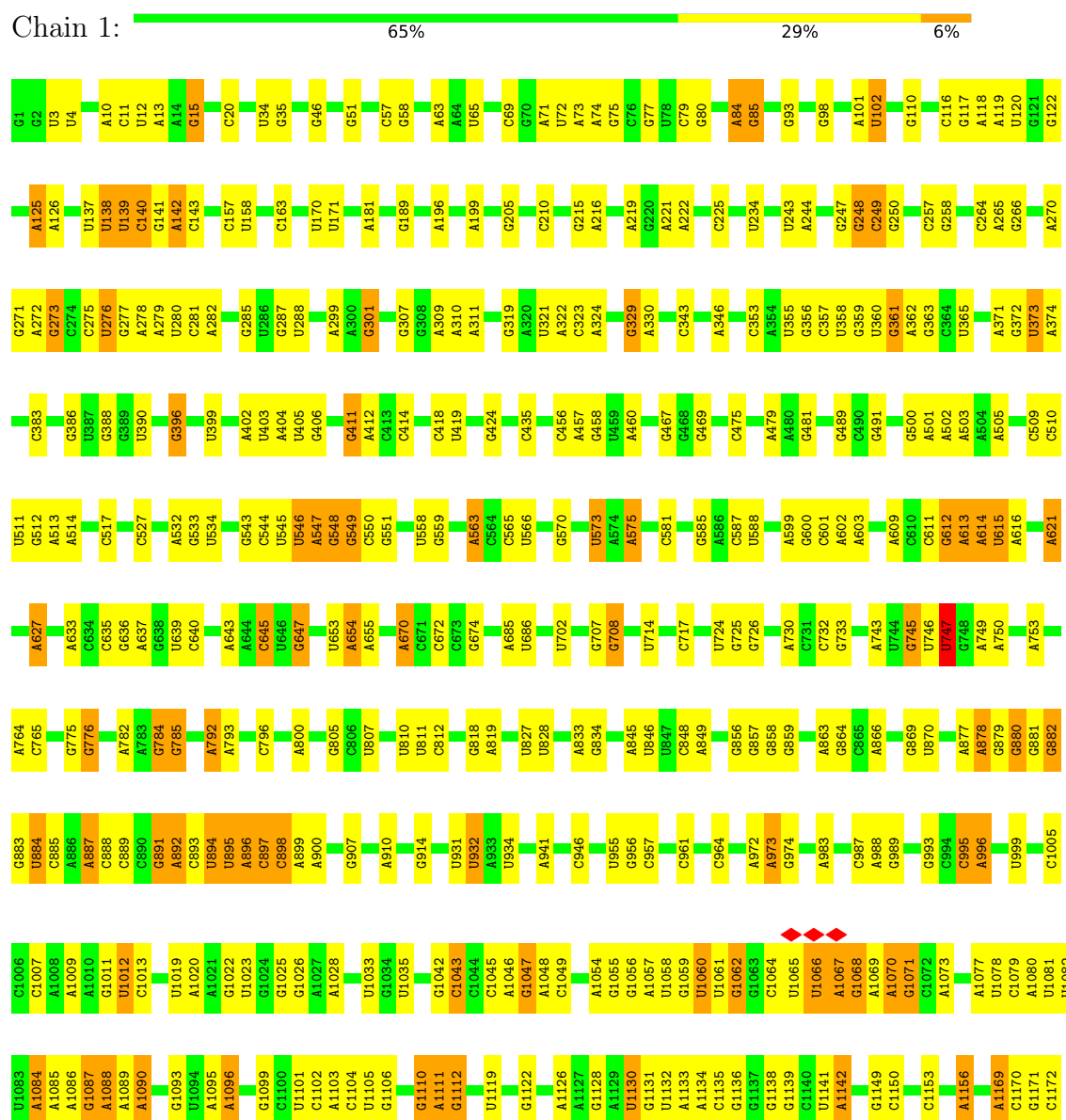
- Molecule 57 is ZINC ION (CCD ID: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms      |         | AltConf |
|-----|-------|----------|------------|---------|---------|
| 57  | Z     | 1        | Total<br>1 | Zn<br>1 | 0       |
| 57  | e     | 1        | Total<br>1 | Zn<br>1 | 0       |

### 3 Residue-property plots

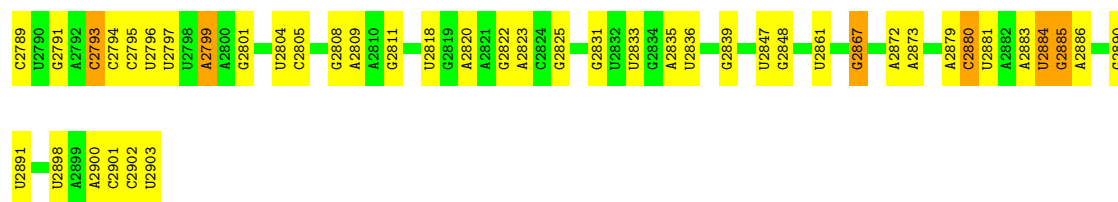
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

#### • Molecule 1: 23S rRNA



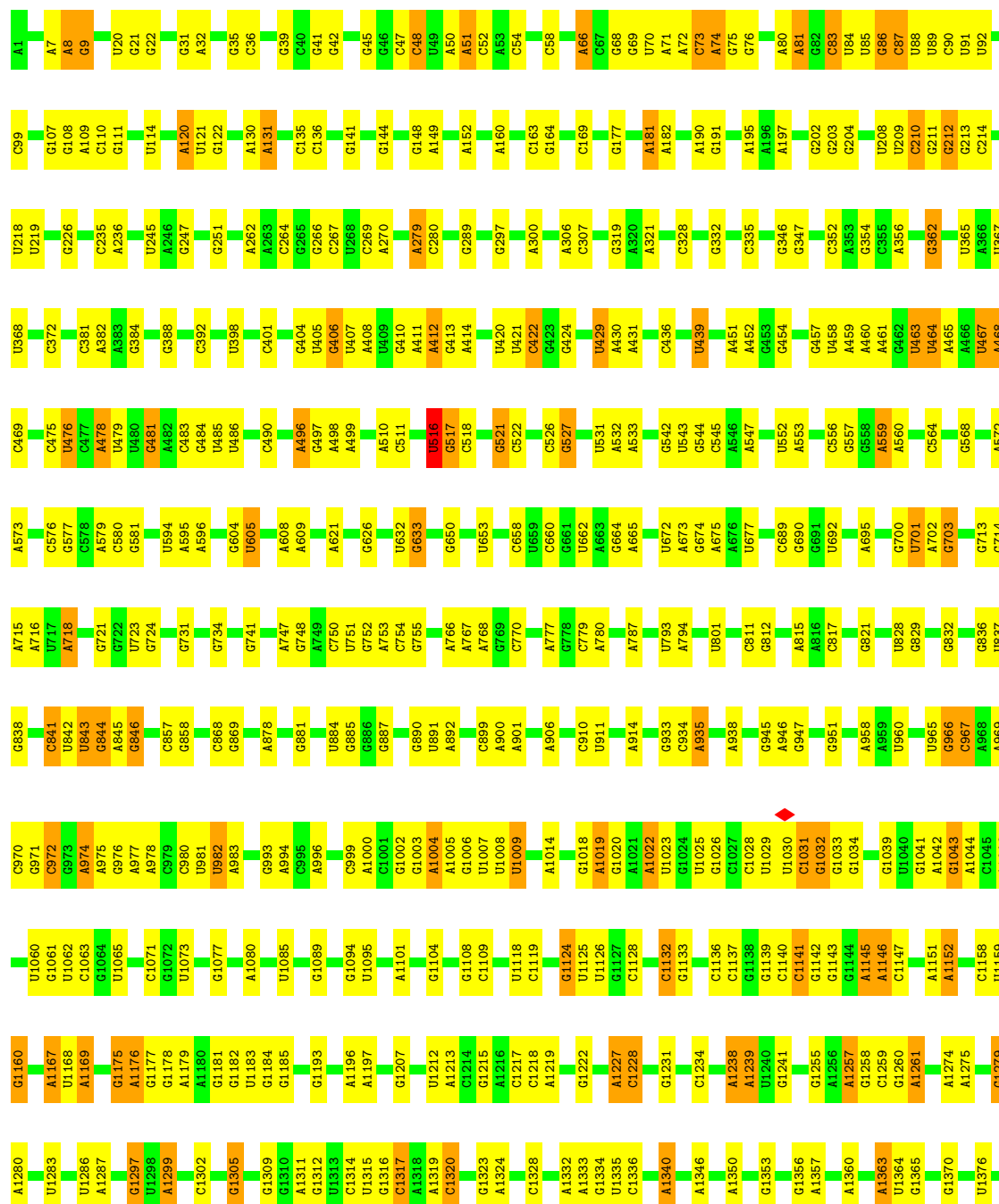
|       |       |       |       |       |       |       |         |       |       |       |       |       |
|-------|-------|-------|-------|-------|-------|-------|---------|-------|-------|-------|-------|-------|
| G2633 | A2530 | U2321 | U2229 | G2143 | A2060 | G1929 | A1808   | A1664 | A1528 | U1411 | A1276 | U1173 |
| G2664 | A2531 | A2322 | U2236 | G2144 | G2061 | G1930 | A1808   | A1668 | G1529 | U1412 | C1298 | U1174 |
| C2676 | G2532 | G2323 | U2237 | C2145 | C2062 | G1931 | G1811   | A1688 | C1531 | C1413 | C1299 | A1175 |
| C2683 | G2535 | U2324 | G2237 | C2146 | C2063 | G1932 | G1814   | U1671 | A1532 | U1415 | C1300 | U1176 |
| U2687 | A2547 | G2326 | G2238 | A2147 | C2065 | G1933 | G1815   | A1672 | U1533 | G1416 | A1301 | G1177 |
| G2688 | U2549 | A2327 | G2239 | G2148 | G2069 | A1936 | A1816   | G1673 | U1534 | C1417 | C1315 | C1178 |
| U2689 | A2450 | U2328 | U2243 | C2150 | A2070 | A1937 | C1816   | G1674 | A1535 | G1418 | C1316 | C1179 |
| U2690 | U2554 | U2329 | U2244 | U2151 | C2072 | U1938 | U1818   | A1676 | G1537 | G1419 | A1321 | U1180 |
| U2696 | U2555 | A2333 | U2249 | A2158 | U2079 | U1939 | U1827   | G1682 | U1539 | G1421 | G1182 | U1181 |
| C2699 | G2556 | U2334 | G2250 | G2159 | U2081 | G1954 | G1828   | G1689 | G1540 | A1427 | G1324 | G1186 |
| G2702 | A2459 | A2335 | G2251 | C2160 | A2082 | U1956 | A1829   | G1699 | U1544 | C1428 | U1325 | U1187 |
| G2708 | U2476 | G2336 | G2253 | G2162 | C2091 | C1962 | C1833   | G1715 | U1554 | G1432 | A1328 | A1189 |
| G2714 | A2477 | A2337 | C2258 | C2164 | U2092 | C1967 | G1835   | A1717 | U1559 | A1433 | C1330 | G1190 |
| C2715 | U2478 | G2338 | A2266 | U2166 | G2093 | U1970 | U1841   | A1722 | U1566 | C1437 | C1335 | C1196 |
| C2716 | U2479 | U2271 | A2267 | G2167 | C2094 | U1971 | G1842   | G1723 | A1569 | G1445 | A1336 | U1203 |
| C2717 | C2480 | G2272 | G2271 | C2168 | A2095 | U1972 | A1847   | U1729 | U1578 | C1446 | G1341 | A1204 |
| G2718 | G2481 | A2273 | A2273 | A2169 | G2100 | G1980 | A1848   | C1730 | A1579 | C1447 | A1342 | A1205 |
| U2721 | C2483 | G2277 | G2277 | G2170 | A2101 | A1981 | U1866   | G1731 | G1577 | G1450 | G1343 | G1206 |
| G2722 | G2484 | A2278 | A2278 | U2172 | G2102 | U1982 | G1857   | G1732 | A1578 | G1451 | C1344 | G1212 |
| A2725 | G2485 | C2283 | C2283 | C2174 | C2103 | U1991 | A1858   | G1738 | G1581 | G1452 | C1345 | G1215 |
| A2726 | C2486 | G2286 | G2286 | G2175 | G2107 | U1992 | U1864   | G1743 | G1582 | U1460 | U1352 | G1218 |
| A2727 | U2490 | A2287 | A2287 | C2177 | G2110 | U1993 | U1865   | A1746 | A1583 | U1468 | C1357 | G1219 |
| U2728 | U2491 | U2288 | U2288 | C2179 | U2111 | U1997 | C1868   | U1747 | U1584 | A1469 | G1358 | G1223 |
| A2733 | G2494 | U2291 | U2291 | U2182 | G2113 | G2002 | G1869   | A1754 | A1586 | G1475 | G1364 | U1231 |
| G2744 | C2496 | G2292 | G2292 | A2183 | A2114 | G2003 | C1870   | A1755 | G1587 | U1476 | A1365 | U1232 |
| A2748 | A2497 | G2293 | G2293 | U2184 | G2115 | A2014 | A1871   | G1756 | G1588 | G1482 | A1366 | G1233 |
| G2751 | C2498 | G2294 | G2294 | U2185 | A2116 | A2015 | A1872   | G1764 | U1589 | U1490 | A1367 | U1234 |
| C2752 | U2502 | A2297 | A2297 | U2186 | U2118 | C2021 | G1873   | C1764 | A1590 | A1503 | G1368 | U1235 |
| A2753 | A2503 | G2300 | G2300 | U2187 | A2119 | U2022 | U1883   | A1773 | A1591 | C1493 | G1370 | G1236 |
| U2754 | G2504 | C2301 | C2301 | U2188 | G2120 | C2023 | G1884   | A1779 | C1604 | A1504 | G1371 | A1237 |
| C2755 | U2505 | U2302 | U2302 | G2190 | G2121 | G2024 | G1896   | U1779 | C1607 | C1494 | C1376 | G1238 |
| U2756 | G2506 | U2305 | U2305 | A2191 | U2122 | C2025 | A1901   | U1782 | A1608 | A1495 | G1377 | U1242 |
| A2757 | C2507 | G2306 | G2306 | G2192 | G2123 | U2026 | G1906   | A1783 | A1609 | A1496 | C1243 | A1244 |
| U2764 | U2511 | G2309 | G2309 | U2194 | G2125 | A2030 | U1907   | A1784 | A1610 | A1503 | G1380 | U1247 |
| A2765 | C2512 | U2310 | U2310 | U2195 | A2126 | A2031 | G1911   | A1769 | A1618 | A1504 | A1383 | G1248 |
| C2767 | A2513 | A2311 | A2311 | C2196 | G2127 | G2032 | A1912   | C1790 | A1634 | A1508 | C1386 | U1249 |
| U2777 | U2518 | U2312 | U2312 | U2197 | C2128 | A2033 | A1913   | A1791 | U1647 | A1509 | A1387 | G1250 |
| A2778 | G2519 | C2313 | C2313 | U2198 | U2130 | C2043 | C1914   | C1795 | U1648 | A1510 | A1392 | A1253 |
| U2779 | C2520 | A2314 | A2314 | U2199 | U2131 | C2050 | 3TD1915 | U1796 | G1649 | A1515 | U1405 | G1256 |
| G2780 | U2521 | G2315 | G2315 | G2120 | U2132 | A2051 | A1916   | G1797 | A1650 | A1522 | U1407 | G1266 |
| A2788 | C2522 | A2316 | A2316 | A2220 | G2133 | A2052 | U1917   | C1800 | G1651 | U1523 | G1407 | U1408 |
| U2789 | G2523 | G2317 | G2317 | G2221 | A2134 | C2055 | G1922   | A1801 | A1652 | G1524 | A1409 | A1271 |
| U2790 | U2524 | G2318 | G2318 | A2225 | U2139 | G2056 | U1923   | A1802 | G1659 | G1527 | G1410 | A1272 |
| G2788 | G2529 | U2320 | U2320 | C2226 | G2140 | G2056 | C1924   | A1803 |       |       |       |       |
|       |       |       |       |       | A2142 |       |         |       |       |       |       |       |





• Molecule 2: 16S rRNA

Chain 2: 66% 28% 6%

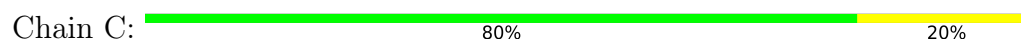




- Molecule 3: 5S rRNA



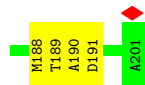
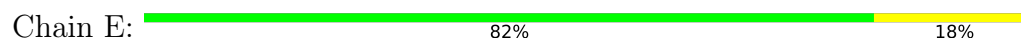
- Molecule 4: 50S ribosomal protein L2



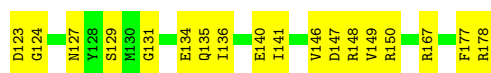
- Molecule 5: 50S ribosomal protein L3



- Molecule 6: 50S ribosomal protein L4

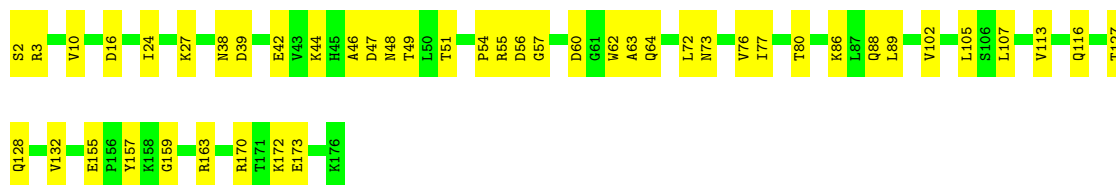


- Molecule 7: 50S ribosomal protein L5



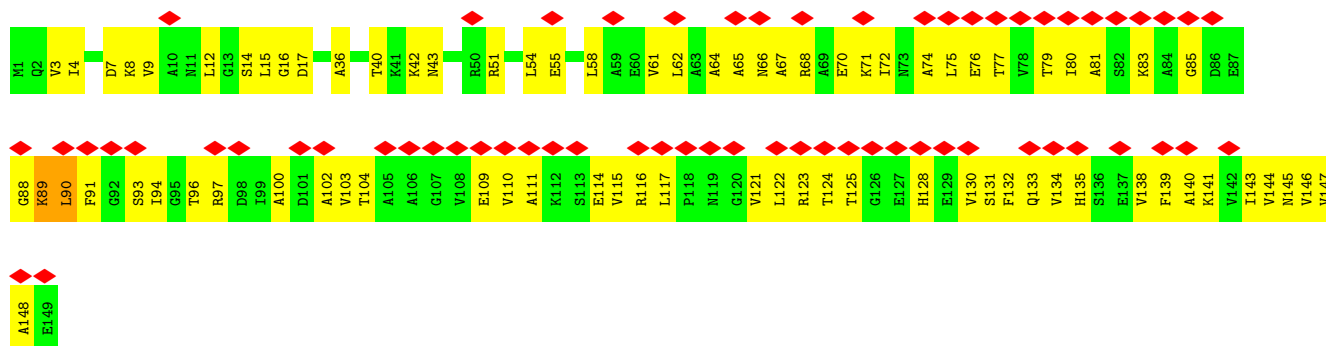
- Molecule 8: 50S ribosomal protein L6

Chain G:  74% 26%



• Molecule 9: 50S ribosomal protein L9

Chain H:  42% 48% 51%



• Molecule 10: 50S ribosomal protein L13

Chain I:  86% 14%



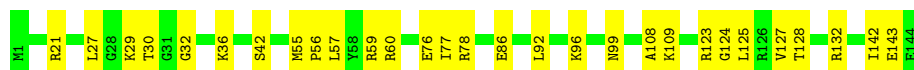
• Molecule 11: 50S ribosomal protein L14

Chain J:  84% 16%



• Molecule 12: 50S ribosomal protein L15

Chain K:  80% 20%



• Molecule 13: 50S ribosomal protein L16

Chain L:  84% 16%



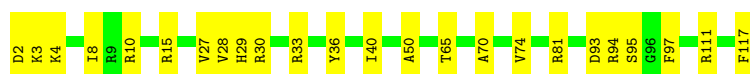
- Molecule 14: 50S ribosomal protein L17

Chain M: 82% 18%



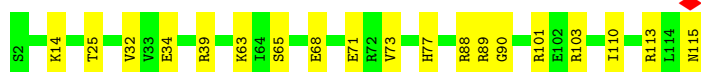
- Molecule 15: 50S ribosomal protein L18

Chain N: 79% 21%



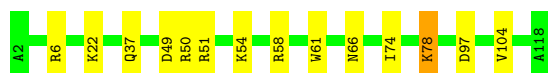
- Molecule 16: 50S ribosomal protein L19

Chain O: 83% 17%



- Molecule 17: 50S ribosomal protein L20

Chain P: 88% 11%



- Molecule 18: 50S ribosomal protein L21

Chain Q: 81% 17%



- Molecule 19: 50S ribosomal protein L22

Chain R: 76% 24%



- Molecule 20: 50S ribosomal protein L23

Chain S: 82% 18%



- Molecule 21: 50S ribosomal protein L24

Chain T: 75% 25%



- Molecule 22: 50S ribosomal protein L25

Chain U: 86% 14%



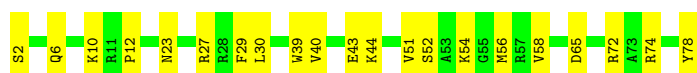
- Molecule 23: 50S ribosomal protein L27

Chain V: 5% 77% 21%



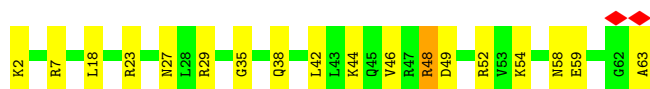
- Molecule 24: 50S ribosomal protein L28

Chain W: 73% 27%



- Molecule 25: 50S ribosomal protein L29

Chain X: 71% 27%

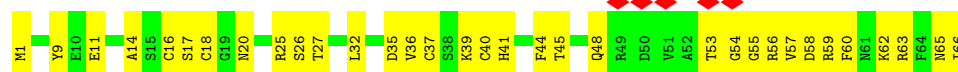


- Molecule 26: 50S ribosomal protein L30

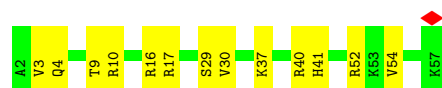
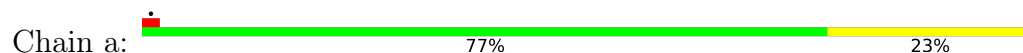
Chain Y: 84% 16%



- Molecule 27: 50S ribosomal protein L31



- Molecule 28: 50S ribosomal protein L32



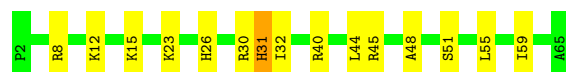
- Molecule 29: 50S ribosomal protein L33



- Molecule 30: 50S ribosomal protein L34



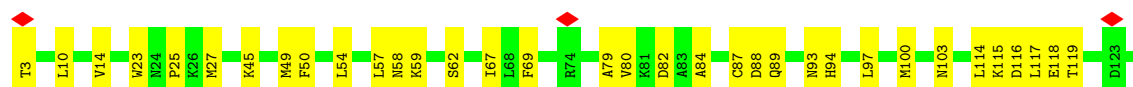
- Molecule 31: 50S ribosomal protein L35

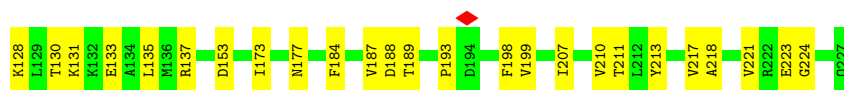


- Molecule 32: 50S ribosomal protein L36



- Molecule 33: 30S ribosomal protein S2

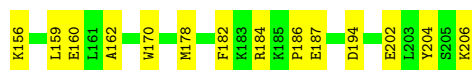
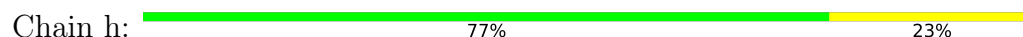




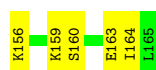
- Molecule 34: 30S ribosomal protein S3



- Molecule 35: 30S ribosomal protein S4



- Molecule 36: 30S ribosomal protein S5

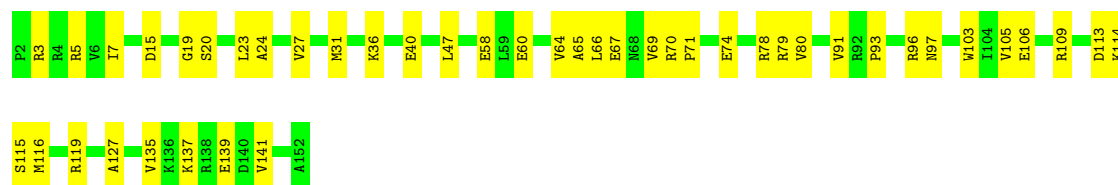


- Molecule 37: 30S ribosomal protein S6



- Molecule 38: 30S ribosomal protein S7





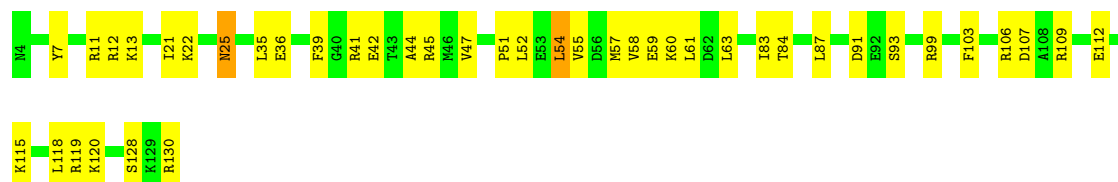
- Molecule 39: 30S ribosomal protein S8

Chain l: 84% 16%



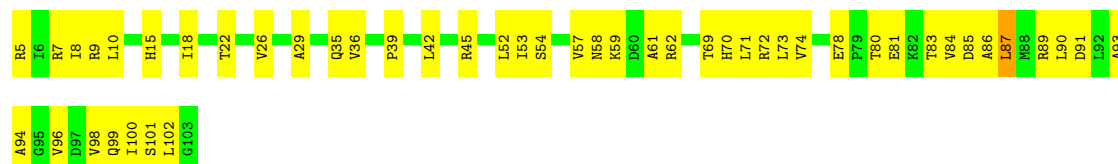
- Molecule 40: 30S ribosomal protein S9

Chain m: 67% 31% .



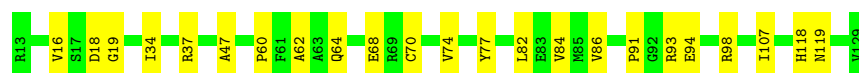
- Molecule 41: 30S ribosomal protein S10

Chain n: 52% 47% .



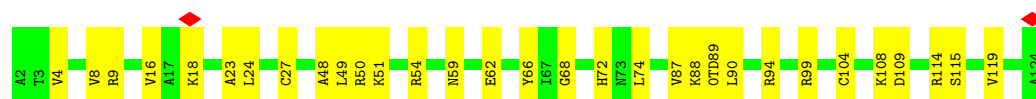
- Molecule 42: 30S ribosomal protein S11

Chain o: 80% 20%



- Molecule 43: 30S ribosomal protein S12

Chain p: 75% 25%



- Molecule 44: 30S ribosomal protein S13

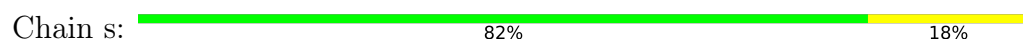




- Molecule 45: 30S ribosomal protein S14



- Molecule 46: 30S ribosomal protein S15



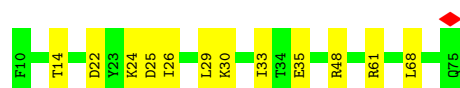
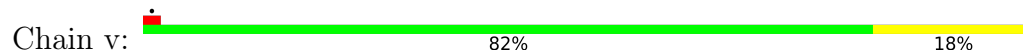
- Molecule 47: 30S ribosomal protein S16



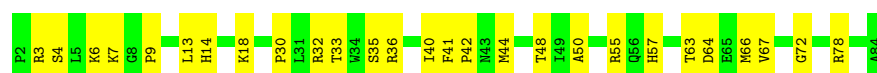
- Molecule 48: 30S ribosomal protein S17



- Molecule 49: 30S ribosomal protein S18

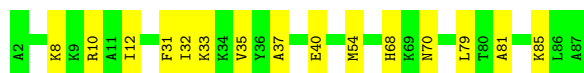


- Molecule 50: 30S ribosomal protein S19



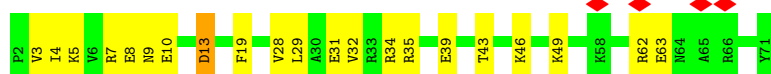
- Molecule 51: 30S ribosomal protein S20

Chain x:  83% 17%



- Molecule 52: 30S ribosomal protein S21

Chain y:  6% 70% 29%

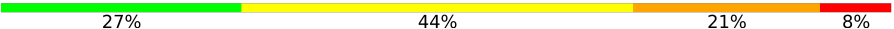


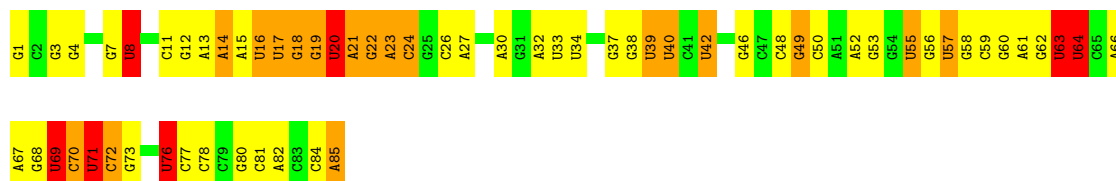
- Molecule 53: mRNA

Chain 4:  67% 17% 17%

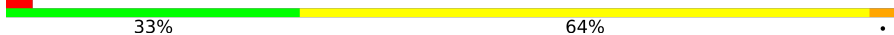


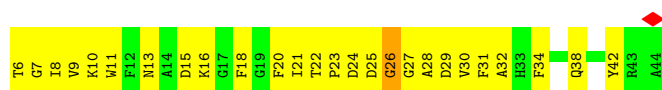
- Molecule 54: tRNA-Leu

Chain z:  27% 44% 21% 8%



- Molecule 55: Cold-shock DNA-binding protein family

Chain B:  33% 64%



## 4 Experimental information

| Property                             | Value                           | Source    |
|--------------------------------------|---------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                 | Depositor |
| Imposed symmetry                     | POINT, C1                       | Depositor |
| Number of particles used             | 23782                           | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF               | Depositor |
| CTF correction method                | NONE                            | Depositor |
| Microscope                           | FEI TITAN KRIOS                 | Depositor |
| Voltage (kV)                         | 300                             | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 2.2                             | Depositor |
| Minimum defocus (nm)                 | 500                             | Depositor |
| Maximum defocus (nm)                 | 2200                            | Depositor |
| Magnification                        | 75000                           | Depositor |
| Image detector                       | FEI FALCON III (4k x 4k)        | Depositor |
| Maximum map value                    | 0.157                           | Depositor |
| Minimum map value                    | -0.078                          | Depositor |
| Average map value                    | -0.000                          | Depositor |
| Map value standard deviation         | 0.009                           | Depositor |
| Recommended contour level            | 0.02                            | Depositor |
| Map size ( $\text{\AA}$ )            | 428.00003, 428.00003, 428.00003 | wwPDB     |
| Map dimensions                       | 400, 400, 400                   | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0                | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 1.07, 1.07, 1.07                | Depositor |

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 0TD, 5MC, 1MG, OMU, MA6, 6MZ, OMC, UR3, 5MU, G7M, MG, 4OC, 2MA, PSU, 2MG, 3TD, ZN, OMG

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   | 1     | 0.75         | 0/69286 | 0.56        | 3/108087 (0.0%) |
| 2   | 2     | 0.67         | 0/36590 | 0.51        | 0/57074         |
| 3   | 3     | 0.65         | 0/2872  | 0.49        | 0/4478          |
| 4   | C     | 1.01         | 0/2121  | 0.68        | 0/2852          |
| 5   | D     | 1.00         | 0/1586  | 0.70        | 1/2134 (0.0%)   |
| 6   | E     | 0.92         | 0/1571  | 0.70        | 0/2113          |
| 7   | F     | 0.72         | 0/1434  | 0.69        | 0/1926          |
| 8   | G     | 0.65         | 0/1333  | 0.67        | 0/1805          |
| 9   | H     | 0.48         | 0/1122  | 0.92        | 0/1515          |
| 10  | I     | 0.96         | 0/1152  | 0.65        | 0/1551          |
| 11  | J     | 0.95         | 0/955   | 0.69        | 0/1279          |
| 12  | K     | 0.97         | 0/1062  | 0.73        | 0/1413          |
| 13  | L     | 0.97         | 0/1093  | 0.68        | 0/1460          |
| 14  | M     | 1.01         | 0/964   | 0.75        | 0/1289          |
| 15  | N     | 0.84         | 0/902   | 0.70        | 0/1209          |
| 16  | O     | 0.94         | 0/929   | 0.67        | 0/1242          |
| 17  | P     | 1.11         | 0/960   | 0.80        | 0/1278          |
| 18  | Q     | 0.90         | 0/829   | 0.68        | 0/1107          |
| 19  | R     | 1.00         | 0/864   | 0.72        | 0/1156          |
| 20  | S     | 0.89         | 0/752   | 0.64        | 0/1005          |
| 21  | T     | 0.81         | 0/796   | 0.68        | 0/1062          |
| 22  | U     | 0.83         | 0/766   | 0.68        | 0/1025          |
| 23  | V     | 0.98         | 0/642   | 0.67        | 0/848           |
| 24  | W     | 0.96         | 0/635   | 0.71        | 0/848           |
| 25  | X     | 0.76         | 0/502   | 0.78        | 1/667 (0.1%)    |
| 26  | Y     | 0.97         | 0/452   | 0.68        | 0/605           |
| 27  | Z     | 0.56         | 0/531   | 0.76        | 0/709           |
| 28  | a     | 0.97         | 0/450   | 0.69        | 0/599           |
| 29  | b     | 0.75         | 0/433   | 0.63        | 0/576           |
| 30  | c     | 1.04         | 0/380   | 0.78        | 0/498           |
| 31  | d     | 1.06         | 0/513   | 0.79        | 0/676           |

| Mol | Chain | Bond lengths |          | Bond angles |                  |
|-----|-------|--------------|----------|-------------|------------------|
|     |       | RMSZ         | # Z  >5  | RMSZ        | # Z  >5          |
| 32  | e     | 0.97         | 0/303    | 0.68        | 0/397            |
| 33  | f     | 0.63         | 0/1791   | 0.74        | 0/2413           |
| 34  | g     | 0.77         | 0/1663   | 0.68        | 0/2241           |
| 35  | h     | 0.76         | 0/1665   | 0.69        | 0/2227           |
| 36  | i     | 0.88         | 0/1165   | 0.75        | 0/1568           |
| 37  | j     | 0.70         | 0/867    | 0.73        | 0/1171           |
| 38  | k     | 0.70         | 0/1195   | 0.74        | 0/1602           |
| 39  | l     | 0.89         | 0/989    | 0.69        | 0/1326           |
| 40  | m     | 0.78         | 0/1034   | 0.78        | 1/1375 (0.1%)    |
| 41  | n     | 0.73         | 0/800    | 0.94        | 2/1082 (0.2%)    |
| 42  | o     | 0.76         | 0/893    | 0.68        | 0/1205           |
| 43  | p     | 0.84         | 0/960    | 0.70        | 0/1286           |
| 44  | q     | 0.73         | 0/909    | 0.74        | 0/1215           |
| 45  | r     | 0.81         | 0/817    | 0.72        | 0/1088           |
| 46  | s     | 0.83         | 0/722    | 0.69        | 0/964            |
| 47  | t     | 0.84         | 0/659    | 0.67        | 0/884            |
| 48  | u     | 0.75         | 0/657    | 0.67        | 0/881            |
| 49  | v     | 0.81         | 0/553    | 0.69        | 0/743            |
| 50  | w     | 0.66         | 0/680    | 0.66        | 0/915            |
| 51  | x     | 0.83         | 0/675    | 0.77        | 0/895            |
| 52  | y     | 0.65         | 0/597    | 0.72        | 0/792            |
| 53  | 4     | 0.79         | 0/134    | 0.87        | 1/205 (0.5%)     |
| 54  | z     | 0.66         | 0/1768   | 0.57        | 0/2759           |
| 55  | B     | 0.60         | 0/255    | 0.80        | 1/347 (0.3%)     |
| All | All   | 0.76         | 0/156228 | 0.59        | 10/233667 (0.0%) |

There are no bond length outliers.

All (10) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 41  | n     | 54   | SER  | CA-C-N      | 8.52  | 128.50      | 119.05   |
| 41  | n     | 54   | SER  | C-N-CA      | 8.52  | 128.50      | 119.05   |
| 1   | 1     | 708  | G    | O3'-P-O5'   | -7.33 | 93.01       | 104.00   |
| 5   | D     | 152  | PRO  | CA-N-CD     | -5.79 | 103.89      | 112.00   |
| 25  | X     | 48   | ARG  | CA-CB-CG    | 5.66  | 125.42      | 114.10   |
| 40  | m     | 54   | LEU  | N-CA-C      | -5.28 | 105.17      | 111.03   |
| 55  | B     | 26   | GLY  | N-CA-C      | -5.26 | 108.65      | 115.59   |
| 1   | 1     | 1534 | U    | C2'-C3'-O3' | -5.04 | 106.14      | 113.70   |
| 1   | 1     | 2164 | C    | P-O3'-C3'   | -5.04 | 112.63      | 120.20   |
| 53  | 4     | 3    | U    | C4'-C3'-O3' | 5.01  | 120.52      | 113.00   |

There are no chirality outliers.

There are no planarity outliers.

## 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   | 1     | 62336 | 0        | 31349    | 578     | 0            |
| 2   | 2     | 32929 | 0        | 16586    | 284     | 0            |
| 3   | 3     | 2569  | 0        | 1299     | 15      | 0            |
| 4   | C     | 2082  | 0        | 2154     | 35      | 0            |
| 5   | D     | 1565  | 0        | 1616     | 26      | 0            |
| 6   | E     | 1552  | 0        | 1619     | 30      | 0            |
| 7   | F     | 1410  | 0        | 1444     | 46      | 0            |
| 8   | G     | 1313  | 0        | 1358     | 28      | 0            |
| 9   | H     | 1111  | 0        | 1148     | 83      | 0            |
| 10  | I     | 1129  | 0        | 1162     | 17      | 0            |
| 11  | J     | 946   | 0        | 1023     | 15      | 0            |
| 12  | K     | 1053  | 0        | 1129     | 26      | 0            |
| 13  | L     | 1074  | 0        | 1157     | 16      | 0            |
| 14  | M     | 951   | 0        | 994      | 20      | 0            |
| 15  | N     | 892   | 0        | 923      | 19      | 0            |
| 16  | O     | 917   | 0        | 962      | 18      | 0            |
| 17  | P     | 947   | 0        | 1019     | 13      | 0            |
| 18  | Q     | 816   | 0        | 839      | 21      | 0            |
| 19  | R     | 857   | 0        | 922      | 19      | 0            |
| 20  | S     | 746   | 0        | 811      | 14      | 0            |
| 21  | T     | 788   | 0        | 844      | 20      | 0            |
| 22  | U     | 753   | 0        | 780      | 7       | 0            |
| 23  | V     | 634   | 0        | 653      | 13      | 0            |
| 24  | W     | 625   | 0        | 652      | 13      | 0            |
| 25  | X     | 501   | 0        | 531      | 18      | 0            |
| 26  | Y     | 448   | 0        | 488      | 5       | 0            |
| 27  | Z     | 522   | 0        | 521      | 27      | 0            |
| 28  | a     | 444   | 0        | 458      | 13      | 0            |
| 29  | b     | 426   | 0        | 464      | 2       | 0            |
| 30  | c     | 377   | 0        | 418      | 11      | 0            |
| 31  | d     | 504   | 0        | 572      | 13      | 0            |
| 32  | e     | 302   | 0        | 340      | 7       | 0            |
| 33  | f     | 1760  | 0        | 1787     | 44      | 0            |
| 34  | g     | 1636  | 0        | 1710     | 50      | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 35  | h     | 1643   | 0        | 1706     | 39      | 0            |
| 36  | i     | 1152   | 0        | 1196     | 30      | 0            |
| 37  | j     | 848    | 0        | 846      | 28      | 0            |
| 38  | k     | 1181   | 0        | 1238     | 31      | 0            |
| 39  | l     | 979    | 0        | 1031     | 20      | 0            |
| 40  | m     | 1022   | 0        | 1070     | 31      | 0            |
| 41  | n     | 790    | 0        | 831      | 43      | 0            |
| 42  | o     | 877    | 0        | 887      | 14      | 0            |
| 43  | p     | 957    | 0        | 1017     | 28      | 0            |
| 44  | q     | 900    | 0        | 965      | 32      | 0            |
| 45  | r     | 805    | 0        | 844      | 27      | 0            |
| 46  | s     | 714    | 0        | 734      | 17      | 0            |
| 47  | t     | 649    | 0        | 666      | 15      | 0            |
| 48  | u     | 648    | 0        | 691      | 14      | 0            |
| 49  | v     | 544    | 0        | 560      | 8       | 0            |
| 50  | w     | 663    | 0        | 688      | 26      | 0            |
| 51  | x     | 669    | 0        | 719      | 9       | 0            |
| 52  | y     | 589    | 0        | 629      | 14      | 0            |
| 53  | 4     | 122    | 0        | 64       | 1       | 0            |
| 54  | z     | 1830   | 0        | 939      | 64      | 0            |
| 55  | B     | 250    | 0        | 199      | 58      | 0            |
| 56  | 1     | 282    | 0        | 0        | 0       | 0            |
| 56  | 2     | 119    | 0        | 0        | 0       | 0            |
| 56  | 3     | 8      | 0        | 0        | 0       | 0            |
| 56  | 4     | 1      | 0        | 0        | 0       | 0            |
| 56  | C     | 1      | 0        | 0        | 0       | 0            |
| 56  | D     | 1      | 0        | 0        | 0       | 0            |
| 56  | M     | 1      | 0        | 0        | 0       | 0            |
| 56  | P     | 1      | 0        | 0        | 0       | 0            |
| 56  | a     | 2      | 0        | 0        | 0       | 0            |
| 56  | h     | 1      | 0        | 0        | 0       | 0            |
| 56  | q     | 1      | 0        | 0        | 0       | 0            |
| 56  | z     | 4      | 0        | 0        | 0       | 0            |
| 57  | Z     | 1      | 0        | 0        | 0       | 0            |
| 57  | e     | 1      | 0        | 0        | 0       | 0            |
| All | All   | 145171 | 0        | 97252    | 1843    | 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 (1843) 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) |
|------------------|-------------------|--------------------------|-------------------|
| 1:1:1335:C:HO2'  | 55:B:6:THR:N      | 1.36                     | 1.22              |
| 5:D:151:THR:HG23 | 5:D:152:PRO:HD3   | 1.25                     | 1.17              |
| 54:z:21:A:N7     | 54:z:56:G:N2      | 2.07                     | 1.02              |
| 1:1:2483:C:N3    | 13:L:123:LYS:NZ   | 2.09                     | 1.01              |
| 40:m:57:MET:HE2  | 40:m:61:LEU:HD11  | 1.48                     | 0.95              |
| 2:2:412:A:N6     | 2:2:431:A:N1      | 2.17                     | 0.92              |
| 1:1:1870:C:O2'   | 1:1:1871:A:O5'    | 1.89                     | 0.90              |
| 2:2:951:G:OP2    | 44:q:101:ARG:NH2  | 2.06                     | 0.89              |
| 1:1:2478:A:OP2   | 32:e:2:LYS:NZ     | 2.06                     | 0.89              |
| 55:B:8:ILE:O     | 55:B:22:THR:N     | 2.06                     | 0.89              |
| 1:1:2130:U:O3'   | 1:1:2158:A:N6     | 2.06                     | 0.89              |
| 2:2:203:G:O2'    | 2:2:465:A:N1      | 2.06                     | 0.88              |
| 1:1:891:G:O2'    | 1:1:892:A:OP1     | 1.91                     | 0.88              |
| 1:1:1223:G:OP1   | 18:Q:68:ARG:NH2   | 2.06                     | 0.88              |
| 33:f:115:LYS:O   | 33:f:119:THR:HG23 | 1.72                     | 0.88              |
| 1:1:2571:U:O2'   | 5:D:151:THR:HG21  | 1.73                     | 0.87              |
| 2:2:1031:C:O3'   | 2:2:1032:G:N2     | 2.08                     | 0.87              |
| 20:S:72:GLN:NE2  | 55:B:30:VAL:O     | 2.08                     | 0.87              |
| 2:2:356:A:N3     | 2:2:368:U:O2'     | 2.07                     | 0.86              |
| 38:k:40:GLU:OE1  | 40:m:41:ARG:NH1   | 2.08                     | 0.86              |
| 2:2:1439:G:OP2   | 51:x:33:LYS:NZ    | 2.07                     | 0.86              |
| 11:J:51:LYS:NZ   | 11:J:95:ILE:O     | 2.07                     | 0.86              |
| 1:1:2140:G:O6    | 1:1:2151:U:C4     | 2.28                     | 0.86              |
| 27:Z:35:ASP:OD2  | 44:q:57:ARG:NE    | 2.09                     | 0.86              |
| 41:n:29:ALA:HB2  | 41:n:87:LEU:HD21  | 1.58                     | 0.86              |
| 1:1:1450:G:N2    | 1:1:1452:G:O6     | 2.09                     | 0.85              |
| 2:2:81:A:H62     | 2:2:87:C:N4       | 1.74                     | 0.85              |
| 1:1:2204:G:OP2   | 4:C:147:LYS:NZ    | 2.09                     | 0.85              |
| 9:H:104:THR:HG23 | 9:H:109:GLU:OE2   | 1.76                     | 0.84              |
| 55:B:28:ALA:O    | 55:B:32:ALA:N     | 2.10                     | 0.84              |
| 44:q:9:ILE:HG23  | 44:q:18:ALA:HB1   | 1.57                     | 0.84              |
| 1:1:956:G:O6     | 13:L:14:LYS:NZ    | 2.10                     | 0.84              |
| 1:1:125:A:OP2    | 30:c:19:ARG:NH2   | 2.11                     | 0.84              |
| 35:h:47:ARG:NH1  | 35:h:48:LEU:O     | 2.11                     | 0.84              |
| 1:1:1062:G:N7    | 1:1:1088:A:O2'    | 2.09                     | 0.84              |
| 1:1:1335:C:O2'   | 55:B:6:THR:N      | 2.10                     | 0.83              |
| 1:1:1172:C:O2'   | 1:1:1173:U:O4'    | 1.95                     | 0.82              |
| 52:y:31:GLU:OE2  | 52:y:35:ARG:NE    | 2.12                     | 0.82              |
| 37:j:17:GLN:OE1  | 37:j:17:GLN:N     | 2.12                     | 0.81              |
| 1:1:475:C:O2     | 1:1:479:A:N6      | 2.13                     | 0.81              |
| 1:1:2530:A:N7    | 8:G:172:LYS:NZ    | 2.28                     | 0.81              |
| 2:2:1168:U:O2'   | 2:2:1169:A:OP1    | 1.99                     | 0.81              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 34:g:28:GLU:OE1  | 34:g:28:GLU:N     | 2.14                     | 0.81              |
| 36:i:151:GLU:OE1 | 36:i:151:GLU:N    | 2.12                     | 0.81              |
| 40:m:36:GLU:OE1  | 40:m:45:ARG:NH1   | 2.14                     | 0.80              |
| 1:1:2220:U:O3'   | 9:H:97:ARG:NH2    | 2.13                     | 0.80              |
| 1:1:1668:A:O2'   | 1:1:1674:G:N7     | 2.15                     | 0.80              |
| 10:I:49:ASP:OD1  | 10:I:121:LYS:NZ   | 2.14                     | 0.80              |
| 37:j:69:GLU:OE1  | 37:j:69:GLU:N     | 2.14                     | 0.80              |
| 33:f:57:LEU:HD13 | 33:f:217:VAL:HG13 | 1.63                     | 0.80              |
| 3:3:31:C:O2      | 3:3:53:A:N6       | 2.15                     | 0.79              |
| 7:F:117:LEU:N    | 7:F:177:PHE:O     | 2.14                     | 0.79              |
| 1:1:1779:U:OP2   | 1:1:1784:A:N6     | 2.13                     | 0.79              |
| 20:S:69:ARG:NH1  | 20:S:72:GLN:OE1   | 2.15                     | 0.79              |
| 1:1:1914:C:N4    | 2:2:1409:C:O2'    | 2.16                     | 0.78              |
| 30:c:31:LEU:HD22 | 30:c:42:LEU:CD2   | 2.13                     | 0.78              |
| 18:Q:70:GLU:OE1  | 18:Q:70:GLU:N     | 2.17                     | 0.78              |
| 15:N:50:ALA:O    | 15:N:81:ARG:NH2   | 2.17                     | 0.78              |
| 2:2:1145:A:O2'   | 2:2:1146:A:OP2    | 2.02                     | 0.78              |
| 16:O:89:ARG:NH2  | 16:O:115:ASN:OD1  | 2.16                     | 0.78              |
| 1:1:1364:G:OP2   | 24:W:2:SER:N      | 2.16                     | 0.77              |
| 2:2:81:A:N6      | 2:2:87:C:N4       | 2.33                     | 0.77              |
| 34:g:156:ARG:NE  | 34:g:160:ALA:O    | 2.16                     | 0.77              |
| 40:m:106:ARG:NH1 | 40:m:107:ASP:O    | 2.18                     | 0.77              |
| 1:1:1754:A:N1    | 1:1:2716:C:O2'    | 2.17                     | 0.76              |
| 9:H:62:LEU:O     | 9:H:66:ASN:ND2    | 2.16                     | 0.76              |
| 9:H:54:LEU:HD12  | 9:H:55:GLU:N      | 2.01                     | 0.76              |
| 2:2:974:A:OP1    | 45:r:69:ARG:NH1   | 2.19                     | 0.76              |
| 1:1:747:5MU:O2'  | 19:R:92:ARG:NH1   | 2.18                     | 0.76              |
| 1:1:2051:A:N6    | 1:1:2614:A:O2'    | 2.19                     | 0.76              |
| 55:B:27:GLY:O    | 55:B:30:VAL:N     | 2.18                     | 0.76              |
| 1:1:1169:A:N6    | 1:1:1180:U:O4     | 2.18                     | 0.76              |
| 20:S:6:ARG:O     | 20:S:10:VAL:HG23  | 1.86                     | 0.76              |
| 35:h:58:LYS:NZ   | 35:h:69:GLU:OE1   | 2.16                     | 0.76              |
| 1:1:249:C:O2     | 31:d:12:LYS:NZ    | 2.19                     | 0.75              |
| 45:r:41:ARG:NH2  | 50:w:6:LYS:O      | 2.19                     | 0.75              |
| 7:F:134:GLU:HG2  | 7:F:136:ILE:HD12  | 1.68                     | 0.75              |
| 50:w:33:THR:HG22 | 50:w:35:SER:H     | 1.50                     | 0.75              |
| 54:z:70:C:H6     | 54:z:70:C:H5''    | 1.51                     | 0.75              |
| 55:B:24:ASP:O    | 55:B:27:GLY:N     | 2.20                     | 0.75              |
| 2:2:71:A:N1      | 2:2:99:C:O2'      | 2.20                     | 0.74              |
| 1:1:65:U:O2'     | 1:1:456:C:N3      | 2.20                     | 0.74              |
| 1:1:627:A:OP1    | 12:K:78:ARG:NH1   | 2.19                     | 0.74              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 19:R:25:ARG:NH1   | 19:R:74:ILE:O    | 2.20                     | 0.74              |
| 37:j:35:LYS:O     | 37:j:36:ILE:HD13 | 1.86                     | 0.74              |
| 2:2:1516:2MG:N2   | 2:2:1519:MA6:OP2 | 2.21                     | 0.74              |
| 1:1:276:U:O2'     | 1:1:277:G:N7     | 2.17                     | 0.74              |
| 2:2:626:G:O3'     | 47:t:51:ARG:NH1  | 2.20                     | 0.74              |
| 7:F:121:SER:OG    | 7:F:129:SER:O    | 2.06                     | 0.74              |
| 2:2:107:G:N7      | 51:x:10:ARG:NH2  | 2.36                     | 0.74              |
| 30:c:31:LEU:HD22  | 30:c:42:LEU:HD21 | 1.68                     | 0.74              |
| 8:G:173:GLU:N     | 8:G:173:GLU:OE1  | 2.21                     | 0.74              |
| 5:D:25:THR:OG1    | 5:D:191:GLY:O    | 2.05                     | 0.74              |
| 39:l:96:MET:SD    | 39:l:130:ALA:HB1 | 2.27                     | 0.74              |
| 1:1:1203:U:N3     | 1:1:1242:U:O4    | 2.19                     | 0.74              |
| 19:R:82:MET:SD    | 19:R:84:ARG:NH1  | 2.60                     | 0.74              |
| 1:1:585:G:N7      | 17:P:6:ARG:NH1   | 2.36                     | 0.73              |
| 1:1:894:U:O2'     | 1:1:895:U:O4'    | 2.05                     | 0.73              |
| 1:1:2377:A:O2'    | 15:N:117:PHE:O   | 2.04                     | 0.73              |
| 1:1:2683:C:O2     | 11:J:70:ARG:NH2  | 2.21                     | 0.73              |
| 42:o:94:GLU:OE1   | 42:o:98:ARG:NE   | 2.22                     | 0.73              |
| 1:1:1416:G:O6     | 1:1:1583:A:N6    | 2.21                     | 0.73              |
| 1:1:2182:U:O2'    | 1:1:2183:A:N7    | 2.21                     | 0.73              |
| 9:H:7:ASP:OD1     | 9:H:8:LYS:N      | 2.22                     | 0.73              |
| 38:k:5:ARG:NH1    | 38:k:7:ILE:HG22  | 2.04                     | 0.73              |
| 44:q:16:VAL:O     | 44:q:20:THR:HG23 | 1.88                     | 0.73              |
| 1:1:1055:G:O6     | 1:1:1105:U:O4    | 2.06                     | 0.72              |
| 2:2:938:A:N3      | 2:2:1376:U:O2'   | 2.21                     | 0.72              |
| 9:H:14:SER:N      | 9:H:17:ASP:OD2   | 2.22                     | 0.72              |
| 15:N:4:LYS:NZ     | 15:N:8:ILE:HD11  | 2.05                     | 0.72              |
| 1:1:1007:C:OP1    | 10:I:37:ARG:NH2  | 2.22                     | 0.72              |
| 1:1:1335:C:O2'    | 55:B:6:THR:OG1   | 2.07                     | 0.72              |
| 2:2:1005:A:H3'    | 2:2:1006:G:C8    | 2.25                     | 0.72              |
| 2:2:1167:A:O2'    | 2:2:1169:A:N7    | 2.23                     | 0.72              |
| 2:2:1311:A:OP1    | 27:Z:59:ARG:NH1  | 2.22                     | 0.72              |
| 33:f:27:MET:HE2   | 33:f:193:PRO:HD3 | 1.72                     | 0.72              |
| 1:1:1068:G:O2'    | 1:1:1070:A:N6    | 2.22                     | 0.72              |
| 2:2:1317:C:OP2    | 45:r:28:LYS:NZ   | 2.21                     | 0.72              |
| 2:2:401:C:O2'     | 2:2:621:A:N3     | 2.21                     | 0.71              |
| 2:2:673:A:O3'     | 37:j:86:ARG:NH2  | 2.23                     | 0.71              |
| 34:g:138:VAL:HG11 | 34:g:170:GLU:OE1 | 1.90                     | 0.71              |
| 25:X:59:GLU:O     | 25:X:63:ALA:HB3  | 1.91                     | 0.71              |
| 2:2:58:C:O2'      | 2:2:388:G:N7     | 2.21                     | 0.71              |
| 2:2:544:G:OP1     | 35:h:56:ARG:NH2  | 2.24                     | 0.71              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 8:G:56:ASP:OD1   | 8:G:57:GLY:N     | 2.24                     | 0.71              |
| 23:V:11:ARG:O    | 23:V:14:ARG:NH2  | 2.21                     | 0.71              |
| 33:f:59:LYS:O    | 33:f:62:SER:OG   | 2.07                     | 0.71              |
| 1:1:870:U:OP1    | 13:L:6:ARG:NH1   | 2.23                     | 0.71              |
| 54:z:63:5MU:H3'  | 54:z:63:5MU:C6   | 2.25                     | 0.71              |
| 1:1:1028:A:OP2   | 1:1:1126:A:N6    | 2.25                     | 0.70              |
| 55:B:24:ASP:O    | 55:B:26:GLY:N    | 2.24                     | 0.70              |
| 1:1:621:A:OP2    | 12:K:99:ASN:ND2  | 2.25                     | 0.70              |
| 15:N:94:ARG:NH2  | 15:N:97:PHE:O    | 2.24                     | 0.70              |
| 2:2:842:U:C2'    | 2:2:844:G:H21    | 2.03                     | 0.70              |
| 34:g:14:ILE:HG22 | 34:g:15:VAL:HG13 | 1.73                     | 0.70              |
| 1:1:563:A:N3     | 17:P:37:GLN:NE2  | 2.40                     | 0.70              |
| 18:Q:29:THR:O    | 18:Q:29:THR:HG22 | 1.90                     | 0.70              |
| 54:z:71:5MU:H6   | 54:z:71:5MU:H5'  | 1.55                     | 0.70              |
| 1:1:2148:G:N1    | 1:1:2149:U:O4    | 2.25                     | 0.70              |
| 1:1:1266:G:OP1   | 28:a:16:ARG:NE   | 2.21                     | 0.70              |
| 1:1:2640:G:OP1   | 10:I:95:ARG:NH2  | 2.25                     | 0.70              |
| 1:1:2125:G:H22   | 1:1:2171:A:P     | 2.14                     | 0.69              |
| 4:C:142:HIS:ND1  | 4:C:193:GLY:O    | 2.24                     | 0.69              |
| 23:V:33:ALA:N    | 23:V:64:ASP:OD1  | 2.25                     | 0.69              |
| 34:g:40:ARG:O    | 34:g:44:THR:HG23 | 1.92                     | 0.69              |
| 37:j:51:ILE:O    | 37:j:54:LEU:HD23 | 1.92                     | 0.69              |
| 1:1:2125:G:N2    | 1:1:2171:A:OP1   | 2.22                     | 0.69              |
| 2:2:8:A:N6       | 35:h:202:GLU:O   | 2.22                     | 0.69              |
| 40:m:59:GLU:OE1  | 40:m:59:GLU:N    | 2.25                     | 0.69              |
| 54:z:69:5MU:H3'  | 54:z:70:C:H5''   | 1.74                     | 0.69              |
| 21:T:36:VAL:CG1  | 21:T:39:ILE:HD12 | 2.23                     | 0.69              |
| 1:1:877:A:O2'    | 1:1:900:A:N6     | 2.26                     | 0.69              |
| 33:f:10:LEU:HD23 | 33:f:10:LEU:O    | 1.93                     | 0.69              |
| 1:1:2126:A:N6    | 1:1:2171:A:OP2   | 2.26                     | 0.69              |
| 1:1:2635:A:O2'   | 5:D:49:GLN:NE2   | 2.26                     | 0.69              |
| 6:E:153:LEU:HD12 | 6:E:153:LEU:O    | 1.92                     | 0.69              |
| 1:1:776:G:N7     | 1:1:793:A:O2'    | 2.26                     | 0.68              |
| 1:1:2116:G:N2    | 1:1:2161:C:OP1   | 2.25                     | 0.68              |
| 4:C:258:ARG:NH1  | 4:C:264:ASP:OD1  | 2.25                     | 0.68              |
| 2:2:933:G:O6     | 38:k:3:ARG:NH2   | 2.26                     | 0.68              |
| 11:J:121:GLU:OE1 | 16:O:65:SER:OG   | 2.11                     | 0.68              |
| 48:u:7:THR:C     | 48:u:8:LEU:HD12  | 2.18                     | 0.68              |
| 2:2:346:G:OP1    | 16:O:39:ARG:NH2  | 2.27                     | 0.68              |
| 2:2:980:C:O2'    | 45:r:13:ARG:NH1  | 2.27                     | 0.68              |
| 25:X:49:ASP:OD1  | 25:X:52:ARG:NH2  | 2.27                     | 0.68              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 40:m:84:THR:HG21 | 40:m:103:PHE:HB3  | 1.75                     | 0.68              |
| 36:i:136:VAL:O   | 36:i:140:THR:HG23 | 1.94                     | 0.68              |
| 1:1:2140:G:O6    | 1:1:2151:U:O4     | 2.11                     | 0.68              |
| 39:l:5:ASP:OD2   | 39:l:77:ARG:NH1   | 2.26                     | 0.67              |
| 2:2:1006:G:H8    | 2:2:1006:G:O5'    | 1.77                     | 0.67              |
| 1:1:2102:G:O6    | 1:1:2187:U:C4     | 2.47                     | 0.67              |
| 2:2:970:C:N4     | 40:m:130:ARG:O    | 2.28                     | 0.67              |
| 38:k:78:ARG:HG2  | 38:k:80:VAL:HG23  | 1.76                     | 0.67              |
| 4:C:71:LYS:O     | 4:C:118:SER:OG    | 2.12                     | 0.67              |
| 2:2:890:G:O2'    | 2:2:906:A:N6      | 2.27                     | 0.67              |
| 1:1:77:G:O3'     | 25:X:7:ARG:NH2    | 2.28                     | 0.67              |
| 54:z:71:5MU:C5'  | 54:z:71:5MU:C6    | 2.77                     | 0.67              |
| 2:2:1181:G:O2'   | 2:2:1182:G:N7     | 2.25                     | 0.67              |
| 2:2:1014:A:OP2   | 50:w:18:LYS:NZ    | 2.27                     | 0.67              |
| 54:z:15:A:O2'    | 54:z:16:U:OP1     | 2.13                     | 0.67              |
| 33:f:67:ILE:N    | 33:f:89:GLN:OE1   | 2.24                     | 0.67              |
| 39:l:74:SER:OG   | 39:l:130:ALA:HB3  | 1.95                     | 0.66              |
| 4:C:66:ASP:OD2   | 4:C:102:ARG:NH1   | 2.29                     | 0.66              |
| 11:J:1:MET:SD    | 11:J:67:LYS:NZ    | 2.68                     | 0.66              |
| 50:w:50:ALA:HB1  | 50:w:57:HIS:HB3   | 1.77                     | 0.66              |
| 1:1:500:G:N1     | 1:1:503:A:OP2     | 2.27                     | 0.66              |
| 1:1:1047:G:HO2'  | 1:1:1110:G:H1     | 1.37                     | 0.66              |
| 6:E:1:MET:HB3    | 6:E:14:VAL:HG23   | 1.77                     | 0.66              |
| 18:Q:38:VAL:HG13 | 18:Q:54:VAL:HB    | 1.76                     | 0.66              |
| 50:w:64:ASP:O    | 50:w:67:VAL:HG23  | 1.95                     | 0.66              |
| 1:1:517:C:OP2    | 28:a:10:ARG:NH2   | 2.28                     | 0.66              |
| 55:B:8:ILE:HB    | 55:B:22:THR:HG23  | 1.78                     | 0.66              |
| 1:1:102:U:O4     | 25:X:2:LYS:N      | 2.29                     | 0.66              |
| 5:D:151:THR:HG23 | 5:D:152:PRO:CD    | 2.16                     | 0.66              |
| 52:y:4:ILE:HD12  | 52:y:19:PHE:HD1   | 1.61                     | 0.66              |
| 9:H:125:THR:HA   | 9:H:146:VAL:HG13  | 1.78                     | 0.65              |
| 1:1:545:U:O2'    | 1:1:546:U:O3'     | 2.13                     | 0.65              |
| 1:1:2258:C:O2'   | 1:1:2427:C:OP2    | 2.14                     | 0.65              |
| 2:2:131:A:O2'    | 2:2:262:A:N3      | 2.27                     | 0.65              |
| 54:z:69:5MU:H3'  | 54:z:70:C:C5'     | 2.25                     | 0.65              |
| 1:1:1055:G:N1    | 1:1:1105:U:C4     | 2.64                     | 0.65              |
| 4:C:180:GLU:OE2  | 4:C:267:ILE:HD12  | 1.97                     | 0.65              |
| 50:w:36:ARG:NH2  | 50:w:72:GLY:O     | 2.29                     | 0.65              |
| 21:T:74:ASN:ND2  | 21:T:81:ASP:OD2   | 2.26                     | 0.65              |
| 38:k:67:GLU:OE1  | 38:k:70:ARG:NH1   | 2.29                     | 0.65              |
| 2:2:1305:G:H21   | 2:2:1332:A:H2     | 1.43                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 35:h:27:ALA:O    | 35:h:30:THR:OG1  | 2.11                     | 0.65              |
| 38:k:15:ASP:OD1  | 38:k:20:SER:N    | 2.30                     | 0.65              |
| 1:1:611:C:C2'    | 1:1:612:G:H5'    | 2.27                     | 0.65              |
| 9:H:121:VAL:HG11 | 9:H:123:ARG:CZ   | 2.26                     | 0.65              |
| 19:R:34:ASP:OD2  | 28:a:37:LYS:NZ   | 2.30                     | 0.65              |
| 37:j:35:LYS:C    | 37:j:36:ILE:HD13 | 2.21                     | 0.65              |
| 1:1:72:U:OP2     | 25:X:54:LYS:NZ   | 2.29                     | 0.64              |
| 1:1:714:U:OP2    | 46:s:88:ARG:NH1  | 2.30                     | 0.64              |
| 1:1:897:C:H2'    | 1:1:898:C:O4'    | 1.97                     | 0.64              |
| 40:m:12:ARG:HG3  | 40:m:13:LYS:H    | 1.62                     | 0.64              |
| 43:p:24:LEU:HD23 | 43:p:27:CYS:O    | 1.98                     | 0.64              |
| 1:1:2839:G:O2'   | 14:M:49:GLU:OE1  | 2.10                     | 0.64              |
| 54:z:70:C:H3'    | 54:z:71:5MU:H5'  | 1.80                     | 0.64              |
| 2:2:841:C:H2'    | 2:2:843:U:H5'    | 1.79                     | 0.64              |
| 2:2:1060:U:OP1   | 45:r:85:ARG:NH1  | 2.29                     | 0.64              |
| 2:2:1124:G:O2'   | 2:2:1145:A:N1    | 2.31                     | 0.64              |
| 1:1:2278:A:OP2   | 23:V:12:ASN:ND2  | 2.31                     | 0.64              |
| 11:J:71:ARG:NH2  | 11:J:123:LEU:O   | 2.30                     | 0.64              |
| 18:Q:51:VAL:HB   | 18:Q:52:PRO:HD3  | 1.78                     | 0.64              |
| 37:j:38:ARG:NH2  | 37:j:63:ASN:OD1  | 2.30                     | 0.64              |
| 45:r:47:LYS:O    | 45:r:50:THR:HG22 | 1.97                     | 0.64              |
| 1:1:743:A:O2'    | 1:1:1659:G:OP1   | 2.16                     | 0.64              |
| 15:N:28:VAL:HG12 | 15:N:93:ASP:O    | 1.97                     | 0.64              |
| 16:O:34:GLU:OE1  | 16:O:34:GLU:N    | 2.31                     | 0.64              |
| 29:b:29:THR:HG23 | 29:b:30:LYS:HG2  | 1.80                     | 0.64              |
| 39:l:11:LEU:HD22 | 39:l:75:ILE:HD11 | 1.80                     | 0.64              |
| 1:1:2220:U:H2'   | 1:1:2221:G:H8    | 1.63                     | 0.64              |
| 2:2:109:A:H5'    | 2:2:110:C:H5     | 1.63                     | 0.64              |
| 33:f:27:MET:HE1  | 33:f:187:VAL:CG1 | 2.28                     | 0.64              |
| 1:1:1069:A:N6    | 1:1:1096:A:OP1   | 2.31                     | 0.64              |
| 16:O:14:LYS:HE2  | 16:O:77:HIS:HA   | 1.79                     | 0.64              |
| 34:g:40:ARG:NH1  | 34:g:55:ILE:O    | 2.30                     | 0.64              |
| 43:p:68:GLY:O    | 43:p:99:ARG:NH1  | 2.31                     | 0.64              |
| 54:z:61:A:H5''   | 54:z:61:A:H8     | 1.62                     | 0.64              |
| 1:1:301:G:H4'    | 1:1:301:G:OP1    | 1.98                     | 0.63              |
| 2:2:405:U:O4     | 35:h:2:ALA:N     | 2.31                     | 0.63              |
| 33:f:49:MET:HE2  | 33:f:199:VAL:O   | 1.98                     | 0.63              |
| 1:1:511:U:H2'    | 1:1:512:G:H5'    | 1.79                     | 0.63              |
| 9:H:40:THR:OG1   | 9:H:43:ASN:OD1   | 2.13                     | 0.63              |
| 1:1:894:U:O2'    | 1:1:895:U:P      | 2.57                     | 0.63              |
| 38:k:60:GLU:O    | 38:k:64:VAL:HG23 | 1.98                     | 0.63              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:1:1378:A:O2'   | 1:1:1380:G:N7     | 2.32                     | 0.63              |
| 1:1:672:C:OP2    | 12:K:42:SER:OG    | 2.15                     | 0.63              |
| 2:2:1317:C:OP1   | 45:r:24:ARG:NH2   | 2.29                     | 0.63              |
| 17:P:74:ILE:HD11 | 17:P:78:LYS:HB3   | 1.80                     | 0.63              |
| 2:2:81:A:N6      | 2:2:87:C:C4       | 2.66                     | 0.63              |
| 1:1:2121:G:O6    | 1:1:2176:A:N6     | 2.32                     | 0.63              |
| 54:z:71:5MU:H6   | 54:z:71:5MU:C5'   | 2.11                     | 0.63              |
| 1:1:1020:A:N1    | 1:1:1141:U:O2'    | 2.25                     | 0.63              |
| 2:2:1145:A:O2'   | 2:2:1146:A:P      | 2.57                     | 0.63              |
| 13:L:49:ALA:HB1  | 13:L:120:ALA:HB1  | 1.81                     | 0.63              |
| 5:D:152:PRO:O    | 5:D:154:LYS:N     | 2.32                     | 0.62              |
| 38:k:115:SER:O   | 38:k:119:ARG:HD3  | 1.98                     | 0.62              |
| 41:n:10:LEU:HG   | 41:n:98:VAL:HG12  | 1.81                     | 0.62              |
| 52:y:31:GLU:OE2  | 52:y:34:ARG:NH2   | 2.31                     | 0.62              |
| 54:z:49:G:H2'    | 54:z:52:A:H61     | 1.64                     | 0.62              |
| 13:L:47:GLU:OE2  | 13:L:51:ARG:NE    | 2.29                     | 0.62              |
| 1:1:2194:U:H2'   | 1:1:2195:U:C6     | 2.34                     | 0.62              |
| 2:2:412:A:H62    | 2:2:431:A:H61     | 1.48                     | 0.62              |
| 14:M:56:LYS:NZ   | 14:M:94:TYR:OH    | 2.23                     | 0.62              |
| 50:w:3:ARG:NH1   | 50:w:9:PRO:O      | 2.31                     | 0.62              |
| 33:f:207:ILE:H   | 33:f:207:ILE:HD12 | 1.64                     | 0.62              |
| 36:i:46:VAL:O    | 36:i:72:ILE:N     | 2.28                     | 0.62              |
| 1:1:324:A:OP2    | 1:1:1205:A:N6     | 2.33                     | 0.62              |
| 1:1:636:G:N7     | 12:K:109:LYS:HE2  | 2.14                     | 0.62              |
| 1:1:1084:A:N3    | 1:1:1105:U:O2'    | 2.33                     | 0.62              |
| 8:G:38:ASN:HD22  | 8:G:64:GLN:HG3    | 1.64                     | 0.62              |
| 1:1:1901:A:OP2   | 4:C:253:LYS:NZ    | 2.32                     | 0.62              |
| 1:1:1915:3TD:H2' | 1:1:1916:A:O4'    | 2.00                     | 0.62              |
| 1:1:2102:G:O6    | 1:1:2187:U:O4     | 2.17                     | 0.62              |
| 1:1:2521:C:O2'   | 1:1:2564:A:N3     | 2.32                     | 0.62              |
| 35:h:50:ASP:OD1  | 35:h:51:TYR:N     | 2.33                     | 0.62              |
| 8:G:2:SER:OG     | 8:G:3:ARG:N       | 2.27                     | 0.62              |
| 1:1:1754:A:O3'   | 16:O:103:ARG:NH2  | 2.31                     | 0.62              |
| 1:1:2831:G:N2    | 1:1:2884:U:OP2    | 2.32                     | 0.62              |
| 5:D:17:GLU:OE1   | 5:D:17:GLU:N      | 2.32                     | 0.62              |
| 23:V:37:ILE:HG22 | 23:V:38:VAL:HG23  | 1.81                     | 0.62              |
| 40:m:42:GLU:OE2  | 40:m:45:ARG:NH1   | 2.33                     | 0.62              |
| 1:1:1324:G:OP1   | 1:1:1324:G:H4'    | 1.99                     | 0.62              |
| 21:T:4:LYS:O     | 21:T:94:ARG:NH2   | 2.33                     | 0.62              |
| 1:1:1869:G:N2    | 1:1:1871:A:O2'    | 2.33                     | 0.61              |
| 7:F:95:ARG:NH1   | 27:Z:1:MET:SD     | 2.72                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 54:z:70:C:H5''   | 54:z:70:C:C6     | 2.34                     | 0.61              |
| 1:1:1042:G:O2'   | 1:1:1043:C:H5''  | 2.00                     | 0.61              |
| 2:2:1003:G:N2    | 2:2:1004:A:O2'   | 2.32                     | 0.61              |
| 38:k:116:MET:HA  | 38:k:119:ARG:HE  | 1.66                     | 0.61              |
| 44:q:16:VAL:HG23 | 44:q:17:ILE:HD12 | 1.82                     | 0.61              |
| 2:2:71:A:H61     | 2:2:99:C:H1'     | 1.65                     | 0.61              |
| 26:Y:45:ARG:NH1  | 26:Y:59:GLU:OE1  | 2.33                     | 0.61              |
| 2:2:1193:G:O6    | 34:g:3:GLN:NE2   | 2.34                     | 0.61              |
| 2:2:1320:C:N3    | 50:w:36:ARG:NH1  | 2.48                     | 0.61              |
| 13:L:47:GLU:OE2  | 13:L:50:ARG:NH1  | 2.34                     | 0.61              |
| 14:M:114:GLU:OE1 | 14:M:118:ARG:NH1 | 2.33                     | 0.61              |
| 2:2:1261:A:N6    | 2:2:1274:A:O2'   | 2.34                     | 0.61              |
| 45:r:42:TRP:O    | 45:r:46:LEU:HD23 | 2.01                     | 0.60              |
| 52:y:13:ASP:N    | 52:y:13:ASP:OD1  | 2.34                     | 0.60              |
| 1:1:1754:A:O2'   | 16:O:103:ARG:NH2 | 2.34                     | 0.60              |
| 11:J:80:ASP:N    | 16:O:68:GLU:OE1  | 2.31                     | 0.60              |
| 17:P:50:ARG:O    | 17:P:54:LYS:NZ   | 2.34                     | 0.60              |
| 1:1:792:A:N3     | 1:1:2072:C:O2'   | 2.31                     | 0.60              |
| 24:W:72:ARG:NH1  | 24:W:78:TYR:OH   | 2.28                     | 0.60              |
| 10:I:114:LEU:HG  | 10:I:118:MET:HE3 | 1.83                     | 0.60              |
| 35:h:124:MET:HE3 | 35:h:146:ARG:HG3 | 1.83                     | 0.60              |
| 43:p:48:ALA:C    | 43:p:49:LEU:HD12 | 2.26                     | 0.60              |
| 1:1:894:U:O2'    | 1:1:895:U:OP1    | 2.18                     | 0.60              |
| 1:1:2655:G:O2'   | 1:1:2664:G:O6    | 2.17                     | 0.60              |
| 55:B:13:ASN:OD1  | 55:B:15:ASP:CG   | 2.45                     | 0.60              |
| 2:2:1073:U:O2    | 33:f:103:ASN:ND2 | 2.35                     | 0.60              |
| 39:l:77:ARG:NE   | 39:l:79:SER:O    | 2.34                     | 0.60              |
| 47:t:18:GLN:OE1  | 47:t:35:ARG:NE   | 2.27                     | 0.60              |
| 55:B:7:GLY:HA2   | 55:B:25:ASP:H    | 1.67                     | 0.60              |
| 55:B:10:LYS:H    | 55:B:22:THR:H    | 1.49                     | 0.60              |
| 8:G:86:LYS:HG2   | 8:G:132:VAL:HG22 | 1.84                     | 0.60              |
| 21:T:36:VAL:HG11 | 21:T:39:ILE:HD12 | 1.82                     | 0.60              |
| 1:1:891:G:O2'    | 1:1:892:A:P      | 2.60                     | 0.60              |
| 1:1:2142:A:N6    | 1:1:2150:C:N3    | 2.49                     | 0.60              |
| 1:1:2168:G:H2'   | 1:1:2168:G:N3    | 2.17                     | 0.60              |
| 40:m:130:ARG:NH1 | 54:z:34:U:OP2    | 2.30                     | 0.60              |
| 9:H:77:THR:HA    | 9:H:143:ILE:O    | 2.02                     | 0.60              |
| 38:k:66:LEU:HD21 | 38:k:97:ASN:OD1  | 2.01                     | 0.60              |
| 2:2:1217:C:OP2   | 45:r:9:ARG:NH2   | 2.34                     | 0.60              |
| 37:j:5:GLU:OE2   | 49:v:24:LYS:NZ   | 2.35                     | 0.60              |
| 55:B:22:THR:O    | 55:B:24:ASP:N    | 2.31                     | 0.60              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 4:C:125:LYS:HG2   | 4:C:128:ASN:OD1  | 2.02                     | 0.59              |
| 10:I:19:ASP:OD1   | 10:I:58:ASN:ND2  | 2.33                     | 0.59              |
| 21:T:38:GLY:N     | 21:T:62:GLU:OE2  | 2.33                     | 0.59              |
| 30:c:24:THR:HG23  | 30:c:27:GLY:H    | 1.67                     | 0.59              |
| 1:1:138:U:O2'     | 1:1:139:U:O2     | 2.16                     | 0.59              |
| 2:2:842:U:O2'     | 2:2:844:G:N2     | 2.35                     | 0.59              |
| 33:f:153:ASP:OD1  | 33:f:153:ASP:N   | 2.35                     | 0.59              |
| 44:q:4:ILE:HG12   | 44:q:9:ILE:HD12  | 1.83                     | 0.59              |
| 47:t:34:GLU:OE1   | 47:t:60:TRP:NE1  | 2.34                     | 0.59              |
| 48:u:48:ASP:CG    | 48:u:75:LEU:HD21 | 2.27                     | 0.59              |
| 1:1:570:G:OP1     | 1:1:972:A:O2'    | 2.17                     | 0.59              |
| 1:1:1055:G:N1     | 1:1:1105:U:N3    | 2.51                     | 0.59              |
| 1:1:2880:C:O3'    | 14:M:90:ARG:NH2  | 2.36                     | 0.59              |
| 34:g:16:LYS:NZ    | 34:g:181:ASP:OD1 | 2.26                     | 0.59              |
| 2:2:673:A:H2'     | 2:2:674:G:C8     | 2.37                     | 0.59              |
| 8:G:10:VAL:HA     | 8:G:49:THR:HG22  | 1.83                     | 0.59              |
| 22:U:75:GLN:HB2   | 22:U:92:VAL:HG23 | 1.85                     | 0.59              |
| 1:1:2445:2MG:OP1  | 6:E:69:ARG:NH1   | 2.28                     | 0.59              |
| 27:Z:57:VAL:HG23  | 50:w:64:ASP:OD1  | 2.02                     | 0.59              |
| 13:L:7:THR:OG1    | 13:L:9:PHE:O     | 2.16                     | 0.59              |
| 7:F:134:GLU:CG    | 7:F:136:ILE:HD12 | 2.32                     | 0.59              |
| 45:r:33:ASP:OD1   | 45:r:33:ASP:O    | 2.21                     | 0.59              |
| 2:2:1152:A:OP1    | 41:n:70:HIS:ND1  | 2.35                     | 0.58              |
| 5:D:151:THR:CG2   | 5:D:152:PRO:HD3  | 2.17                     | 0.58              |
| 9:H:89:LYS:C      | 9:H:91:PHE:H     | 2.11                     | 0.58              |
| 41:n:7:ARG:HB2    | 41:n:101:SER:OG  | 2.02                     | 0.58              |
| 42:o:19:GLY:C     | 42:o:82:LEU:HD12 | 2.28                     | 0.58              |
| 1:1:534:U:O2'     | 17:P:49:ASP:OD2  | 2.18                     | 0.58              |
| 1:1:2316:G:H2'    | 1:1:2317:A:H8    | 1.69                     | 0.58              |
| 11:J:110:GLU:N    | 11:J:110:GLU:OE2 | 2.36                     | 0.58              |
| 1:1:811:U:H2'     | 12:K:21:ARG:HA   | 1.84                     | 0.58              |
| 1:1:2848:G:O2'    | 1:1:2867:G:N2    | 2.33                     | 0.58              |
| 2:2:454:G:H1      | 2:2:478:A:H61    | 1.51                     | 0.58              |
| 2:2:1147:C:HO2'   | 40:m:7:TYR:HH    | 1.48                     | 0.58              |
| 11:J:76:VAL:HG12  | 16:O:73:VAL:HB   | 1.85                     | 0.58              |
| 1:1:1019:U:OP1    | 1:1:1035:U:O2'   | 2.21                     | 0.58              |
| 2:2:1168:U:H3'    | 2:2:1169:A:H5'   | 1.86                     | 0.58              |
| 9:H:64:ALA:O      | 9:H:68:ARG:HG3   | 2.03                     | 0.58              |
| 33:f:173:ILE:HG22 | 33:f:177:ASN:OD1 | 2.03                     | 0.58              |
| 1:1:514:A:N3      | 1:1:581:C:O2'    | 2.34                     | 0.58              |
| 1:1:2052:A:O2'    | 5:D:148:GLN:O    | 2.18                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:1:2134:A:O2'   | 1:1:2159:G:O2'   | 2.11                     | 0.58              |
| 5:D:33:ARG:NH1   | 5:D:53:GLY:O     | 2.35                     | 0.58              |
| 6:E:6:LYS:O      | 6:E:9:GLN:NE2    | 2.35                     | 0.58              |
| 9:H:51:ARG:HA    | 9:H:54:LEU:HG    | 1.84                     | 0.58              |
| 27:Z:48:GLN:N    | 27:Z:48:GLN:OE1  | 2.36                     | 0.58              |
| 41:n:42:LEU:HB2  | 41:n:71:LEU:HB3  | 1.86                     | 0.58              |
| 46:s:78:TYR:OH   | 46:s:89:ARG:O    | 2.14                     | 0.58              |
| 44:q:81:MET:SD   | 44:q:92:ARG:HB3  | 2.44                     | 0.58              |
| 1:1:63:A:C2      | 55:B:22:THR:HG21 | 2.39                     | 0.58              |
| 1:1:611:C:H2'    | 1:1:612:G:H5'    | 1.84                     | 0.58              |
| 41:n:90:LEU:HD23 | 41:n:91:ASP:N    | 2.19                     | 0.58              |
| 2:2:1297:G:O2'   | 38:k:114:LYS:NZ  | 2.37                     | 0.57              |
| 38:k:24:ALA:HA   | 38:k:27:VAL:HG22 | 1.85                     | 0.57              |
| 1:1:2780:G:OP2   | 10:I:120:ARG:NE  | 2.31                     | 0.57              |
| 2:2:662:U:O2'    | 2:2:836:G:OP1    | 2.21                     | 0.57              |
| 1:1:1068:G:HO2'  | 1:1:1070:A:N6    | 2.00                     | 0.57              |
| 1:1:2148:G:C2    | 1:1:2149:U:O4    | 2.57                     | 0.57              |
| 1:1:2469:A:N6    | 1:1:2481:G:O2'   | 2.37                     | 0.57              |
| 10:I:7:LYS:HB2   | 10:I:10:THR:HG22 | 1.85                     | 0.57              |
| 15:N:27:VAL:HG21 | 15:N:40:ILE:HD12 | 1.85                     | 0.57              |
| 20:S:65:GLY:N    | 20:S:79:ASP:OD1  | 2.35                     | 0.57              |
| 1:1:1936:A:OP2   | 1:1:1962:5MC:N4  | 2.36                     | 0.57              |
| 1:1:2185:U:H2'   | 1:1:2186:G:C8    | 2.39                     | 0.57              |
| 7:F:45:ALA:O     | 7:F:46:ASP:OD1   | 2.22                     | 0.57              |
| 1:1:219:A:N3     | 1:1:234:U:O2'    | 2.37                     | 0.57              |
| 2:2:1340:A:O2'   | 54:z:32:A:O2'    | 2.14                     | 0.57              |
| 21:T:7:ARG:O     | 21:T:25:VAL:HB   | 2.03                     | 0.57              |
| 27:Z:44:PHE:CD2  | 27:Z:45:THR:HG23 | 2.39                     | 0.57              |
| 38:k:105:VAL:O   | 38:k:109:ARG:HG2 | 2.04                     | 0.57              |
| 54:z:21:A:O2'    | 54:z:22:G:O5'    | 2.16                     | 0.57              |
| 34:g:24:ALA:HB1  | 34:g:28:GLU:HG2  | 1.87                     | 0.57              |
| 1:1:79:C:O2'     | 1:1:346:A:N3     | 2.32                     | 0.56              |
| 1:1:85:G:OP2     | 21:T:7:ARG:HB2   | 2.04                     | 0.56              |
| 1:1:280:U:O4     | 1:1:361:G:N2     | 2.38                     | 0.56              |
| 1:1:1028:A:N3    | 1:1:2486:C:O2'   | 2.30                     | 0.56              |
| 1:1:1335:C:O2'   | 55:B:6:THR:CB    | 2.53                     | 0.56              |
| 46:s:21:ASP:OD1  | 46:s:22:THR:N    | 2.37                     | 0.56              |
| 1:1:2477:U:O2    | 32:e:4:ARG:NH2   | 2.37                     | 0.56              |
| 2:2:844:G:N1     | 2:2:846:G:H1'    | 2.20                     | 0.56              |
| 33:f:50:PHE:CE2  | 33:f:54:LEU:HD11 | 2.39                     | 0.56              |
| 1:1:1335:C:O2'   | 55:B:6:THR:CA    | 2.53                     | 0.56              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:1:2314:A:OP1   | 7:F:88:LYS:NZ     | 2.39                     | 0.56              |
| 2:2:1255:G:OP2   | 41:n:45:ARG:NH1   | 2.38                     | 0.56              |
| 9:H:15:LEU:HD23  | 9:H:16:GLY:N      | 2.21                     | 0.56              |
| 9:H:58:LEU:HA    | 9:H:61:VAL:HG12   | 1.87                     | 0.56              |
| 14:M:47:VAL:O    | 14:M:51:LEU:HD23  | 2.05                     | 0.56              |
| 37:j:40:GLU:OE1  | 37:j:100:SER:OG   | 2.16                     | 0.56              |
| 43:p:50:ARG:HG3  | 43:p:90:LEU:HD21  | 1.88                     | 0.56              |
| 18:Q:5:PHE:HE1   | 18:Q:14:VAL:HG11  | 1.70                     | 0.56              |
| 34:g:155:GLY:O   | 34:g:196:ILE:HG12 | 2.05                     | 0.56              |
| 43:p:99:ARG:NE   | 43:p:104:CYS:SG   | 2.78                     | 0.56              |
| 1:1:307:G:N1     | 1:1:310:A:OP2     | 2.33                     | 0.56              |
| 1:1:1056:G:O2'   | 1:1:1103:A:N6     | 2.39                     | 0.56              |
| 1:1:1266:G:OP2   | 28:a:17:ARG:NE    | 2.34                     | 0.56              |
| 1:1:1664:A:H2    | 11:J:1:MET:HE1    | 1.70                     | 0.56              |
| 22:U:36:ALA:O    | 22:U:93:ARG:NH2   | 2.36                     | 0.56              |
| 26:Y:23:THR:HG23 | 26:Y:47:MET:HG2   | 1.88                     | 0.56              |
| 41:n:26:VAL:HG13 | 41:n:36:VAL:HG21  | 1.88                     | 0.56              |
| 51:x:37:ALA:O    | 51:x:40:GLU:HG3   | 2.06                     | 0.56              |
| 1:1:2808:G:O2'   | 1:1:2890:G:O6     | 2.23                     | 0.56              |
| 2:2:521:G:N7     | 43:p:50:ARG:NH2   | 2.53                     | 0.56              |
| 9:H:58:LEU:O     | 9:H:62:LEU:HG     | 2.06                     | 0.56              |
| 46:s:2:SER:OG    | 46:s:3:LEU:N      | 2.39                     | 0.56              |
| 2:2:1004:A:H2'   | 2:2:1005:A:O4'    | 2.05                     | 0.56              |
| 16:O:71:GLU:OE2  | 16:O:101:ARG:NE   | 2.38                     | 0.56              |
| 41:n:39:PRO:HA   | 41:n:74:VAL:HG22  | 1.88                     | 0.56              |
| 7:F:149:VAL:HG23 | 7:F:149:VAL:O     | 2.05                     | 0.56              |
| 9:H:4:ILE:HD12   | 9:H:17:ASP:C      | 2.31                     | 0.56              |
| 12:K:132:ARG:HG3 | 12:K:142:ILE:HD12 | 1.87                     | 0.56              |
| 33:f:27:MET:HE1  | 33:f:187:VAL:HG11 | 1.86                     | 0.56              |
| 48:u:15:ASP:OD1  | 48:u:55:ILE:HD11  | 2.06                     | 0.56              |
| 1:1:396:G:OP2    | 24:W:10:LYS:NZ    | 2.39                     | 0.56              |
| 1:1:1779:U:H5    | 1:1:1784:A:N7     | 2.04                     | 0.56              |
| 6:E:32:VAL:HG13  | 6:E:178:VAL:HG12  | 1.88                     | 0.56              |
| 15:N:15:ARG:NH2  | 15:N:95:SER:OG    | 2.38                     | 0.56              |
| 39:l:48:ASP:OD1  | 39:l:49:PHE:N     | 2.39                     | 0.56              |
| 33:f:93:ASN:OD1  | 33:f:94:HIS:N     | 2.38                     | 0.55              |
| 1:1:2249:U:N3    | 1:1:2253:G:OP2    | 2.37                     | 0.55              |
| 2:2:910:C:OP2    | 43:p:18:LYS:NZ    | 2.40                     | 0.55              |
| 3:3:41:G:O6      | 7:F:69:LYS:NZ     | 2.34                     | 0.55              |
| 33:f:97:LEU:H    | 33:f:100:MET:HE3  | 1.71                     | 0.55              |
| 1:1:2523:G:HO2'  | 1:1:2764:A:HO2'   | 1.54                     | 0.55              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:2:496:A:H2'    | 2:2:496:A:N3      | 2.22                     | 0.55              |
| 2:2:1176:A:H2'   | 2:2:1177:G:C8     | 2.42                     | 0.55              |
| 27:Z:16:CYS:SG   | 27:Z:17:SER:N     | 2.79                     | 0.55              |
| 43:p:114:ARG:CG  | 43:p:119:VAL:HB   | 2.36                     | 0.55              |
| 1:1:2189:U:H1'   | 1:1:2190:G:C8     | 2.41                     | 0.55              |
| 2:2:1360:A:OP2   | 45:r:75:ARG:NH2   | 2.38                     | 0.55              |
| 21:T:79:LYS:HG2  | 21:T:80:ALA:H     | 1.72                     | 0.55              |
| 36:i:39:VAL:HG12 | 36:i:40:GLY:N     | 2.21                     | 0.55              |
| 1:1:1056:G:HO2'  | 1:1:1103:A:H61    | 1.53                     | 0.55              |
| 1:1:2159:G:H2'   | 1:1:2160:C:C6     | 2.41                     | 0.55              |
| 6:E:150:THR:HG22 | 6:E:152:GLU:H     | 1.72                     | 0.55              |
| 7:F:8:TYR:OH     | 7:F:29:PRO:O      | 2.24                     | 0.55              |
| 8:G:159:GLY:O    | 8:G:163:ARG:NH1   | 2.35                     | 0.55              |
| 34:g:118:ASP:OD1 | 34:g:119:SER:N    | 2.40                     | 0.55              |
| 1:1:599:A:O2'    | 1:1:600:G:H5'     | 2.07                     | 0.55              |
| 1:1:1584:U:H5'   | 1:1:1585:C:C6     | 2.42                     | 0.55              |
| 2:2:410:G:OP2    | 35:h:31:LYS:NZ    | 2.33                     | 0.55              |
| 1:1:1055:G:C6    | 1:1:1105:U:C4     | 2.95                     | 0.55              |
| 2:2:464:U:N3     | 2:2:467:U:OP2     | 2.33                     | 0.55              |
| 2:2:1141:C:HO2'  | 2:2:1142:G:H8     | 1.54                     | 0.55              |
| 15:N:4:LYS:HZ3   | 15:N:8:ILE:HD11   | 1.70                     | 0.55              |
| 18:Q:52:PRO:HD2  | 18:Q:53:PHE:H     | 1.71                     | 0.55              |
| 36:i:55:GLU:HG3  | 36:i:57:PRO:HD2   | 1.88                     | 0.55              |
| 41:n:52:LEU:O    | 45:r:81:ARG:NH1   | 2.40                     | 0.55              |
| 49:v:26:ILE:HG23 | 49:v:68:LEU:HD21  | 1.88                     | 0.55              |
| 19:R:86:MET:SD   | 19:R:87:PRO:HD2   | 2.47                     | 0.55              |
| 37:j:1:MET:N     | 37:j:1:MET:SD     | 2.80                     | 0.55              |
| 1:1:12:U:H2'     | 1:1:13:A:H5'      | 1.88                     | 0.55              |
| 2:2:542:G:O3'    | 35:h:14:ARG:NH2   | 2.37                     | 0.55              |
| 2:2:999:C:N3     | 2:2:1042:A:N6     | 2.54                     | 0.55              |
| 9:H:15:LEU:HD23  | 9:H:15:LEU:C      | 2.31                     | 0.55              |
| 9:H:96:THR:HG22  | 9:H:117:LEU:CD1   | 2.37                     | 0.55              |
| 33:f:23:TRP:CZ3  | 33:f:25:PRO:HA    | 2.42                     | 0.55              |
| 1:1:301:G:OP2    | 21:T:82:ARG:NH1   | 2.40                     | 0.55              |
| 1:1:2503:2MA:O2' | 1:1:2505:G:OP2    | 2.25                     | 0.55              |
| 5:D:34:VAL:HB    | 5:D:92:VAL:O      | 2.07                     | 0.55              |
| 19:R:13:SER:O    | 19:R:17:VAL:HG23  | 2.06                     | 0.55              |
| 36:i:154:ALA:HA  | 36:i:164:ILE:HD11 | 1.89                     | 0.55              |
| 54:z:56:G:N3     | 54:z:56:G:H2'     | 2.22                     | 0.55              |
| 1:1:2102:G:C2    | 1:1:2188:U:C2     | 2.95                     | 0.54              |
| 2:2:911:U:OP2    | 43:p:94:ARG:NH2   | 2.40                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1:1383:A:N3     | 1:1:1405:U:O2'    | 2.37                     | 0.54              |
| 1:1:2126:A:C6     | 1:1:2171:A:OP2    | 2.60                     | 0.54              |
| 7:F:140:GLU:OE1   | 27:Z:27:THR:OG1   | 2.19                     | 0.54              |
| 18:Q:52:PRO:O     | 18:Q:53:PHE:CG    | 2.61                     | 0.54              |
| 1:1:1447:C:O2'    | 1:1:1544:A:N3     | 2.37                     | 0.54              |
| 2:2:677:U:H3      | 2:2:713:G:H22     | 1.54                     | 0.54              |
| 23:V:4:LYS:O      | 23:V:6:ALA:N      | 2.41                     | 0.54              |
| 1:1:573:U:O2'     | 1:1:575:A:OP1     | 2.22                     | 0.54              |
| 2:2:675:A:H1'     | 42:o:118:HIS:CD2  | 2.42                     | 0.54              |
| 45:r:59:ARG:HG3   | 45:r:59:ARG:O     | 2.08                     | 0.54              |
| 1:1:810:U:N3      | 12:K:29:LYS:O     | 2.40                     | 0.54              |
| 12:K:77:ILE:HD11  | 12:K:108:ALA:HB1  | 1.88                     | 0.54              |
| 35:h:107:PHE:HB3  | 35:h:145:ILE:HD11 | 1.89                     | 0.54              |
| 1:1:2266:A:N6     | 1:1:2273:A:OP2    | 2.41                     | 0.54              |
| 2:2:35:G:N3       | 43:p:115:SER:OG   | 2.40                     | 0.54              |
| 2:2:842:U:O3'     | 2:2:844:G:N2      | 2.40                     | 0.54              |
| 7:F:34:ILE:HD12   | 7:F:96:MET:HG3    | 1.88                     | 0.54              |
| 39:l:74:SER:HG    | 39:l:130:ALA:HB3  | 1.73                     | 0.54              |
| 1:1:1364:G:N2     | 1:1:1367:A:OP2    | 2.31                     | 0.54              |
| 1:1:2220:U:H2'    | 1:1:2221:G:C8     | 2.43                     | 0.54              |
| 18:Q:52:PRO:CD    | 18:Q:53:PHE:H     | 2.21                     | 0.54              |
| 55:B:27:GLY:O     | 55:B:31:PHE:N     | 2.39                     | 0.54              |
| 1:1:1870:C:H2'    | 1:1:1871:A:C8     | 2.42                     | 0.54              |
| 21:T:94:ARG:HB3   | 21:T:103:ILE:HD12 | 1.90                     | 0.54              |
| 1:1:2277:G:OP2    | 23:V:10:THR:OG1   | 2.22                     | 0.54              |
| 5:D:181:ASP:OD2   | 5:D:184:ARG:NH2   | 2.37                     | 0.54              |
| 40:m:25:ASN:O     | 40:m:25:ASN:ND2   | 2.36                     | 0.54              |
| 43:p:114:ARG:HG2  | 43:p:119:VAL:HB   | 1.89                     | 0.54              |
| 1:1:1156:A:C8     | 17:P:51:ARG:HG2   | 2.43                     | 0.54              |
| 1:1:2788:C:O2'    | 1:1:2809:A:N3     | 2.35                     | 0.54              |
| 2:2:86:G:H1'      | 2:2:87:C:O4'      | 2.08                     | 0.54              |
| 2:2:1519:MA6:O5'  | 2:2:1519:MA6:H8   | 2.06                     | 0.54              |
| 19:R:85:ILE:HD13  | 55:B:42:TYR:HA    | 1.90                     | 0.54              |
| 54:z:63:5MU:C6    | 54:z:63:5MU:C3'   | 2.89                     | 0.54              |
| 2:2:770:C:O2'     | 2:2:899:C:N3      | 2.38                     | 0.53              |
| 6:E:125:SER:O     | 6:E:137:LYS:NZ    | 2.42                     | 0.53              |
| 15:N:70:ALA:O     | 15:N:74:VAL:HG23  | 2.07                     | 0.53              |
| 36:i:115:LEU:HD13 | 36:i:123:VAL:HG21 | 1.90                     | 0.53              |
| 46:s:4:SER:O      | 46:s:8:THR:HG23   | 2.08                     | 0.53              |
| 55:B:10:LYS:H     | 55:B:21:ILE:HA    | 1.72                     | 0.53              |
| 41:n:83:THR:O     | 41:n:87:LEU:HG    | 2.07                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 41:n:84:VAL:HG13  | 41:n:85:ASP:N     | 2.22                     | 0.53              |
| 47:t:19:VAL:HG22  | 47:t:37:GLY:C     | 2.34                     | 0.53              |
| 50:w:40:ILE:HD12  | 50:w:66:MET:O     | 2.07                     | 0.53              |
| 1:1:1827:U:OP2    | 4:C:221:ARG:NE    | 2.41                     | 0.53              |
| 1:1:2101:A:N6     | 1:1:2189:U:N3     | 2.56                     | 0.53              |
| 1:1:2753:A:H2'    | 1:1:2754:U:C6     | 2.44                     | 0.53              |
| 2:2:1314:C:OP1    | 50:w:6:LYS:NZ     | 2.29                     | 0.53              |
| 1:1:2103:C:N4     | 1:1:2186:G:O6     | 2.42                     | 0.53              |
| 1:1:2880:C:O2'    | 14:M:90:ARG:NH2   | 2.30                     | 0.53              |
| 9:H:74:ALA:O      | 9:H:76:GLU:OE1    | 2.27                     | 0.53              |
| 39:l:90:ASP:OD1   | 39:l:90:ASP:N     | 2.34                     | 0.53              |
| 52:y:9:ASN:OD1    | 52:y:9:ASN:O      | 2.27                     | 0.53              |
| 2:2:109:A:H5'     | 2:2:110:C:C5      | 2.42                     | 0.53              |
| 34:g:129:MET:SD   | 34:g:132:ARG:NH1  | 2.82                     | 0.53              |
| 2:2:439:U:O2      | 35:h:120:HIS:CD2  | 2.61                     | 0.53              |
| 2:2:545:C:OP1     | 35:h:58:LYS:NZ    | 2.41                     | 0.53              |
| 2:2:1319:A:O2'    | 2:2:1323:G:N7     | 2.36                     | 0.53              |
| 27:Z:66:ILE:O     | 27:Z:66:ILE:HG22  | 2.08                     | 0.53              |
| 34:g:123:GLN:HB3  | 34:g:128:VAL:HG21 | 1.89                     | 0.53              |
| 40:m:118:LEU:HD12 | 40:m:118:LEU:N    | 2.24                     | 0.53              |
| 1:1:402:A:H2'     | 1:1:403:U:H5'     | 1.90                     | 0.53              |
| 9:H:94:ILE:HG13   | 9:H:94:ILE:O      | 2.07                     | 0.53              |
| 15:N:4:LYS:HZ2    | 15:N:8:ILE:HD11   | 1.70                     | 0.53              |
| 41:n:93:ALA:O     | 41:n:96:VAL:HG22  | 2.09                     | 0.53              |
| 1:1:1336:A:OP1    | 55:B:8:ILE:HG12   | 2.09                     | 0.53              |
| 2:2:1043:G:H2'    | 2:2:1044:A:C8     | 2.44                     | 0.53              |
| 7:F:47:LYS:HE2    | 7:F:47:LYS:HA     | 1.90                     | 0.53              |
| 43:p:4:VAL:O      | 43:p:8:VAL:HG23   | 2.08                     | 0.53              |
| 54:z:19:G:C4'     | 54:z:20:5MU:OP2   | 2.57                     | 0.53              |
| 1:1:1328:A:H2'    | 1:1:1330:C:C5     | 2.43                     | 0.53              |
| 22:U:56:PHE:CE1   | 22:U:61:LEU:HD21  | 2.44                     | 0.53              |
| 52:y:8:GLU:O      | 52:y:9:ASN:OD1    | 2.25                     | 0.53              |
| 55:B:8:ILE:O      | 55:B:22:THR:HG22  | 2.09                     | 0.53              |
| 1:1:1045:C:O2     | 1:1:1047:G:N1     | 2.41                     | 0.52              |
| 2:2:1239:A:H62    | 2:2:1299:A:N6     | 2.07                     | 0.52              |
| 46:s:21:ASP:O     | 46:s:22:THR:HG22  | 2.09                     | 0.52              |
| 54:z:49:G:C2'     | 54:z:52:A:H61     | 2.22                     | 0.52              |
| 2:2:878:A:OP1     | 39:l:80:ARG:NH1   | 2.40                     | 0.52              |
| 2:2:1152:A:P      | 41:n:72:ARG:HH22  | 2.32                     | 0.52              |
| 4:C:107:PRO:HD2   | 4:C:110:LEU:HD22  | 1.91                     | 0.52              |
| 7:F:136:ILE:O     | 7:F:136:ILE:HG22  | 2.08                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 9:H:96:THR:HG22  | 9:H:117:LEU:HD11 | 1.91                     | 0.52              |
| 37:j:62:MET:HG2  | 37:j:64:VAL:HG23 | 1.90                     | 0.52              |
| 43:p:48:ALA:O    | 43:p:49:LEU:HD12 | 2.09                     | 0.52              |
| 55:B:8:ILE:O     | 55:B:21:ILE:HG23 | 2.08                     | 0.52              |
| 1:1:287:G:H2'    | 1:1:288:U:C6     | 2.44                     | 0.52              |
| 2:2:1316:G:N1    | 2:2:1319:A:OP2   | 2.42                     | 0.52              |
| 2:2:1328:C:O2'   | 44:q:29:ARG:NH1  | 2.35                     | 0.52              |
| 14:M:114:GLU:OE1 | 14:M:118:ARG:NE  | 2.42                     | 0.52              |
| 34:g:10:ILE:HG23 | 34:g:11:ARG:HD2  | 1.90                     | 0.52              |
| 45:r:30:ILE:O    | 45:r:33:ASP:OD1  | 2.27                     | 0.52              |
| 1:1:1056:G:O2'   | 1:1:1086:A:O2'   | 2.12                     | 0.52              |
| 1:1:2145:C:O2    | 1:1:2145:C:C2'   | 2.56                     | 0.52              |
| 34:g:47:LEU:HD23 | 34:g:76:VAL:HG11 | 1.92                     | 0.52              |
| 55:B:11:TRP:CZ2  | 55:B:20:PHE:HB2  | 2.44                     | 0.52              |
| 1:1:784:G:O2'    | 1:1:785:G:O5'    | 2.26                     | 0.52              |
| 1:1:1582:C:O2'   | 1:1:1585:C:N3    | 2.29                     | 0.52              |
| 1:1:2144:G:N2    | 1:1:2148:G:C6    | 2.77                     | 0.52              |
| 2:2:80:A:H2'     | 2:2:81:A:C8      | 2.44                     | 0.52              |
| 2:2:1309:G:OP2   | 44:q:98:ARG:NH2  | 2.39                     | 0.52              |
| 33:f:133:GLU:O   | 33:f:137:ARG:HG2 | 2.10                     | 0.52              |
| 36:i:56:VAL:HB   | 36:i:57:PRO:HD3  | 1.91                     | 0.52              |
| 41:n:52:LEU:HD23 | 41:n:62:ARG:HG2  | 1.91                     | 0.52              |
| 1:1:2163:A:OP1   | 1:1:2170:A:O2'   | 2.28                     | 0.52              |
| 9:H:67:ALA:O     | 9:H:71:LYS:CD    | 2.58                     | 0.52              |
| 23:V:26:PHE:N    | 23:V:29:GLU:OE1  | 2.40                     | 0.52              |
| 41:n:15:HIS:HA   | 41:n:18:ILE:HG22 | 1.90                     | 0.52              |
| 44:q:29:ARG:O    | 44:q:33:ILE:HG12 | 2.10                     | 0.52              |
| 1:1:11:C:H2'     | 1:1:12:U:H5'     | 1.92                     | 0.52              |
| 1:1:84:A:N1      | 1:1:98:G:O2'     | 2.41                     | 0.52              |
| 1:1:2294:G:OP1   | 15:N:10:ARG:HD3  | 2.10                     | 0.52              |
| 2:2:279:A:H5''   | 2:2:280:C:H3'    | 1.90                     | 0.52              |
| 2:2:559:A:H4'    | 2:2:560:A:H3'    | 1.92                     | 0.52              |
| 9:H:115:VAL:HG12 | 9:H:117:LEU:HD11 | 1.91                     | 0.52              |
| 21:T:15:THR:OG1  | 21:T:69:ASN:OD1  | 2.27                     | 0.52              |
| 40:m:52:LEU:O    | 40:m:58:VAL:HG23 | 2.10                     | 0.52              |
| 8:G:46:ALA:O     | 8:G:47:ASP:OD1   | 2.26                     | 0.52              |
| 1:1:355:U:H2'    | 1:1:356:G:H8     | 1.75                     | 0.52              |
| 1:1:1084:A:C2    | 1:1:1106:G:O4'   | 2.63                     | 0.52              |
| 1:1:2375:G:N2    | 1:1:2378:A:OP2   | 2.34                     | 0.52              |
| 15:N:33:ARG:O    | 15:N:65:THR:OG1  | 2.26                     | 0.52              |
| 16:O:90:GLY:O    | 16:O:113:ARG:NH1 | 2.38                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 54:z:61:A:H5''   | 54:z:61:A:C8     | 2.44                     | 0.52              |
| 1:1:2122:U:H2'   | 1:1:2123:G:C8    | 2.45                     | 0.52              |
| 1:1:2636:C:HO2'  | 5:D:45:TYR:HH    | 1.53                     | 0.52              |
| 6:E:77:ILE:HG22  | 6:E:77:ILE:O     | 2.10                     | 0.52              |
| 1:1:747:5MU:O2   | 19:R:92:ARG:NH1  | 2.41                     | 0.51              |
| 1:1:1105:U:H2'   | 1:1:1106:G:H8    | 1.75                     | 0.51              |
| 2:2:136:C:O2'    | 47:t:64:GLY:O    | 2.26                     | 0.51              |
| 2:2:1363:A:H2'   | 2:2:1365:G:N7    | 2.25                     | 0.51              |
| 7:F:140:GLU:OE2  | 27:Z:26:SER:OG   | 2.25                     | 0.51              |
| 15:N:29:HIS:HB3  | 15:N:36:TYR:HB2  | 1.92                     | 0.51              |
| 7:F:141:ILE:HG23 | 7:F:146:VAL:HG11 | 1.92                     | 0.51              |
| 9:H:121:VAL:HG11 | 9:H:123:ARG:NH1  | 2.25                     | 0.51              |
| 30:c:31:LEU:HD22 | 30:c:42:LEU:HD23 | 1.92                     | 0.51              |
| 42:o:47:ALA:HB1  | 42:o:62:ALA:HB1  | 1.93                     | 0.51              |
| 1:1:707:G:H2'    | 1:1:708:G:O4'    | 2.11                     | 0.51              |
| 1:1:2636:C:O2'   | 5:D:45:TYR:OH    | 2.21                     | 0.51              |
| 1:1:2885:G:O6    | 28:a:29:SER:OG   | 2.28                     | 0.51              |
| 2:2:701:U:O2     | 2:2:703:G:N1     | 2.43                     | 0.51              |
| 2:2:958:A:OP1    | 50:w:55:ARG:NH1  | 2.39                     | 0.51              |
| 2:2:1145:A:C2'   | 2:2:1146:A:OP2   | 2.58                     | 0.51              |
| 19:R:33:LEU:O    | 19:R:37:THR:OG1  | 2.19                     | 0.51              |
| 47:t:44:SER:N    | 47:t:47:GLU:OE2  | 2.32                     | 0.51              |
| 2:2:521:G:OP2    | 43:p:51:LYS:NZ   | 2.43                     | 0.51              |
| 3:3:48:U:OP1     | 15:N:30:ARG:NH2  | 2.43                     | 0.51              |
| 9:H:51:ARG:HG3   | 9:H:54:LEU:HD11  | 1.92                     | 0.51              |
| 38:k:71:PRO:O    | 38:k:96:ARG:HG2  | 2.11                     | 0.51              |
| 41:n:57:VAL:O    | 41:n:57:VAL:HG22 | 2.09                     | 0.51              |
| 55:B:25:ASP:C    | 55:B:27:GLY:H    | 2.17                     | 0.51              |
| 29:b:13:SER:HA   | 29:b:49:TYR:CD1  | 2.45                     | 0.51              |
| 37:j:37:HIS:NE2  | 37:j:65:GLU:HB2  | 2.25                     | 0.51              |
| 41:n:35:GLN:HB3  | 41:n:78:GLU:OE1  | 2.11                     | 0.51              |
| 1:1:69:C:O2      | 1:1:73:A:O2'     | 2.26                     | 0.51              |
| 1:1:137:U:H2'    | 1:1:138:U:H5'    | 1.92                     | 0.51              |
| 1:1:2756:U:OP2   | 32:e:19:ARG:NE   | 2.37                     | 0.51              |
| 2:2:1062:U:H2'   | 2:2:1063:C:C6    | 2.46                     | 0.51              |
| 3:3:74:U:O2      | 22:U:29:ILE:HD13 | 2.10                     | 0.51              |
| 27:Z:55:GLY:O    | 27:Z:58:ASP:OD1  | 2.29                     | 0.51              |
| 48:u:76:VAL:HG23 | 48:u:77:ARG:HG2  | 1.92                     | 0.51              |
| 55:B:9:VAL:HG22  | 55:B:21:ILE:HG12 | 1.92                     | 0.51              |
| 1:1:877:A:C6     | 1:1:899:A:C6     | 2.99                     | 0.51              |
| 1:1:1173:U:H4'   | 1:1:1174:U:H5'   | 1.93                     | 0.51              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:1:2902:C:C3'   | 1:1:2903:U:H5''   | 2.40                     | 0.51              |
| 2:2:626:G:OP1    | 47:t:35:ARG:NH2   | 2.44                     | 0.51              |
| 2:2:1314:C:OP2   | 50:w:4:SER:OG     | 2.22                     | 0.51              |
| 4:C:80:ARG:NH1   | 4:C:82:GLU:OE2    | 2.36                     | 0.51              |
| 7:F:40:VAL:O     | 7:F:40:VAL:HG12   | 2.11                     | 0.51              |
| 14:M:38:LEU:HB3  | 14:M:39:PRO:HD3   | 1.93                     | 0.51              |
| 33:f:62:SER:HA   | 33:f:224:GLY:O    | 2.11                     | 0.51              |
| 41:n:86:ALA:O    | 41:n:89:ARG:HG2   | 2.11                     | 0.51              |
| 1:1:2591:C:H2'   | 1:1:2592:G:C8     | 2.46                     | 0.51              |
| 1:1:2753:A:O2'   | 32:e:15:LYS:NZ    | 2.44                     | 0.51              |
| 2:2:580:C:H2'    | 2:2:581:G:O4'     | 2.11                     | 0.51              |
| 2:2:811:C:O2'    | 2:2:901:A:N1      | 2.43                     | 0.51              |
| 9:H:67:ALA:O     | 9:H:71:LYS:HD3    | 2.11                     | 0.51              |
| 12:K:123:ARG:NH1 | 12:K:143:GLU:OE2  | 2.43                     | 0.51              |
| 35:h:47:ARG:HG3  | 35:h:47:ARG:O     | 2.11                     | 0.51              |
| 37:j:9:MET:HG2   | 37:j:59:TYR:CE1   | 2.46                     | 0.51              |
| 45:r:39:GLU:OE2  | 45:r:43:ASN:ND2   | 2.43                     | 0.51              |
| 55:B:20:PHE:C    | 55:B:21:ILE:HG13  | 2.35                     | 0.51              |
| 1:1:1818:U:O2'   | 4:C:153:GLN:O     | 2.18                     | 0.50              |
| 2:2:36:C:O2'     | 43:p:114:ARG:NH2  | 2.44                     | 0.50              |
| 2:2:1014:A:P     | 50:w:18:LYS:HZ1   | 2.34                     | 0.50              |
| 9:H:89:LYS:O     | 9:H:91:PHE:N      | 2.44                     | 0.50              |
| 34:g:19:ASN:OD1  | 34:g:54:ARG:NE    | 2.38                     | 0.50              |
| 44:q:59:GLU:OE1  | 44:q:62:LYS:NZ    | 2.41                     | 0.50              |
| 55:B:7:GLY:HA3   | 55:B:21:ILE:HG22  | 1.93                     | 0.50              |
| 1:1:527:C:O2'    | 1:1:2779:U:O2'    | 2.26                     | 0.50              |
| 1:1:1172:C:H2'   | 1:1:1173:U:C2     | 2.46                     | 0.50              |
| 5:D:3:GLY:C      | 5:D:4:LEU:HD12    | 2.36                     | 0.50              |
| 24:W:54:LYS:O    | 24:W:58:VAL:HG23  | 2.11                     | 0.50              |
| 28:a:40:ARG:HG3  | 28:a:41:HIS:ND1   | 2.27                     | 0.50              |
| 33:f:207:ILE:HA  | 33:f:210:VAL:HG22 | 1.94                     | 0.50              |
| 1:1:137:U:C2'    | 1:1:138:U:H5'     | 2.40                     | 0.50              |
| 1:1:411:G:OP2    | 1:1:2406:A:O2'    | 2.27                     | 0.50              |
| 1:1:1358:G:C8    | 1:1:1371:G:O6     | 2.64                     | 0.50              |
| 1:1:1914:C:H2'   | 1:1:1915:3TD:O4   | 2.12                     | 0.50              |
| 1:1:2145:C:O2    | 1:1:2145:C:O2'    | 2.28                     | 0.50              |
| 1:1:2394:C:P     | 31:d:30:ARG:NH2   | 2.84                     | 0.50              |
| 2:2:1126:U:O4    | 41:n:9:ARG:NH1    | 2.44                     | 0.50              |
| 16:O:32:VAL:HG12 | 16:O:34:GLU:OE1   | 2.11                     | 0.50              |
| 33:f:58:ASN:OD1  | 33:f:224:GLY:CA   | 2.60                     | 0.50              |
| 36:i:156:LYS:HG2 | 39:l:71:VAL:HG13  | 1.93                     | 0.50              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 54:z:34:U:H5     | 54:z:37:G:OP2     | 1.95                     | 0.50              |
| 1:1:1141:U:H4'   | 1:1:1142:A:O4'    | 2.12                     | 0.50              |
| 1:1:2140:G:C6    | 1:1:2151:U:N3     | 2.80                     | 0.50              |
| 1:1:2308:G:O6    | 1:1:2311:A:N7     | 2.45                     | 0.50              |
| 2:2:108:G:H5'    | 2:2:109:A:H5''    | 1.93                     | 0.50              |
| 2:2:604:G:H2'    | 2:2:605:U:O4'     | 2.11                     | 0.50              |
| 2:2:713:G:H2'    | 2:2:714:G:C8      | 2.46                     | 0.50              |
| 2:2:718:A:O5'    | 42:o:119:ASN:OD1  | 2.29                     | 0.50              |
| 18:Q:37:GLU:OE1  | 18:Q:37:GLU:O     | 2.30                     | 0.50              |
| 39:l:55:THR:HG23 | 39:l:56:LYS:H     | 1.77                     | 0.50              |
| 54:z:38:G:H2'    | 54:z:39:5MU:O4'   | 2.12                     | 0.50              |
| 54:z:48:C:H2'    | 54:z:49:G:O4'     | 2.10                     | 0.50              |
| 1:1:2050:C:H2'   | 1:1:2051:A:O4'    | 2.12                     | 0.50              |
| 2:2:1518:MA6:N6  | 2:2:1519:MA6:H93  | 2.27                     | 0.50              |
| 33:f:87:CYS:O    | 33:f:88:ASP:OD1   | 2.29                     | 0.50              |
| 33:f:114:LEU:C   | 33:f:114:LEU:HD23 | 2.37                     | 0.50              |
| 41:n:57:VAL:O    | 41:n:57:VAL:HG13  | 2.12                     | 0.50              |
| 55:B:7:GLY:CA    | 55:B:25:ASP:H     | 2.24                     | 0.50              |
| 1:1:2114:A:N7    | 1:1:2167:U:H4'    | 2.26                     | 0.50              |
| 1:1:2753:A:H8    | 1:1:2753:A:O5'    | 1.95                     | 0.50              |
| 2:2:982:U:H5''   | 45:r:6:MET:HE3    | 1.93                     | 0.50              |
| 2:2:1003:G:N2    | 2:2:1005:A:O5'    | 2.41                     | 0.50              |
| 41:n:22:THR:O    | 41:n:26:VAL:HG23  | 2.11                     | 0.50              |
| 41:n:80:THR:O    | 41:n:84:VAL:HG12  | 2.11                     | 0.50              |
| 51:x:31:PHE:O    | 51:x:35:VAL:HG23  | 2.11                     | 0.50              |
| 1:1:749:A:N1     | 1:1:753:A:O2'     | 2.37                     | 0.50              |
| 1:1:1538:G:H2'   | 1:1:1539:U:C6     | 2.47                     | 0.50              |
| 1:1:2161:C:O2'   | 1:1:2173:A:H5''   | 2.10                     | 0.50              |
| 2:2:20:U:H2'     | 2:2:21:G:O4'      | 2.11                     | 0.50              |
| 2:2:202:G:O2'    | 2:2:468:A:H8      | 1.93                     | 0.50              |
| 2:2:1382:C:O2'   | 38:k:79:ARG:NH1   | 2.45                     | 0.50              |
| 12:K:124:GLY:C   | 12:K:125:LEU:HD12 | 2.37                     | 0.50              |
| 23:V:10:THR:O    | 23:V:10:THR:HG23  | 2.12                     | 0.50              |
| 25:X:44:LYS:O    | 25:X:48:ARG:HD2   | 2.11                     | 0.50              |
| 1:1:210:C:OP1    | 30:c:29:GLN:NE2   | 2.45                     | 0.50              |
| 1:1:2182:U:O2'   | 1:1:2183:A:C8     | 2.60                     | 0.50              |
| 2:2:1391:U:H2'   | 2:2:1392:G:C8     | 2.47                     | 0.50              |
| 34:g:47:LEU:HD12 | 34:g:47:LEU:N     | 2.26                     | 0.50              |
| 1:1:1055:G:C6    | 1:1:1105:U:O4     | 2.65                     | 0.50              |
| 1:1:2394:C:OP2   | 31:d:30:ARG:NH2   | 2.45                     | 0.50              |
| 2:2:110:C:H2'    | 2:2:111:G:O4'     | 2.12                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:2:404:G:N7      | 35:h:2:ALA:HB3    | 2.27                     | 0.50              |
| 2:2:1005:A:H3'    | 2:2:1006:G:H8     | 1.76                     | 0.50              |
| 2:2:1259:C:O2'    | 2:2:1283:U:O2     | 2.23                     | 0.50              |
| 4:C:84:ASP:OD2    | 4:C:87:ARG:NE     | 2.32                     | 0.50              |
| 34:g:73:PRO:HA    | 34:g:76:VAL:HG22  | 1.93                     | 0.50              |
| 38:k:78:ARG:HE    | 38:k:80:VAL:HG21  | 1.77                     | 0.50              |
| 1:1:247:G:OP2     | 1:1:249:C:N4      | 2.42                     | 0.49              |
| 19:R:108:SER:OG   | 19:R:109:ASP:N    | 2.44                     | 0.49              |
| 33:f:79:ALA:HA    | 33:f:82:ASP:OD2   | 2.12                     | 0.49              |
| 34:g:151:VAL:HG12 | 34:g:200:VAL:HG22 | 1.93                     | 0.49              |
| 41:n:59:LYS:HE2   | 41:n:62:ARG:NH2   | 2.27                     | 0.49              |
| 1:1:1652:A:OP1    | 14:M:8:ARG:NH2    | 2.40                     | 0.49              |
| 1:1:2350:C:OP2    | 31:d:45:ARG:NH2   | 2.45                     | 0.49              |
| 2:2:1126:U:O4     | 41:n:73:LEU:HD12  | 2.12                     | 0.49              |
| 9:H:121:VAL:CG1   | 9:H:123:ARG:HG3   | 2.42                     | 0.49              |
| 34:g:155:GLY:HA2  | 34:g:163:ALA:HB1  | 1.93                     | 0.49              |
| 55:B:10:LYS:HG3   | 55:B:22:THR:CA    | 2.42                     | 0.49              |
| 55:B:27:GLY:C     | 55:B:29:ASP:N     | 2.68                     | 0.49              |
| 2:2:692:U:H1'     | 2:2:695:A:N7      | 2.27                     | 0.49              |
| 6:E:152:GLU:CD    | 6:E:153:LEU:N     | 2.71                     | 0.49              |
| 34:g:80:LYS:HG3   | 34:g:80:LYS:O     | 2.12                     | 0.49              |
| 47:t:61:VAL:HG21  | 47:t:67:ILE:HD11  | 1.94                     | 0.49              |
| 1:1:964:C:O2'     | 1:1:2273:A:N3     | 2.39                     | 0.49              |
| 2:2:1257:A:C2     | 45:r:21:PHE:CE1   | 3.01                     | 0.49              |
| 3:3:1:U:O2'       | 3:3:2:G:H8        | 1.96                     | 0.49              |
| 20:S:31:VAL:HG22  | 20:S:84:TYR:CD1   | 2.47                     | 0.49              |
| 44:q:4:ILE:CG1    | 44:q:9:ILE:HD12   | 2.42                     | 0.49              |
| 52:y:3:VAL:HG23   | 52:y:3:VAL:O      | 2.12                     | 0.49              |
| 54:z:20:5MU:H3'   | 54:z:21:A:H5''    | 1.94                     | 0.49              |
| 54:z:77:C:O2'     | 54:z:78:C:H5'     | 2.12                     | 0.49              |
| 1:1:279:A:N6      | 1:1:361:G:H1'     | 2.27                     | 0.49              |
| 2:2:451:A:H61     | 2:2:481:G:H5'     | 1.77                     | 0.49              |
| 2:2:714:G:H2'     | 2:2:715:A:C8      | 2.47                     | 0.49              |
| 2:2:881:G:OP2     | 43:p:9:ARG:NH1    | 2.45                     | 0.49              |
| 2:2:1031:C:H4'    | 2:2:1032:G:H22    | 1.77                     | 0.49              |
| 36:i:13:GLU:OE2   | 36:i:68:ARG:NH1   | 2.46                     | 0.49              |
| 49:v:35:GLU:OE1   | 49:v:35:GLU:N     | 2.37                     | 0.49              |
| 1:1:402:A:H2'     | 1:1:403:U:C5'     | 2.43                     | 0.49              |
| 1:1:545:U:HO2'    | 1:1:547:A:P       | 2.35                     | 0.49              |
| 1:1:549:G:H2'     | 1:1:550:C:C6      | 2.48                     | 0.49              |
| 1:1:1722:A:N6     | 1:1:1738:G:H1'    | 2.28                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:1:2186:G:H2'   | 1:1:2187:U:C6    | 2.48                     | 0.49              |
| 1:1:2728:U:O2'   | 1:1:2729:G:H8    | 1.96                     | 0.49              |
| 2:2:608:A:H2'    | 2:2:609:A:O4'    | 2.12                     | 0.49              |
| 2:2:1350:A:OP2   | 40:m:120:LYS:NZ  | 2.44                     | 0.49              |
| 8:G:105:LEU:HB2  | 8:G:113:VAL:HB   | 1.95                     | 0.49              |
| 9:H:135:HIS:CB   | 9:H:138:VAL:HG22 | 2.42                     | 0.49              |
| 48:u:14:SER:HA   | 48:u:55:ILE:HD12 | 1.95                     | 0.49              |
| 54:z:11:C:O2'    | 54:z:12:G:H5'    | 2.11                     | 0.49              |
| 55:B:7:GLY:C     | 55:B:21:ILE:CG2  | 2.86                     | 0.49              |
| 1:1:388:G:N7     | 1:1:390:U:H2'    | 2.27                     | 0.49              |
| 2:2:516:PSU:H4'  | 2:2:517:G:OP1    | 2.12                     | 0.49              |
| 2:2:1077:G:N2    | 2:2:1080:A:OP2   | 2.36                     | 0.49              |
| 7:F:122:PHE:O    | 7:F:123:ASP:OD1  | 2.31                     | 0.49              |
| 8:G:42:GLU:HA    | 8:G:55:ARG:NH2   | 2.27                     | 0.49              |
| 8:G:155:GLU:HG2  | 8:G:157:TYR:H    | 1.77                     | 0.49              |
| 35:h:184:ARG:NH1 | 35:h:187:GLU:OE1 | 2.46                     | 0.49              |
| 36:i:149:SER:OG  | 36:i:151:GLU:OE1 | 2.31                     | 0.49              |
| 38:k:135:VAL:O   | 38:k:139:GLU:HG2 | 2.12                     | 0.49              |
| 55:B:8:ILE:C     | 55:B:21:ILE:HG23 | 2.37                     | 0.49              |
| 1:1:1715:G:O2'   | 1:1:1743:G:O6    | 2.24                     | 0.49              |
| 1:1:2144:G:O3'   | 1:1:2145:C:H2'   | 2.12                     | 0.49              |
| 2:2:80:A:N6      | 2:2:87:C:C5      | 2.81                     | 0.49              |
| 4:C:225:MET:SD   | 4:C:230:HIS:HB2  | 2.53                     | 0.49              |
| 26:Y:13:ALA:O    | 26:Y:21:LYS:HE2  | 2.13                     | 0.49              |
| 1:1:13:A:O2'     | 1:1:15:G:O6      | 2.30                     | 0.49              |
| 1:1:278:A:C6     | 1:1:362:A:C8     | 3.01                     | 0.49              |
| 1:1:357:C:C2     | 1:1:358:U:C5     | 3.01                     | 0.49              |
| 2:2:90:C:H2'     | 2:2:91:U:C6      | 2.48                     | 0.49              |
| 2:2:1234:C:OP1   | 40:m:119:ARG:NH2 | 2.41                     | 0.49              |
| 12:K:55:MET:SD   | 12:K:59:ARG:HD2  | 2.53                     | 0.49              |
| 38:k:5:ARG:CZ    | 38:k:7:ILE:HG22  | 2.42                     | 0.49              |
| 47:t:51:ARG:C    | 47:t:52:LEU:HD12 | 2.38                     | 0.49              |
| 1:1:357:C:H2'    | 1:1:358:U:H6     | 1.77                     | 0.49              |
| 1:1:548:G:H3'    | 1:1:549:G:O4'    | 2.12                     | 0.49              |
| 1:1:895:U:O2'    | 1:1:896:A:O4'    | 2.18                     | 0.49              |
| 1:1:1244:A:O2'   | 6:E:29:HIS:NE2   | 2.42                     | 0.49              |
| 1:1:2102:G:C2    | 1:1:2103:C:C2    | 3.01                     | 0.49              |
| 1:1:2123:G:H2'   | 1:1:2124:G:C8    | 2.48                     | 0.49              |
| 2:2:1008:U:O2    | 2:2:1009:U:C2    | 2.66                     | 0.49              |
| 2:2:1317:C:P     | 45:r:28:LYS:HZ3  | 2.34                     | 0.49              |
| 9:H:4:ILE:HD12   | 9:H:17:ASP:O     | 2.12                     | 0.49              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 9:H:79:THR:HG22  | 9:H:145:ASN:HB3   | 1.95                     | 0.49              |
| 9:H:115:VAL:HG12 | 9:H:117:LEU:CD1   | 2.43                     | 0.49              |
| 22:U:58:SER:O    | 22:U:73:LYS:NZ    | 2.46                     | 0.49              |
| 35:h:3:ARG:NH1   | 35:h:5:LEU:HD21   | 2.28                     | 0.49              |
| 1:1:714:U:OP2    | 46:s:88:ARG:NH2   | 2.45                     | 0.48              |
| 1:1:1055:G:C6    | 1:1:1105:U:N3     | 2.81                     | 0.48              |
| 1:1:1445:G:C5    | 1:1:1446:C:C5     | 3.01                     | 0.48              |
| 1:1:2571:U:C2'   | 5:D:151:THR:HG21  | 2.42                     | 0.48              |
| 6:E:189:THR:HG22 | 6:E:191:ASP:H     | 1.77                     | 0.48              |
| 9:H:51:ARG:O     | 9:H:55:GLU:HG3    | 2.12                     | 0.48              |
| 31:d:32:ILE:O    | 31:d:32:ILE:HG22  | 2.13                     | 0.48              |
| 1:1:1054:A:C6    | 1:1:1106:G:C6     | 3.01                     | 0.48              |
| 7:F:123:ASP:OD2  | 7:F:127:ASN:HB2   | 2.14                     | 0.48              |
| 25:X:23:ARG:O    | 25:X:27:ASN:ND2   | 2.36                     | 0.48              |
| 26:Y:47:MET:O    | 26:Y:51:VAL:HG22  | 2.13                     | 0.48              |
| 27:Z:11:GLU:HA   | 27:Z:25:ARG:HA    | 1.95                     | 0.48              |
| 52:y:28:VAL:HG23 | 52:y:29:LEU:N     | 2.28                     | 0.48              |
| 1:1:1590:A:H2'   | 1:1:1591:A:C8     | 2.48                     | 0.48              |
| 1:1:1722:A:H2'   | 1:1:1723:G:O4'    | 2.13                     | 0.48              |
| 2:2:1417:G:C6    | 2:2:1482:G:C6     | 3.01                     | 0.48              |
| 14:M:59:SER:OG   | 14:M:62:ASN:OD1   | 2.23                     | 0.48              |
| 24:W:6:GLN:O     | 24:W:74:ARG:NH2   | 2.46                     | 0.48              |
| 51:x:32:ILE:HG12 | 51:x:54:MET:SD    | 2.54                     | 0.48              |
| 1:1:126:A:OP1    | 30:c:45:SER:OG    | 2.23                     | 0.48              |
| 1:1:993:G:OP1    | 17:P:50:ARG:NE    | 2.46                     | 0.48              |
| 1:1:2902:C:H3'   | 1:1:2903:U:H5''   | 1.94                     | 0.48              |
| 2:2:1168:U:C3'   | 2:2:1169:A:H5'    | 2.43                     | 0.48              |
| 35:h:107:PHE:CD1 | 35:h:159:LEU:HD21 | 2.47                     | 0.48              |
| 41:n:102:LEU:C   | 41:n:102:LEU:HD23 | 2.38                     | 0.48              |
| 1:1:2584:U:H2'   | 1:1:2585:U:C2     | 2.48                     | 0.48              |
| 25:X:38:GLN:OE1  | 55:B:16:LYS:NZ    | 2.46                     | 0.48              |
| 36:i:145:GLU:HA  | 36:i:145:GLU:OE1  | 2.13                     | 0.48              |
| 42:o:34:ILE:HG12 | 42:o:70:CYS:SG    | 2.53                     | 0.48              |
| 44:q:53:ILE:HG22 | 44:q:57:ARG:NH1   | 2.27                     | 0.48              |
| 44:q:98:ARG:HB2  | 44:q:100:GLN:OE1  | 2.14                     | 0.48              |
| 55:B:24:ASP:C    | 55:B:26:GLY:N     | 2.70                     | 0.48              |
| 1:1:639:U:H2'    | 1:1:640:C:C6      | 2.47                     | 0.48              |
| 1:1:957:C:N4     | 1:1:2459:A:C8     | 2.82                     | 0.48              |
| 2:2:235:C:H2'    | 2:2:236:A:C8      | 2.49                     | 0.48              |
| 2:2:779:C:H2'    | 2:2:780:A:O4'     | 2.13                     | 0.48              |
| 4:C:205:LEU:N    | 4:C:205:LEU:HD12  | 2.29                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:E:77:ILE:O     | 6:E:77:ILE:CG2   | 2.61                     | 0.48              |
| 21:T:33:LYS:HB3  | 21:T:64:ALA:HB1  | 1.96                     | 0.48              |
| 34:g:10:ILE:HG23 | 34:g:11:ARG:CD   | 2.43                     | 0.48              |
| 35:h:140:ASN:N   | 35:h:182:PHE:O   | 2.47                     | 0.48              |
| 43:p:72:HIS:HB2  | 43:p:74:LEU:HD23 | 1.96                     | 0.48              |
| 1:1:309:A:N3     | 1:1:329:G:O2'    | 2.41                     | 0.48              |
| 1:1:810:U:C2     | 12:K:29:LYS:O    | 2.67                     | 0.48              |
| 2:2:152:A:N6     | 2:2:169:C:C2     | 2.82                     | 0.48              |
| 2:2:1006:G:C8    | 2:2:1006:G:O5'   | 2.62                     | 0.48              |
| 4:C:161:TYR:HB3  | 4:C:194:GLU:HG2  | 1.96                     | 0.48              |
| 9:H:65:ALA:HA    | 9:H:68:ARG:HH21  | 1.78                     | 0.48              |
| 47:t:61:VAL:CG2  | 47:t:67:ILE:HD11 | 2.43                     | 0.48              |
| 55:B:11:TRP:CE2  | 55:B:20:PHE:HB2  | 2.49                     | 0.48              |
| 1:1:1077:A:N6    | 1:1:1078:U:O2    | 2.47                     | 0.48              |
| 1:1:2402:U:O2'   | 1:1:2403:C:H5''  | 2.13                     | 0.48              |
| 2:2:490:C:OP1    | 35:h:146:ARG:NH2 | 2.47                     | 0.48              |
| 3:3:43:C:O2      | 7:F:92:ARG:NH2   | 2.46                     | 0.48              |
| 34:g:134:MET:HE2 | 34:g:168:TYR:HD2 | 1.79                     | 0.48              |
| 36:i:88:VAL:HG12 | 36:i:93:ARG:HG3  | 1.96                     | 0.48              |
| 39:l:75:ILE:HG23 | 39:l:75:ILE:O    | 2.12                     | 0.48              |
| 42:o:64:GLN:O    | 42:o:68:GLU:HG3  | 2.14                     | 0.48              |
| 46:s:21:ASP:O    | 46:s:23:GLY:N    | 2.47                     | 0.48              |
| 54:z:76:5MU:OP2  | 54:z:76:5MU:H6   | 1.97                     | 0.48              |
| 1:1:2170:A:C2    | 1:1:2171:A:C4    | 3.02                     | 0.48              |
| 1:1:2236:U:H2'   | 1:1:2237:G:O4'   | 2.13                     | 0.48              |
| 1:1:2635:A:O2'   | 5:D:81:GLU:OE1   | 2.21                     | 0.48              |
| 1:1:2766:A:C5    | 1:1:2767:C:C5    | 3.01                     | 0.48              |
| 13:L:110:GLU:O   | 13:L:114:ARG:HG2 | 2.13                     | 0.48              |
| 19:R:86:MET:N    | 19:R:94:ASP:O    | 2.35                     | 0.48              |
| 22:U:64:VAL:HG22 | 22:U:69:GLU:HG3  | 1.94                     | 0.48              |
| 34:g:51:SER:HB2  | 34:g:71:ALA:HB3  | 1.94                     | 0.48              |
| 40:m:128:SER:OG  | 40:m:130:ARG:OXT | 2.19                     | 0.48              |
| 1:1:1584:U:H4'   | 1:1:1585:C:H5''  | 1.95                     | 0.48              |
| 1:1:2144:G:N7    | 1:1:2146:C:N4    | 2.61                     | 0.48              |
| 2:2:412:A:H62    | 2:2:431:A:N6     | 2.10                     | 0.48              |
| 9:H:54:LEU:O     | 9:H:58:LEU:HD12  | 2.14                     | 0.48              |
| 38:k:15:ASP:OD1  | 38:k:19:GLY:N    | 2.47                     | 0.48              |
| 40:m:51:PRO:O    | 40:m:55:VAL:HG22 | 2.14                     | 0.48              |
| 1:1:2178:C:H2'   | 1:1:2179:C:C5    | 2.49                     | 0.47              |
| 2:2:496:A:O2'    | 2:2:497:G:C8     | 2.64                     | 0.47              |
| 7:F:38:MET:HE1   | 7:F:53:ALA:O     | 2.14                     | 0.47              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 33:f:217:VAL:O   | 33:f:221:VAL:HG22 | 2.14                     | 0.47              |
| 34:g:42:TYR:CE2  | 34:g:90:VAL:HG21  | 2.48                     | 0.47              |
| 36:i:111:MET:HA  | 36:i:114:VAL:HG12 | 1.95                     | 0.47              |
| 1:1:1410:G:H2'   | 1:1:1411:U:C6     | 2.50                     | 0.47              |
| 8:G:39:ASP:O     | 8:G:55:ARG:HD2    | 2.14                     | 0.47              |
| 1:1:321:U:O3'    | 6:E:162:ARG:NH1   | 2.42                     | 0.47              |
| 1:1:2297:A:N1    | 1:1:2321:U:H5     | 2.12                     | 0.47              |
| 2:2:689:C:H2'    | 2:2:690:G:O4'     | 2.14                     | 0.47              |
| 3:3:40:U:N3      | 3:3:44:G:OP2      | 2.28                     | 0.47              |
| 9:H:90:LEU:HD23  | 9:H:90:LEU:O      | 2.15                     | 0.47              |
| 15:N:2:ASP:CG    | 15:N:3:LYS:H      | 2.22                     | 0.47              |
| 27:Z:37:CYS:SG   | 27:Z:39:LYS:HB3   | 2.54                     | 0.47              |
| 31:d:15:LYS:HB2  | 31:d:23:LYS:HE2   | 1.96                     | 0.47              |
| 1:1:116:C:H2'    | 1:1:117:G:O4'     | 2.14                     | 0.47              |
| 1:1:460:A:P      | 30:c:41:ARG:HH22  | 2.37                     | 0.47              |
| 1:1:2116:G:H22   | 1:1:2161:C:C5'    | 2.27                     | 0.47              |
| 2:2:946:A:H2'    | 2:2:947:G:C8      | 2.50                     | 0.47              |
| 2:2:1160:G:H22   | 2:2:1176:A:H2     | 1.61                     | 0.47              |
| 3:3:48:U:P       | 15:N:30:ARG:HH22  | 2.37                     | 0.47              |
| 21:T:49:VAL:HG22 | 21:T:54:GLN:HB2   | 1.95                     | 0.47              |
| 33:f:115:LYS:O   | 33:f:118:GLU:HG2  | 2.13                     | 0.47              |
| 1:1:2425:A:H5''  | 1:1:2427:C:O4'    | 2.15                     | 0.47              |
| 2:2:945:G:C2     | 2:2:946:A:C8      | 3.02                     | 0.47              |
| 1:1:170:U:H2'    | 1:1:171:U:C6      | 2.50                     | 0.47              |
| 1:1:1077:A:H61   | 1:1:1088:A:H2'    | 1.80                     | 0.47              |
| 1:1:1370:C:H2'   | 1:1:1371:G:O4'    | 2.15                     | 0.47              |
| 2:2:459:A:H2'    | 2:2:460:A:C8      | 2.50                     | 0.47              |
| 6:E:12:LEU:HD11  | 6:E:190:ALA:HB1   | 1.97                     | 0.47              |
| 6:E:126:VAL:HG12 | 6:E:128:ALA:O     | 2.14                     | 0.47              |
| 6:E:152:GLU:OE1  | 6:E:153:LEU:C     | 2.58                     | 0.47              |
| 44:q:9:ILE:CG2   | 44:q:18:ALA:HB1   | 2.36                     | 0.47              |
| 45:r:46:LEU:HD12 | 50:w:13:LEU:HB3   | 1.97                     | 0.47              |
| 47:t:70:ARG:O    | 47:t:74:LEU:HG    | 2.15                     | 0.47              |
| 1:1:244:A:OP2    | 31:d:8:ARG:NH2    | 2.39                     | 0.47              |
| 1:1:635:C:H2'    | 1:1:636:G:O4'     | 2.15                     | 0.47              |
| 1:1:856:G:H2'    | 1:1:857:G:C8      | 2.49                     | 0.47              |
| 1:1:1469:A:H2'   | 1:1:1470:A:C8     | 2.49                     | 0.47              |
| 1:1:1954:G:O2'   | 1:1:1956:U:O4     | 2.28                     | 0.47              |
| 1:1:2119:A:N6    | 1:1:2167:U:O2     | 2.48                     | 0.47              |
| 1:1:2158:A:O2'   | 1:1:2159:G:C8     | 2.67                     | 0.47              |
| 1:1:2376:A:N3    | 15:N:111:ARG:NH1  | 2.63                     | 0.47              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:2:1168:U:HO2'  | 2:2:1169:A:P      | 2.35                     | 0.47              |
| 6:E:48:THR:O     | 6:E:52:VAL:HG23   | 2.14                     | 0.47              |
| 7:F:7:TYR:CE1    | 7:F:11:GLU:OE1    | 2.68                     | 0.47              |
| 21:T:99:ASN:C    | 21:T:99:ASN:OD1   | 2.57                     | 0.47              |
| 40:m:60:LYS:HB3  | 40:m:61:LEU:HD12  | 1.97                     | 0.47              |
| 42:o:60:PRO:HD3  | 42:o:91:PRO:HB2   | 1.96                     | 0.47              |
| 54:z:23:A:H3'    | 54:z:24:C:H5''    | 1.97                     | 0.47              |
| 54:z:70:C:C3'    | 54:z:71:5MU:H5'   | 2.44                     | 0.47              |
| 55:B:8:ILE:O     | 55:B:22:THR:CG2   | 2.62                     | 0.47              |
| 55:B:26:GLY:O    | 55:B:27:GLY:C     | 2.58                     | 0.47              |
| 1:1:510:C:C2'    | 1:1:511:U:H5'     | 2.45                     | 0.47              |
| 1:1:878:A:N7     | 1:1:899:A:H2      | 2.13                     | 0.47              |
| 1:1:1066:U:H2'   | 1:1:1067:A:H2'    | 1.95                     | 0.47              |
| 1:1:2195:U:O2'   | 1:1:2196:C:H5'    | 2.15                     | 0.47              |
| 2:2:632:U:H5''   | 2:2:633:G:C8      | 2.50                     | 0.47              |
| 2:2:1356:G:H2'   | 2:2:1357:A:C8     | 2.50                     | 0.47              |
| 4:C:20:VAL:HG23  | 4:C:20:VAL:O      | 2.14                     | 0.47              |
| 36:i:133:PRO:HA  | 36:i:136:VAL:HG12 | 1.96                     | 0.47              |
| 41:n:86:ALA:HA   | 41:n:89:ARG:HG2   | 1.97                     | 0.47              |
| 44:q:46:SER:C    | 44:q:47:GLU:HG3   | 2.40                     | 0.47              |
| 1:1:888:C:O4'    | 44:q:92:ARG:HB2   | 2.14                     | 0.47              |
| 1:1:1215:G:H1    | 1:1:1234:U:H3     | 1.62                     | 0.47              |
| 1:1:1818:U:OP2   | 4:C:156:ARG:NE    | 2.47                     | 0.47              |
| 7:F:149:VAL:O    | 7:F:149:VAL:CG2   | 2.63                     | 0.47              |
| 9:H:83:LYS:C     | 9:H:89:LYS:O      | 2.58                     | 0.47              |
| 34:g:43:LEU:HD23 | 34:g:68:ILE:HD11  | 1.97                     | 0.47              |
| 37:j:21:MET:HG2  | 37:j:24:ARG:HH21  | 1.80                     | 0.47              |
| 1:1:2118:U:OP1   | 1:1:2148:G:O2'    | 2.30                     | 0.47              |
| 1:1:2301:C:H2'   | 1:1:2302:U:H6     | 1.80                     | 0.47              |
| 1:1:2831:G:OP2   | 5:D:59:ARG:NH1    | 2.30                     | 0.47              |
| 2:2:9:G:OP2      | 36:i:126:LYS:NZ   | 2.32                     | 0.47              |
| 2:2:90:C:H2'     | 2:2:91:U:H6       | 1.80                     | 0.47              |
| 2:2:463:U:H3'    | 2:2:464:U:C6      | 2.50                     | 0.47              |
| 3:3:42:C:C5      | 7:F:66:LEU:HD22   | 2.50                     | 0.47              |
| 4:C:174:LEU:O    | 4:C:181:MET:HA    | 2.14                     | 0.47              |
| 8:G:73:ASN:O     | 8:G:77:ILE:HG12   | 2.15                     | 0.47              |
| 18:Q:69:GLY:O    | 18:Q:90:ARG:NE    | 2.41                     | 0.47              |
| 21:T:98:SER:O    | 21:T:99:ASN:OD1   | 2.33                     | 0.47              |
| 34:g:47:LEU:HD23 | 34:g:76:VAL:CG1   | 2.45                     | 0.47              |
| 40:m:107:ASP:CG  | 40:m:109:ARG:HE   | 2.24                     | 0.47              |
| 1:1:587:C:OP2    | 12:K:21:ARG:NH2   | 2.34                     | 0.46              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:1:732:C:H2'    | 1:1:733:G:O4'     | 2.14                     | 0.46              |
| 1:1:1417:C:O2'   | 1:1:1587:G:O2'    | 2.33                     | 0.46              |
| 1:1:1607:C:H4'   | 1:1:1608:A:H5'    | 1.97                     | 0.46              |
| 1:1:1872:A:H8    | 1:1:1872:A:O5'    | 1.99                     | 0.46              |
| 1:1:2065:C:H42   | 1:1:2445:2MG:HN1  | 1.63                     | 0.46              |
| 2:2:297:G:N2     | 2:2:300:A:OP2     | 2.41                     | 0.46              |
| 2:2:475:C:H2'    | 2:2:476:U:C6      | 2.50                     | 0.46              |
| 2:2:664:G:H22    | 2:2:741:G:H1      | 1.63                     | 0.46              |
| 7:F:54:ALA:HB1   | 7:F:65:PRO:HG2    | 1.97                     | 0.46              |
| 10:I:31:GLU:OE2  | 10:I:35:ARG:NE    | 2.48                     | 0.46              |
| 23:V:34:GLY:N    | 23:V:61:ALA:O     | 2.39                     | 0.46              |
| 36:i:150:PRO:HA  | 36:i:153:VAL:HG22 | 1.97                     | 0.46              |
| 39:l:30:SER:O    | 39:l:34:VAL:HG23  | 2.14                     | 0.46              |
| 48:u:12:VAL:N    | 48:u:57:ASP:O     | 2.48                     | 0.46              |
| 54:z:26:C:H2'    | 54:z:27:A:O4'     | 2.15                     | 0.46              |
| 1:1:1007:C:H5''  | 10:I:37:ARG:NH2   | 2.30                     | 0.46              |
| 1:1:1087:G:H1    | 1:1:1102:C:H42    | 1.64                     | 0.46              |
| 1:1:1445:G:C6    | 1:1:1446:C:C4     | 3.04                     | 0.46              |
| 2:2:1018:G:H2'   | 2:2:1019:A:O4'    | 2.15                     | 0.46              |
| 4:C:144:VAL:HB   | 4:C:154:LEU:HB2   | 1.97                     | 0.46              |
| 40:m:91:ASP:OD2  | 40:m:93:SER:OG    | 2.33                     | 0.46              |
| 41:n:8:ILE:HG12  | 41:n:100:ILE:HG22 | 1.98                     | 0.46              |
| 48:u:17:MET:HG3  | 48:u:20:SER:HB2   | 1.95                     | 0.46              |
| 55:B:10:LYS:HE3  | 55:B:21:ILE:N     | 2.31                     | 0.46              |
| 1:1:882:G:C6     | 1:1:895:U:O2      | 2.69                     | 0.46              |
| 1:1:2113:U:N3    | 1:1:2114:A:N7     | 2.62                     | 0.46              |
| 1:1:2167:U:O5'   | 1:1:2167:U:H6     | 1.97                     | 0.46              |
| 1:1:2300:C:O2'   | 1:1:2301:C:H5'    | 2.15                     | 0.46              |
| 7:F:115:ARG:O    | 7:F:178:ARG:NH1   | 2.44                     | 0.46              |
| 7:F:147:ASP:OD1  | 7:F:148:ARG:N     | 2.48                     | 0.46              |
| 25:X:35:GLY:O    | 55:B:15:ASP:OD1   | 2.33                     | 0.46              |
| 37:j:29:ILE:HG21 | 37:j:36:ILE:CD1   | 2.45                     | 0.46              |
| 42:o:18:ASP:OD2  | 42:o:37:ARG:NE    | 2.36                     | 0.46              |
| 55:B:7:GLY:N     | 55:B:25:ASP:H     | 2.13                     | 0.46              |
| 1:1:601:C:H2'    | 1:1:602:A:O4'     | 2.16                     | 0.46              |
| 1:1:1174:U:OP2   | 1:1:1175:A:N1     | 2.49                     | 0.46              |
| 1:1:1588:G:C2    | 1:1:1589:U:C4     | 3.03                     | 0.46              |
| 1:1:2580:PSU:OP1 | 5:D:137:SER:OG    | 2.23                     | 0.46              |
| 1:1:2788:C:H2'   | 1:1:2789:C:C6     | 2.50                     | 0.46              |
| 4:C:51:THR:HG23  | 4:C:54:ILE:HD12   | 1.98                     | 0.46              |
| 24:W:65:ASP:OD1  | 24:W:65:ASP:N     | 2.45                     | 0.46              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 37:j:45:ARG:HD3  | 37:j:59:TYR:CE2   | 2.50                     | 0.46              |
| 41:n:53:ILE:HD11 | 41:n:61:ALA:HB1   | 1.98                     | 0.46              |
| 43:p:87:VAL:HG11 | 43:p:90:LEU:HD12  | 1.98                     | 0.46              |
| 54:z:19:G:C1'    | 54:z:20:5MU:OP2   | 2.64                     | 0.46              |
| 54:z:23:A:OP2    | 54:z:24:C:C5      | 2.68                     | 0.46              |
| 55:B:10:LYS:HG3  | 55:B:22:THR:HB    | 1.97                     | 0.46              |
| 1:1:1095:A:O2'   | 1:1:1096:A:O4'    | 2.33                     | 0.46              |
| 1:1:1604:C:O2'   | 1:1:1610:A:N1     | 2.43                     | 0.46              |
| 1:1:2103:C:H2'   | 1:1:2186:G:H22    | 1.80                     | 0.46              |
| 1:1:2902:C:H2'   | 1:1:2903:U:H5''   | 1.96                     | 0.46              |
| 6:E:176:ASP:OD1  | 6:E:176:ASP:N     | 2.48                     | 0.46              |
| 9:H:9:VAL:HB     | 9:H:12:LEU:HD21   | 1.98                     | 0.46              |
| 13:L:105:MET:SD  | 13:L:108:VAL:HG21 | 2.55                     | 0.46              |
| 25:X:18:LEU:O    | 25:X:18:LEU:HD23  | 2.15                     | 0.46              |
| 35:h:102:VAL:HB  | 35:h:114:ALA:HB1  | 1.98                     | 0.46              |
| 38:k:69:VAL:HG12 | 38:k:135:VAL:HG12 | 1.96                     | 0.46              |
| 54:z:55:5MU:C2   | 54:z:56:G:C8      | 3.03                     | 0.46              |
| 55:B:10:LYS:H    | 55:B:22:THR:N     | 2.12                     | 0.46              |
| 2:2:1178:G:N2    | 2:2:1181:G:OP2    | 2.48                     | 0.46              |
| 9:H:85:GLY:HA2   | 9:H:125:THR:HG22  | 1.97                     | 0.46              |
| 12:K:86:GLU:OE1  | 12:K:86:GLU:N     | 2.48                     | 0.46              |
| 18:Q:29:THR:O    | 18:Q:29:THR:CG2   | 2.61                     | 0.46              |
| 33:f:223:GLU:N   | 33:f:223:GLU:OE1  | 2.48                     | 0.46              |
| 37:j:4:TYR:CD2   | 37:j:71:ILE:HG13  | 2.51                     | 0.46              |
| 49:v:30:LYS:HA   | 49:v:33:ILE:HG12  | 1.98                     | 0.46              |
| 1:1:2364:C:H2'   | 1:1:2365:G:O4'    | 2.15                     | 0.46              |
| 2:2:31:G:O2'     | 2:2:48:C:N4       | 2.48                     | 0.46              |
| 2:2:522:C:OP2    | 43:p:66:TYR:OH    | 2.20                     | 0.46              |
| 2:2:556:C:H2'    | 2:2:557:G:O4'     | 2.15                     | 0.46              |
| 2:2:857:C:H2'    | 2:2:858:G:O4'     | 2.16                     | 0.46              |
| 4:C:72:ASP:OD2   | 4:C:189:ARG:NH2   | 2.48                     | 0.46              |
| 6:E:8:ALA:HB3    | 6:E:122:GLU:OE2   | 2.15                     | 0.46              |
| 9:H:138:VAL:HG23 | 9:H:138:VAL:O     | 2.15                     | 0.46              |
| 41:n:90:LEU:HD23 | 41:n:90:LEU:C     | 2.40                     | 0.46              |
| 50:w:13:LEU:HD23 | 50:w:14:HIS:H     | 1.80                     | 0.46              |
| 55:B:16:LYS:HB2  | 55:B:18:PHE:CE1   | 2.50                     | 0.46              |
| 1:1:1048:A:C5    | 1:1:1049:C:C5     | 3.03                     | 0.46              |
| 1:1:1357:C:H2'   | 1:1:1358:G:O4'    | 2.16                     | 0.46              |
| 1:1:2063:C:O2    | 1:1:2450:A:N1     | 2.48                     | 0.46              |
| 1:1:2164:C:OP2   | 1:1:2170:A:N7     | 2.48                     | 0.46              |
| 1:1:2189:U:C2    | 1:1:2190:G:N7     | 2.84                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:2:88:U:C6       | 2:2:89:U:C5       | 3.03                     | 0.46              |
| 2:2:978:A:C2      | 2:2:1319:A:C4     | 3.04                     | 0.46              |
| 7:F:57:LEU:HD21   | 7:F:89:VAL:CG2    | 2.45                     | 0.46              |
| 8:G:60:ASP:HB2    | 8:G:63:ALA:HB3    | 1.98                     | 0.46              |
| 8:G:76:VAL:O      | 8:G:80:THR:HG22   | 2.15                     | 0.46              |
| 14:M:65:LEU:O     | 14:M:69:ARG:HG3   | 2.16                     | 0.46              |
| 47:t:42:ILE:O     | 47:t:42:ILE:HG22  | 2.15                     | 0.46              |
| 55:B:7:GLY:HA2    | 55:B:23:PRO:HA    | 1.98                     | 0.46              |
| 1:1:613:A:H4'     | 1:1:614:A:OP1     | 2.16                     | 0.46              |
| 1:1:1584:U:H5''   | 1:1:1585:C:O4'    | 2.16                     | 0.46              |
| 2:2:411:A:OP2     | 35:h:26:ARG:NH1   | 2.48                     | 0.46              |
| 5:D:45:TYR:OH     | 5:D:81:GLU:OE2    | 2.34                     | 0.46              |
| 8:G:24:ILE:HD13   | 8:G:72:LEU:HD21   | 1.98                     | 0.46              |
| 9:H:123:ARG:O     | 9:H:124:THR:HG23  | 2.15                     | 0.46              |
| 36:i:160:SER:OG   | 36:i:163:GLU:HG3  | 2.16                     | 0.46              |
| 48:u:48:ASP:OD2   | 48:u:75:LEU:HD21  | 2.16                     | 0.46              |
| 55:B:11:TRP:O     | 55:B:20:PHE:O     | 2.33                     | 0.46              |
| 1:1:1012:U:O4     | 10:I:30:THR:HG21  | 2.16                     | 0.46              |
| 1:1:1818:U:C5     | 4:C:156:ARG:NH1   | 2.84                     | 0.46              |
| 2:2:1168:U:O2'    | 2:2:1169:A:P      | 2.74                     | 0.46              |
| 7:F:19:GLU:O      | 7:F:19:GLU:HG2    | 2.15                     | 0.46              |
| 17:P:104:VAL:HG11 | 18:Q:45:GLU:OE1   | 2.16                     | 0.46              |
| 25:X:18:LEU:HD23  | 25:X:18:LEU:C     | 2.41                     | 0.46              |
| 37:j:88:MET:HE1   | 49:v:61:ARG:HG2   | 1.98                     | 0.46              |
| 38:k:74:GLU:HG2   | 38:k:91:VAL:HG22  | 1.96                     | 0.46              |
| 46:s:5:THR:O      | 46:s:8:THR:OG1    | 2.29                     | 0.46              |
| 47:t:4:ILE:HG12   | 47:t:21:VAL:HG22  | 1.97                     | 0.46              |
| 55:B:13:ASN:ND2   | 55:B:15:ASP:OD2   | 2.49                     | 0.46              |
| 1:1:299:A:N6      | 1:1:322:A:O2'     | 2.47                     | 0.45              |
| 1:1:2795:C:H2'    | 1:1:2796:U:C6     | 2.51                     | 0.45              |
| 2:2:73:C:H2'      | 2:2:74:A:H5'      | 1.98                     | 0.45              |
| 24:W:12:PRO:HB3   | 24:W:30:LEU:HD23  | 1.98                     | 0.45              |
| 28:a:3:VAL:HG22   | 28:a:4:GLN:N      | 2.31                     | 0.45              |
| 34:g:20:SER:OG    | 34:g:40:ARG:NH2   | 2.49                     | 0.45              |
| 41:n:29:ALA:HB2   | 41:n:87:LEU:CD2   | 2.36                     | 0.45              |
| 1:1:570:G:H2'     | 1:1:2030:6MZ:N7   | 2.30                     | 0.45              |
| 1:1:645:C:H2'     | 1:1:647:G:N7      | 2.32                     | 0.45              |
| 1:1:1814:G:OP2    | 1:1:1815:A:O2'    | 2.18                     | 0.45              |
| 1:1:2060:A:O2'    | 1:1:2061:G:OP2    | 2.34                     | 0.45              |
| 1:1:2128:G:N2     | 1:1:2173:A:O2'    | 2.48                     | 0.45              |
| 2:2:406:G:H21     | 35:h:116:GLN:HE22 | 1.64                     | 0.45              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 9:H:66:ASN:OD1   | 9:H:135:HIS:HB2   | 2.16                     | 0.45              |
| 9:H:133:GLN:HG2  | 9:H:139:PHE:CD1   | 2.51                     | 0.45              |
| 9:H:135:HIS:HB3  | 9:H:138:VAL:HG22  | 1.96                     | 0.45              |
| 30:c:22:MET:SD   | 30:c:31:LEU:HD12  | 2.56                     | 0.45              |
| 36:i:149:SER:H   | 36:i:152:MET:CE   | 2.30                     | 0.45              |
| 54:z:72:C:O2'    | 54:z:73:G:H5'     | 2.16                     | 0.45              |
| 1:1:287:G:H2'    | 1:1:288:U:H6      | 1.82                     | 0.45              |
| 1:1:414:C:O2     | 1:1:1864:U:O2'    | 2.32                     | 0.45              |
| 1:1:633:A:O2'    | 1:1:2404:U:OP1    | 2.33                     | 0.45              |
| 1:1:1047:G:N2    | 1:1:1110:G:O2'    | 2.49                     | 0.45              |
| 1:1:1682:G:OP2   | 1:1:1699:G:N2     | 2.43                     | 0.45              |
| 2:2:1183:U:O2'   | 2:2:1185:G:OP2    | 2.34                     | 0.45              |
| 8:G:105:LEU:HD13 | 8:G:107:LEU:HD11  | 1.98                     | 0.45              |
| 23:V:18:ALA:O    | 23:V:20:ARG:NH1   | 2.38                     | 0.45              |
| 27:Z:44:PHE:O    | 27:Z:48:GLN:NE2   | 2.49                     | 0.45              |
| 35:h:106:GLY:HA3 | 35:h:162:ALA:HB2  | 1.99                     | 0.45              |
| 36:i:99:ALA:HB1  | 36:i:103:THR:HG21 | 1.97                     | 0.45              |
| 1:1:898:C:H2'    | 1:1:899:A:O4'     | 2.17                     | 0.45              |
| 1:1:996:A:OP1    | 18:Q:10:LYS:HD2   | 2.16                     | 0.45              |
| 1:1:1796:U:H2'   | 1:1:1797:G:H8     | 1.82                     | 0.45              |
| 2:2:148:G:O2'    | 2:2:1446:A:N3     | 2.46                     | 0.45              |
| 2:2:264:C:O3'    | 48:u:65:ARG:NH2   | 2.50                     | 0.45              |
| 2:2:1128:C:O2'   | 2:2:1147:C:N3     | 2.41                     | 0.45              |
| 14:M:80:PHE:N    | 14:M:80:PHE:HD1   | 2.15                     | 0.45              |
| 19:R:73:LYS:HB2  | 19:R:106:VAL:HB   | 1.99                     | 0.45              |
| 27:Z:56:ARG:O    | 27:Z:59:ARG:HG2   | 2.16                     | 0.45              |
| 37:j:43:GLY:HA2  | 37:j:58:HIS:CE1   | 2.51                     | 0.45              |
| 44:q:31:LYS:HG2  | 44:q:41:GLU:OE2   | 2.16                     | 0.45              |
| 1:1:458:G:O2'    | 1:1:469:G:O6      | 2.32                     | 0.45              |
| 1:1:796:C:OP1    | 6:E:57:LYS:NZ     | 2.40                     | 0.45              |
| 1:1:888:C:C6     | 44:q:92:ARG:HD2   | 2.51                     | 0.45              |
| 1:1:2147:A:N6    | 1:1:2148:G:N2     | 2.65                     | 0.45              |
| 2:2:1218:C:H2'   | 2:2:1219:A:C8     | 2.52                     | 0.45              |
| 41:n:57:VAL:O    | 41:n:58:ASN:CG    | 2.59                     | 0.45              |
| 42:o:16:VAL:HG12 | 42:o:77:TYR:HB3   | 1.99                     | 0.45              |
| 44:q:46:SER:O    | 44:q:47:GLU:HG3   | 2.17                     | 0.45              |
| 1:1:2127:G:H2'   | 1:1:2128:G:O4'    | 2.17                     | 0.45              |
| 2:2:120:A:O2'    | 2:2:122:G:N7      | 2.36                     | 0.45              |
| 2:2:1061:G:OP2   | 34:g:2:GLY:O      | 2.34                     | 0.45              |
| 8:G:46:ALA:C     | 8:G:48:ASN:H      | 2.25                     | 0.45              |
| 9:H:131:SER:HA   | 9:H:140:ALA:O     | 2.17                     | 0.45              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 35:h:73:ARG:HD3  | 35:h:204:TYR:CE1  | 2.51                     | 0.45              |
| 54:z:71:5MU:H5'  | 54:z:71:5MU:C6    | 2.41                     | 0.45              |
| 1:1:878:A:H3'    | 1:1:879:G:H8      | 1.82                     | 0.45              |
| 1:1:2118:U:H5    | 1:1:2149:U:C4     | 2.35                     | 0.45              |
| 1:1:2142:A:N7    | 1:1:2143:C:C4     | 2.85                     | 0.45              |
| 2:2:552:U:H2'    | 2:2:553:A:H8      | 1.81                     | 0.45              |
| 2:2:1323:G:H2'   | 2:2:1324:A:C8     | 2.52                     | 0.45              |
| 3:3:24:G:N7      | 3:3:56:G:H2'      | 2.32                     | 0.45              |
| 24:W:39:TRP:CH2  | 24:W:44:LYS:C     | 2.95                     | 0.45              |
| 35:h:150:LYS:HG3 | 35:h:178:MET:SD   | 2.57                     | 0.45              |
| 1:1:1138:G:H21   | 10:I:108:MET:HE2  | 1.82                     | 0.45              |
| 1:1:1870:C:C6    | 1:1:1870:C:OP1    | 2.70                     | 0.45              |
| 1:1:2328:A:H2'   | 1:1:2329:U:C6     | 2.52                     | 0.45              |
| 2:2:1436:U:H2'   | 2:2:1437:A:H8     | 1.82                     | 0.45              |
| 7:F:38:MET:HE2   | 7:F:57:LEU:HD13   | 1.98                     | 0.45              |
| 9:H:85:GLY:H     | 9:H:90:LEU:HA     | 1.82                     | 0.45              |
| 33:f:10:LEU:HD23 | 33:f:10:LEU:C     | 2.41                     | 0.45              |
| 34:g:51:SER:HB3  | 34:g:115:LEU:HD22 | 1.99                     | 0.45              |
| 34:g:87:LEU:O    | 34:g:91:VAL:HG23  | 2.16                     | 0.45              |
| 34:g:122:SER:O   | 34:g:126:ARG:HG2  | 2.17                     | 0.45              |
| 38:k:93:PRO:HA   | 38:k:96:ARG:HD3   | 1.98                     | 0.45              |
| 1:1:501:A:H2'    | 1:1:502:A:C8      | 2.52                     | 0.45              |
| 1:1:864:G:O2'    | 1:1:914:G:O6      | 2.33                     | 0.45              |
| 1:1:1077:A:C2    | 1:1:1088:A:C2     | 3.04                     | 0.45              |
| 2:2:878:A:P      | 39:l:80:ARG:HH11  | 2.40                     | 0.45              |
| 16:O:34:GLU:OE2  | 16:O:39:ARG:HG2   | 2.17                     | 0.45              |
| 21:T:7:ARG:O     | 21:T:25:VAL:O     | 2.34                     | 0.45              |
| 27:Z:55:GLY:C    | 27:Z:58:ASP:OD1   | 2.60                     | 0.45              |
| 33:f:128:LYS:HD2 | 33:f:128:LYS:O    | 2.16                     | 0.45              |
| 35:h:95:GLU:HA   | 35:h:100:ASN:HD22 | 1.82                     | 0.45              |
| 37:j:74:LEU:HG   | 37:j:78:PHE:CE2   | 2.52                     | 0.45              |
| 45:r:37:SER:HG   | 45:r:40:ASP:CG    | 2.25                     | 0.45              |
| 51:x:8:LYS:O     | 51:x:12:ILE:HG13  | 2.17                     | 0.45              |
| 1:1:745:1MG:HN22 | 1:1:750:A:H61     | 1.65                     | 0.45              |
| 1:1:2139:U:O2    | 1:1:2140:G:N7     | 2.50                     | 0.45              |
| 1:1:2532:G:O2'   | 1:1:2657:A:N1     | 2.50                     | 0.45              |
| 2:2:269:C:H2'    | 2:2:270:A:C8      | 2.52                     | 0.45              |
| 8:G:102:VAL:HG22 | 8:G:116:GLN:OE1   | 2.17                     | 0.45              |
| 14:M:63:ARG:HD3  | 14:M:80:PHE:CD2   | 2.52                     | 0.45              |
| 25:X:38:GLN:HG2  | 55:B:15:ASP:OD2   | 2.16                     | 0.45              |
| 34:g:123:GLN:HB3 | 34:g:128:VAL:CG2  | 2.47                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 40:m:25:ASN:ND2  | 40:m:25:ASN:C    | 2.74                     | 0.45              |
| 1:1:1081:U:C2    | 1:1:1082:U:C5    | 3.05                     | 0.44              |
| 1:1:1494:A:H2'   | 1:1:1495:A:C8    | 2.52                     | 0.44              |
| 1:1:2140:G:N1    | 1:1:2151:U:N3    | 2.65                     | 0.44              |
| 1:1:2676:C:OP1   | 11:J:31:ARG:NH2  | 2.51                     | 0.44              |
| 9:H:70:GLU:OE1   | 9:H:140:ALA:HB2  | 2.17                     | 0.44              |
| 9:H:70:GLU:CD    | 9:H:140:ALA:HB2  | 2.43                     | 0.44              |
| 11:J:7:MET:SD    | 11:J:20:MET:HB2  | 2.56                     | 0.44              |
| 19:R:70:LYS:N    | 19:R:108:SER:O   | 2.50                     | 0.44              |
| 33:f:3:THR:O     | 33:f:3:THR:HG22  | 2.17                     | 0.44              |
| 44:q:33:ILE:HD11 | 44:q:63:PHE:HE2  | 1.82                     | 0.44              |
| 54:z:49:G:O2'    | 54:z:50:C:C4     | 2.70                     | 0.44              |
| 1:1:645:C:H2'    | 1:1:647:G:C8     | 2.52                     | 0.44              |
| 1:1:863:A:O3'    | 3:3:100:G:N2     | 2.49                     | 0.44              |
| 1:1:995:C:O2     | 10:I:3:THR:OG1   | 2.31                     | 0.44              |
| 1:1:2143:C:H2'   | 1:1:2144:G:O4'   | 2.18                     | 0.44              |
| 1:1:2394:C:OP1   | 31:d:30:ARG:NH2  | 2.50                     | 0.44              |
| 2:2:81:A:OP2     | 2:2:83:C:N4      | 2.48                     | 0.44              |
| 2:2:1000:A:C6    | 2:2:1041:G:C6    | 3.05                     | 0.44              |
| 12:K:29:LYS:HG3  | 12:K:30:THR:HG23 | 1.97                     | 0.44              |
| 33:f:116:ASP:OD1 | 33:f:117:LEU:N   | 2.51                     | 0.44              |
| 37:j:42:TRP:HB2  | 37:j:59:TYR:HB2  | 1.98                     | 0.44              |
| 37:j:42:TRP:HZ2  | 37:j:61:LEU:HD22 | 1.81                     | 0.44              |
| 40:m:83:ILE:O    | 40:m:87:LEU:HD13 | 2.17                     | 0.44              |
| 45:r:10:GLU:O    | 45:r:14:VAL:HG23 | 2.17                     | 0.44              |
| 50:w:32:ARG:HH21 | 50:w:32:ARG:HG3  | 1.82                     | 0.44              |
| 50:w:63:THR:HG22 | 50:w:64:ASP:N    | 2.33                     | 0.44              |
| 1:1:880:G:C2     | 1:1:881:G:C8     | 3.06                     | 0.44              |
| 1:1:1871:A:H1'   | 1:1:1872:A:C8    | 2.53                     | 0.44              |
| 2:2:1317:C:P     | 45:r:28:LYS:NZ   | 2.90                     | 0.44              |
| 7:F:119:ALA:HB1  | 7:F:167:ARG:HE   | 1.82                     | 0.44              |
| 36:i:45:ARG:HA   | 36:i:72:ILE:O    | 2.17                     | 0.44              |
| 38:k:65:ALA:HB1  | 38:k:127:ALA:HB3 | 2.00                     | 0.44              |
| 44:q:49:SER:HB3  | 44:q:52:GLN:HG3  | 1.99                     | 0.44              |
| 1:1:883:G:N2     | 1:1:884:U:C4     | 2.85                     | 0.44              |
| 1:1:1169:A:H62   | 1:1:1180:U:H3    | 1.66                     | 0.44              |
| 1:1:2190:G:C6    | 1:1:2191:A:C6    | 3.06                     | 0.44              |
| 2:2:475:C:H2'    | 2:2:476:U:H6     | 1.82                     | 0.44              |
| 2:2:1006:G:H2'   | 2:2:1007:U:C6    | 2.53                     | 0.44              |
| 7:F:148:ARG:HG2  | 7:F:150:ARG:NH1  | 2.33                     | 0.44              |
| 9:H:68:ARG:O     | 9:H:72:ILE:HG12  | 2.18                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 18:Q:52:PRO:O    | 18:Q:53:PHE:CD2  | 2.71                     | 0.44              |
| 20:S:69:ARG:HH12 | 55:B:34:PHE:CB   | 2.30                     | 0.44              |
| 25:X:35:GLY:O    | 55:B:15:ASP:HA   | 2.16                     | 0.44              |
| 27:Z:18:CYS:SG   | 27:Z:20:ASN:HB2  | 2.57                     | 0.44              |
| 34:g:8:ASN:O     | 34:g:12:LEU:HG   | 2.18                     | 0.44              |
| 34:g:140:ASN:OD1 | 34:g:143:ARG:NH2 | 2.51                     | 0.44              |
| 50:w:3:ARG:HH21  | 50:w:7:LYS:HD3   | 1.83                     | 0.44              |
| 54:z:21:A:H1'    | 54:z:22:G:O5'    | 2.17                     | 0.44              |
| 1:1:636:G:N2     | 12:K:76:GLU:OE1  | 2.38                     | 0.44              |
| 1:1:1149:G:H2'   | 1:1:1150:C:C6    | 2.52                     | 0.44              |
| 1:1:1527:G:N1    | 1:1:1544:A:OP2   | 2.35                     | 0.44              |
| 1:1:2127:G:P     | 1:1:2162:G:H22   | 2.40                     | 0.44              |
| 2:2:672:U:H2'    | 2:2:673:A:C8     | 2.53                     | 0.44              |
| 2:2:1071:C:OP1   | 36:i:54:ARG:NH2  | 2.50                     | 0.44              |
| 2:2:1414:U:H2'   | 2:2:1415:G:H8    | 1.80                     | 0.44              |
| 2:2:1530:G:H2'   | 2:2:1531:A:H8    | 1.83                     | 0.44              |
| 4:C:41:GLY:O     | 4:C:43:ARG:NH1   | 2.50                     | 0.44              |
| 8:G:89:LEU:HD12  | 8:G:89:LEU:N     | 2.32                     | 0.44              |
| 14:M:80:PHE:N    | 14:M:80:PHE:CD1  | 2.84                     | 0.44              |
| 27:Z:53:THR:HG23 | 27:Z:54:GLY:N    | 2.32                     | 0.44              |
| 28:a:30:VAL:HG22 | 28:a:37:LYS:HG2  | 1.99                     | 0.44              |
| 34:g:131:ARG:O   | 34:g:135:LYS:HG3 | 2.18                     | 0.44              |
| 41:n:5:ARG:HD3   | 41:n:5:ARG:N     | 2.33                     | 0.44              |
| 54:z:3:G:O2'     | 54:z:4:G:H5'     | 2.18                     | 0.44              |
| 1:1:1298:C:H2'   | 1:1:1299:G:O4'   | 2.17                     | 0.44              |
| 1:1:1588:G:N1    | 1:1:1589:U:O4    | 2.51                     | 0.44              |
| 1:1:2134:A:O2'   | 1:1:2159:G:H1'   | 2.18                     | 0.44              |
| 1:1:2511:U:O4    | 1:1:2575:C:N3    | 2.51                     | 0.44              |
| 1:1:2512:C:H2'   | 1:1:2513:A:O4'   | 2.17                     | 0.44              |
| 1:1:2847:U:H2'   | 1:1:2848:G:O4'   | 2.17                     | 0.44              |
| 2:2:1126:U:P     | 41:n:7:ARG:HH22  | 2.40                     | 0.44              |
| 2:2:1238:A:H2    | 2:2:1241:G:N3    | 2.15                     | 0.44              |
| 5:D:48:ILE:HG23  | 5:D:84:LEU:HD11  | 2.00                     | 0.44              |
| 14:M:54:LEU:HD11 | 14:M:62:ASN:HD22 | 1.83                     | 0.44              |
| 31:d:55:LEU:O    | 31:d:59:ILE:HG13 | 2.17                     | 0.44              |
| 42:o:86:VAL:HG11 | 42:o:93:ARG:HE   | 1.83                     | 0.44              |
| 54:z:84:C:H2'    | 54:z:85:A:O4'    | 2.16                     | 0.44              |
| 1:1:1196:C:H2'   | 1:1:1197:G:O4'   | 2.18                     | 0.44              |
| 1:1:1587:G:C2    | 1:1:1588:G:C8    | 3.05                     | 0.44              |
| 1:1:2188:U:O4    | 1:1:2189:U:C4    | 2.71                     | 0.44              |
| 2:2:1425:U:H2'   | 2:2:1426:G:H8    | 1.82                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 12:K:57:LEU:HD13  | 12:K:60:ARG:HH11  | 1.82                     | 0.44              |
| 15:N:93:ASP:OD1   | 15:N:95:SER:N     | 2.50                     | 0.44              |
| 35:h:170:TRP:CD2  | 35:h:186:PRO:HB3  | 2.53                     | 0.44              |
| 38:k:23:LEU:O     | 38:k:27:VAL:HG13  | 2.17                     | 0.44              |
| 39:l:5:ASP:CG     | 39:l:77:ARG:HH12  | 2.25                     | 0.44              |
| 41:n:73:LEU:C     | 41:n:73:LEU:HD23  | 2.42                     | 0.44              |
| 44:q:52:GLN:O     | 44:q:56:LEU:HG    | 2.17                     | 0.44              |
| 44:q:81:MET:HE2   | 44:q:91:HIS:HB3   | 1.98                     | 0.44              |
| 48:u:68:SER:OG    | 48:u:69:LYS:N     | 2.49                     | 0.44              |
| 1:1:565:C:H2'     | 1:1:566:U:O4'     | 2.17                     | 0.44              |
| 1:1:1190:G:H5''   | 12:K:32:GLY:HA2   | 1.99                     | 0.44              |
| 1:1:2286:G:H4'    | 1:1:2287:A:O4'    | 2.18                     | 0.44              |
| 1:1:2496:C:H2'    | 1:1:2497:A:O4'    | 2.18                     | 0.44              |
| 9:H:125:THR:O     | 9:H:125:THR:HG23  | 2.17                     | 0.44              |
| 13:L:47:GLU:CD    | 13:L:51:ARG:NE    | 2.76                     | 0.44              |
| 27:Z:58:ASP:O     | 27:Z:62:LYS:HB2   | 2.18                     | 0.44              |
| 37:j:1:MET:HE2    | 37:j:67:PRO:HD3   | 2.00                     | 0.44              |
| 41:n:81:GLU:OE1   | 41:n:81:GLU:N     | 2.48                     | 0.44              |
| 1:1:2031:A:C6     | 1:1:2498:OMC:H1'  | 2.53                     | 0.44              |
| 1:1:2116:G:N2     | 1:1:2161:C:P      | 2.91                     | 0.44              |
| 1:1:2189:U:C2     | 1:1:2190:G:C8     | 3.06                     | 0.44              |
| 1:1:2561:U:O3'    | 11:J:40:LYS:HE3   | 2.18                     | 0.44              |
| 2:2:1402:4OC:HM22 | 2:2:1403:C:H5'    | 2.00                     | 0.44              |
| 7:F:57:LEU:HD21   | 7:F:89:VAL:HG23   | 2.00                     | 0.44              |
| 34:g:76:VAL:O     | 34:g:83:ASP:HB2   | 2.17                     | 0.44              |
| 40:m:112:GLU:OE2  | 40:m:115:LYS:NZ   | 2.46                     | 0.44              |
| 1:1:356:G:C5      | 1:1:357:C:C5      | 3.06                     | 0.43              |
| 1:1:2030:6MZ:H2   | 1:1:2499:C:H5''   | 2.00                     | 0.43              |
| 9:H:85:GLY:HA2    | 9:H:125:THR:H     | 1.82                     | 0.43              |
| 33:f:218:ALA:HA   | 33:f:221:VAL:HG22 | 2.00                     | 0.43              |
| 34:g:118:ASP:OD1  | 34:g:118:ASP:C    | 2.61                     | 0.43              |
| 41:n:96:VAL:O     | 41:n:96:VAL:HG23  | 2.18                     | 0.43              |
| 43:p:54:ARG:HD2   | 43:p:62:GLU:HG3   | 2.00                     | 0.43              |
| 54:z:39:5MU:H2'   | 54:z:40:5MU:O4'   | 2.17                     | 0.43              |
| 1:1:273:G:N2      | 1:1:365:U:C2      | 2.86                     | 0.43              |
| 1:1:1955:U:C5     | 1:1:2552:OMU:H1'  | 2.54                     | 0.43              |
| 25:X:42:LEU:O     | 25:X:46:VAL:HG23  | 2.18                     | 0.43              |
| 27:Z:36:VAL:HA    | 27:Z:40:CYS:SG    | 2.58                     | 0.43              |
| 39:l:9:ASP:O      | 39:l:13:ARG:HG3   | 2.18                     | 0.43              |
| 39:l:55:THR:HG23  | 39:l:56:LYS:N     | 2.33                     | 0.43              |
| 41:n:45:ARG:HB3   | 41:n:69:THR:HB    | 2.01                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 52:y:7:ARG:N     | 52:y:10:GLU:OE1  | 2.44                     | 0.43              |
| 52:y:39:GLU:OE2  | 52:y:43:THR:HG22 | 2.18                     | 0.43              |
| 54:z:55:5MU:N3   | 54:z:56:G:C8     | 2.86                     | 0.43              |
| 1:1:57:C:H2'     | 1:1:58:G:O4'     | 2.18                     | 0.43              |
| 1:1:243:U:OP2    | 31:d:8:ARG:NH1   | 2.52                     | 0.43              |
| 1:1:323:C:H2'    | 6:E:163:ASN:OD1  | 2.17                     | 0.43              |
| 1:1:1789:A:OP2   | 4:C:221:ARG:NH1  | 2.51                     | 0.43              |
| 1:1:2021:C:OP1   | 28:a:9:THR:HG21  | 2.18                     | 0.43              |
| 1:1:2079:U:O2'   | 24:W:23:ASN:OD1  | 2.32                     | 0.43              |
| 2:2:135:C:O2     | 47:t:1:MET:N     | 2.51                     | 0.43              |
| 2:2:837:U:H2'    | 2:2:838:G:H8     | 1.84                     | 0.43              |
| 2:2:1217:C:P     | 45:r:9:ARG:HH21  | 2.40                     | 0.43              |
| 2:2:1222:G:H5''  | 50:w:78:ARG:HD2  | 2.00                     | 0.43              |
| 2:2:1518:MA6:O5' | 2:2:1518:MA6:H8  | 2.19                     | 0.43              |
| 8:G:60:ASP:OD1   | 8:G:60:ASP:N     | 2.50                     | 0.43              |
| 9:H:85:GLY:O     | 9:H:88:GLY:O     | 2.35                     | 0.43              |
| 9:H:116:ARG:HG3  | 9:H:133:GLN:HB2  | 2.01                     | 0.43              |
| 9:H:117:LEU:HG   | 9:H:130:VAL:HG23 | 2.00                     | 0.43              |
| 14:M:71:ARG:HD2  | 14:M:71:ARG:HA   | 1.86                     | 0.43              |
| 16:O:88:ARG:NH2  | 16:O:110:ILE:O   | 2.46                     | 0.43              |
| 18:Q:9:GLY:C     | 18:Q:10:LYS:HG3  | 2.42                     | 0.43              |
| 36:i:64:MET:O    | 36:i:68:ARG:HG3  | 2.18                     | 0.43              |
| 49:v:25:ASP:O    | 49:v:29:LEU:HD13 | 2.19                     | 0.43              |
| 1:1:807:U:OP1    | 12:K:36:LYS:HE2  | 2.18                     | 0.43              |
| 1:1:811:U:O4     | 12:K:21:ARG:NH1  | 2.51                     | 0.43              |
| 1:1:882:G:N1     | 1:1:895:U:O2     | 2.51                     | 0.43              |
| 1:1:1056:G:N2    | 1:1:1104:C:N4    | 2.67                     | 0.43              |
| 1:1:1722:A:O2'   | 1:1:1723:G:H5'   | 2.19                     | 0.43              |
| 1:1:2687:U:H2'   | 1:1:2688:G:O4'   | 2.19                     | 0.43              |
| 2:2:51:A:N7      | 2:2:114:U:O2'    | 2.51                     | 0.43              |
| 2:2:181:A:N6     | 2:2:195:A:C8     | 2.86                     | 0.43              |
| 2:2:420:U:N3     | 2:2:422:C:N3     | 2.66                     | 0.43              |
| 2:2:451:A:H4'    | 2:2:452:A:O4'    | 2.18                     | 0.43              |
| 7:F:117:LEU:O    | 7:F:177:PHE:O    | 2.36                     | 0.43              |
| 9:H:14:SER:OG    | 9:H:15:LEU:N     | 2.51                     | 0.43              |
| 9:H:70:GLU:OE2   | 9:H:140:ALA:HA   | 2.18                     | 0.43              |
| 34:g:130:PHE:O   | 34:g:134:MET:HG3 | 2.18                     | 0.43              |
| 35:h:3:ARG:HH12  | 35:h:5:LEU:HD21  | 1.83                     | 0.43              |
| 1:1:72:U:O4      | 25:X:58:ASN:ND2  | 2.51                     | 0.43              |
| 1:1:373:U:H2'    | 1:1:374:A:H8     | 1.82                     | 0.43              |
| 1:1:887:A:O2'    | 1:1:889:C:H5     | 2.02                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1:1138:G:N2     | 10:I:108:MET:HE2  | 2.33                     | 0.43              |
| 1:1:1496:A:N3     | 1:1:1577:C:O2'    | 2.46                     | 0.43              |
| 1:1:1883:U:H2'    | 1:1:1884:G:O4'    | 2.19                     | 0.43              |
| 1:1:2125:G:H21    | 1:1:2174:C:N4     | 2.15                     | 0.43              |
| 1:1:2190:G:H2'    | 1:1:2191:A:C8     | 2.54                     | 0.43              |
| 1:1:2322:A:H2'    | 1:1:2323:G:O4'    | 2.18                     | 0.43              |
| 1:1:2497:A:N3     | 1:1:2498:OMC:N4   | 2.62                     | 0.43              |
| 2:2:1128:C:H1'    | 2:2:1147:C:H42    | 1.83                     | 0.43              |
| 7:F:57:LEU:HD22   | 7:F:65:PRO:HB3    | 2.00                     | 0.43              |
| 7:F:141:ILE:HG23  | 7:F:146:VAL:CG1   | 2.48                     | 0.43              |
| 11:J:12:ASP:OD2   | 11:J:14:SER:OG    | 2.37                     | 0.43              |
| 14:M:29:VAL:O     | 14:M:78:LYS:NZ    | 2.39                     | 0.43              |
| 20:S:93:LEU:HD23  | 20:S:94:ASP:C     | 2.43                     | 0.43              |
| 27:Z:60:PHE:CE2   | 50:w:42:PRO:HD3   | 2.54                     | 0.43              |
| 34:g:111:LEU:HD22 | 34:g:146:ALA:HB2  | 1.99                     | 0.43              |
| 35:h:124:MET:HE3  | 35:h:146:ARG:CG   | 2.47                     | 0.43              |
| 38:k:47:LEU:HD23  | 38:k:58:GLU:HB3   | 1.99                     | 0.43              |
| 38:k:137:LYS:O    | 38:k:141:VAL:HG23 | 2.19                     | 0.43              |
| 50:w:30:PRO:HA    | 50:w:48:THR:O     | 2.19                     | 0.43              |
| 1:1:973:A:OP2     | 18:Q:81:LYS:HE3   | 2.18                     | 0.43              |
| 1:1:2498:OMC:HM22 | 1:1:2499:C:H5'    | 2.00                     | 0.43              |
| 1:1:2884:U:O2'    | 1:1:2885:G:C8     | 2.72                     | 0.43              |
| 2:2:910:C:H2'     | 2:2:911:U:O4'     | 2.18                     | 0.43              |
| 2:2:1119:C:OP2    | 40:m:11:ARG:NH1   | 2.51                     | 0.43              |
| 2:2:1309:G:OP2    | 44:q:98:ARG:NE    | 2.44                     | 0.43              |
| 34:g:7:PRO:HA     | 34:g:10:ILE:HG22  | 1.99                     | 0.43              |
| 34:g:186:THR:HG23 | 34:g:198:VAL:O    | 2.18                     | 0.43              |
| 36:i:137:VAL:O    | 36:i:141:ILE:HG12 | 2.18                     | 0.43              |
| 36:i:154:ALA:HB2  | 36:i:164:ILE:HD12 | 2.00                     | 0.43              |
| 45:r:80:SER:O     | 45:r:84:VAL:HG23  | 2.18                     | 0.43              |
| 1:1:102:U:H5''    | 1:1:102:U:O2      | 2.19                     | 0.43              |
| 1:1:1980:G:O2'    | 1:1:1982:U:OP2    | 2.33                     | 0.43              |
| 1:1:2128:G:H2'    | 1:1:2129:C:O4'    | 2.17                     | 0.43              |
| 1:1:2150:C:H2'    | 1:1:2151:U:C6     | 2.54                     | 0.43              |
| 2:2:1175:G:N3     | 2:2:1176:A:C8     | 2.86                     | 0.43              |
| 6:E:113:VAL:HG22  | 6:E:118:LEU:HD23  | 2.01                     | 0.43              |
| 9:H:4:ILE:HA      | 9:H:17:ASP:O      | 2.19                     | 0.43              |
| 30:c:12:ARG:HG2   | 30:c:44:VAL:HG11  | 2.00                     | 0.43              |
| 43:p:23:ALA:O     | 43:p:59:ASN:ND2   | 2.52                     | 0.43              |
| 46:s:78:TYR:O     | 46:s:82:ILE:HG12  | 2.18                     | 0.43              |
| 55:B:8:ILE:O      | 55:B:21:ILE:CG2   | 2.67                     | 0.43              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:1:880:G:C6     | 1:1:881:G:N7      | 2.87                     | 0.43              |
| 1:1:1060:U:O2    | 1:1:1088:A:C8     | 2.72                     | 0.43              |
| 1:1:1539:U:H2'   | 1:1:1540:G:H8     | 1.84                     | 0.43              |
| 2:2:335:C:O2'    | 2:2:1433:A:N3     | 2.50                     | 0.43              |
| 11:J:108:ARG:HG2 | 11:J:116:ILE:HG21 | 2.00                     | 0.43              |
| 34:g:58:GLU:OE2  | 41:n:94:ALA:HB3   | 2.17                     | 0.43              |
| 35:h:107:PHE:CE1 | 35:h:159:LEU:HD21 | 2.52                     | 0.43              |
| 43:p:88:LYS:C    | 43:p:90:LEU:H     | 2.27                     | 0.43              |
| 54:z:1:G:C5      | 54:z:82:A:C2      | 3.07                     | 0.43              |
| 54:z:8:5MU:O4    | 54:z:14:A:C8      | 2.71                     | 0.43              |
| 1:1:3:U:H2'      | 1:1:4:U:C6        | 2.54                     | 0.43              |
| 1:1:12:U:H2'     | 1:1:12:U:O2       | 2.18                     | 0.43              |
| 1:1:189:G:O6     | 1:1:205:G:O2'     | 2.31                     | 0.43              |
| 1:1:588:U:O4     | 1:1:670:A:H1'     | 2.19                     | 0.43              |
| 1:1:818:G:N1     | 1:1:1188:U:OP2    | 2.39                     | 0.43              |
| 1:1:1342:A:O2'   | 1:1:1344:U:OP2    | 2.27                     | 0.43              |
| 1:1:1675:C:H2'   | 1:1:1676:A:O4'    | 2.18                     | 0.43              |
| 1:1:1841:U:C4    | 1:1:1842:G:N7     | 2.87                     | 0.43              |
| 1:1:1932:A:H2'   | 1:1:1933:G:O4'    | 2.19                     | 0.43              |
| 1:1:2092:U:N3    | 1:1:2226:C:OP2    | 2.42                     | 0.43              |
| 1:1:2102:G:N1    | 1:1:2188:U:N3     | 2.66                     | 0.43              |
| 1:1:2184:A:H2'   | 1:1:2185:U:C6     | 2.54                     | 0.43              |
| 1:1:2192:U:H2'   | 1:1:2193:G:O4'    | 2.19                     | 0.43              |
| 1:1:2301:C:H2'   | 1:1:2302:U:C6     | 2.53                     | 0.43              |
| 1:1:2639:A:H2'   | 1:1:2640:G:O4'    | 2.19                     | 0.43              |
| 1:1:2793:C:H2'   | 1:1:2794:C:H6     | 1.84                     | 0.43              |
| 2:2:429:U:O2     | 2:2:430:A:C8      | 2.72                     | 0.43              |
| 8:G:88:GLN:C     | 8:G:89:LEU:HD12   | 2.44                     | 0.43              |
| 19:R:15:GLN:O    | 19:R:19:LEU:HD13  | 2.19                     | 0.43              |
| 19:R:85:ILE:HD12 | 19:R:85:ILE:N     | 2.33                     | 0.43              |
| 33:f:131:LYS:O   | 33:f:135:LEU:HD23 | 2.18                     | 0.43              |
| 40:m:54:LEU:HD12 | 40:m:54:LEU:HA    | 1.86                     | 0.43              |
| 44:q:20:THR:HA   | 44:q:25:VAL:HG23  | 2.01                     | 0.43              |
| 46:s:3:LEU:HB2   | 46:s:35:GLN:OE1   | 2.19                     | 0.43              |
| 1:1:894:U:HO2'   | 1:1:895:U:P       | 2.35                     | 0.43              |
| 1:1:1130:U:N3    | 1:1:2025:C:OP1    | 2.43                     | 0.43              |
| 1:1:1413:A:C5    | 1:1:1414:C:C5     | 3.07                     | 0.43              |
| 2:2:526:C:OP2    | 43:p:88:LYS:HE3   | 2.19                     | 0.43              |
| 2:2:958:A:C8     | 50:w:55:ARG:NH1   | 2.87                     | 0.43              |
| 2:2:1380:U:C4    | 38:k:3:ARG:HG2    | 2.53                     | 0.43              |
| 6:E:117:ARG:NH2  | 6:E:183:PHE:O     | 2.46                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:H:135:HIS:HB3   | 9:H:138:VAL:H     | 1.82                     | 0.43              |
| 38:k:103:TRP:HA   | 38:k:106:GLU:HG2  | 2.01                     | 0.43              |
| 48:u:19:LYS:HA    | 48:u:48:ASP:O     | 2.19                     | 0.43              |
| 55:B:8:ILE:N      | 55:B:22:THR:O     | 2.52                     | 0.43              |
| 1:1:2025:C:H2'    | 1:1:2026:U:C6     | 2.54                     | 0.42              |
| 1:1:2822:G:OP1    | 5:D:164:GLN:NE2   | 2.50                     | 0.42              |
| 2:2:212:G:C2      | 2:2:213:G:C8      | 3.07                     | 0.42              |
| 2:2:891:U:H2'     | 2:2:892:A:H8      | 1.83                     | 0.42              |
| 2:2:1518:MA6:H103 | 2:2:1519:MA6:N6   | 2.34                     | 0.42              |
| 4:C:69:ARG:NH1    | 4:C:129:THR:OG1   | 2.52                     | 0.42              |
| 7:F:7:TYR:O       | 7:F:10:ASP:OD1    | 2.36                     | 0.42              |
| 7:F:135:GLN:CD    | 7:F:150:ARG:H     | 2.27                     | 0.42              |
| 21:T:36:VAL:HG12  | 21:T:39:ILE:HD12  | 1.99                     | 0.42              |
| 32:e:3:VAL:HA     | 32:e:36:ARG:O     | 2.19                     | 0.42              |
| 33:f:130:THR:O    | 33:f:133:GLU:N    | 2.50                     | 0.42              |
| 36:i:159:LYS:NZ   | 39:l:42:GLU:O     | 2.44                     | 0.42              |
| 44:q:89:LEU:HD23  | 44:q:92:ARG:NE    | 2.34                     | 0.42              |
| 1:1:281:C:H2'     | 1:1:282:A:H8      | 1.84                     | 0.42              |
| 1:1:1419:A:O2'    | 1:1:1421:G:N7     | 2.37                     | 0.42              |
| 1:1:2081:U:H2'    | 1:1:2082:A:H8     | 1.83                     | 0.42              |
| 2:2:439:U:O2      | 2:2:439:U:O4'     | 2.36                     | 0.42              |
| 2:2:460:A:H2'     | 2:2:461:A:H8      | 1.84                     | 0.42              |
| 3:3:15:A:O4'      | 3:3:109:A:C8      | 2.72                     | 0.42              |
| 9:H:70:GLU:OE2    | 9:H:139:PHE:O     | 2.37                     | 0.42              |
| 9:H:89:LYS:HG3    | 9:H:148:ALA:HB1   | 2.01                     | 0.42              |
| 18:Q:93:PHE:C     | 18:Q:93:PHE:CD1   | 2.97                     | 0.42              |
| 34:g:47:LEU:HB3   | 34:g:50:ALA:HB3   | 2.01                     | 0.42              |
| 39:l:7:ILE:O      | 39:l:11:LEU:HG    | 2.18                     | 0.42              |
| 42:o:84:VAL:HG23  | 42:o:107:ILE:HD11 | 2.01                     | 0.42              |
| 50:w:41:PHE:N     | 50:w:44:MET:SD    | 2.72                     | 0.42              |
| 1:1:1266:G:N7     | 19:R:16:LYS:HE3   | 2.34                     | 0.42              |
| 1:1:1407:G:H3'    | 1:1:1408:G:H5''   | 2.00                     | 0.42              |
| 1:1:2070:A:H2'    | 1:1:2071:A:O4'    | 2.20                     | 0.42              |
| 1:1:2147:A:H62    | 1:1:2148:G:N2     | 2.17                     | 0.42              |
| 1:1:2412:A:H2'    | 1:1:2413:G:O4'    | 2.20                     | 0.42              |
| 2:2:45:G:H5''     | 2:2:307:C:O2'     | 2.19                     | 0.42              |
| 2:2:81:A:N1       | 2:2:88:U:O4       | 2.52                     | 0.42              |
| 2:2:481:G:O2'     | 2:2:483:C:N4      | 2.43                     | 0.42              |
| 2:2:552:U:H2'     | 2:2:553:A:C8      | 2.53                     | 0.42              |
| 2:2:1518:MA6:H103 | 2:2:1519:MA6:C9   | 2.48                     | 0.42              |
| 4:C:145:GLU:HB2   | 4:C:188:CYS:HB3   | 2.01                     | 0.42              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 13:L:53:MET:O     | 13:L:57:VAL:HG22 | 2.19                     | 0.42              |
| 16:O:63:LYS:HE2   | 16:O:65:SER:HB2  | 2.02                     | 0.42              |
| 20:S:72:GLN:NE2   | 55:B:34:PHE:N    | 2.67                     | 0.42              |
| 27:Z:59:ARG:O     | 27:Z:63:ARG:HG3  | 2.19                     | 0.42              |
| 43:p:16:VAL:HG23  | 43:p:16:VAL:O    | 2.19                     | 0.42              |
| 52:y:28:VAL:O     | 52:y:32:VAL:HG23 | 2.19                     | 0.42              |
| 1:1:362:A:C4      | 1:1:363:G:C8     | 3.08                     | 0.42              |
| 1:1:2102:G:N2     | 1:1:2188:U:C2    | 2.88                     | 0.42              |
| 1:1:2591:C:H2'    | 1:1:2592:G:H8    | 1.82                     | 0.42              |
| 4:C:202:LEU:HD23  | 4:C:202:LEU:HA   | 1.89                     | 0.42              |
| 7:F:61:SER:HB2    | 7:F:91:LEU:HD21  | 2.01                     | 0.42              |
| 10:I:118:MET:HA   | 10:I:121:LYS:HE2 | 2.00                     | 0.42              |
| 23:V:53:CYS:SG    | 23:V:57:HIS:HA   | 2.60                     | 0.42              |
| 24:W:40:VAL:HG12  | 24:W:43:GLU:H    | 1.84                     | 0.42              |
| 27:Z:41:HIS:O     | 27:Z:44:PHE:CE1  | 2.73                     | 0.42              |
| 36:i:13:GLU:HG2   | 36:i:39:VAL:HG22 | 2.01                     | 0.42              |
| 43:p:108:LYS:NZ   | 43:p:109:ASP:HB2 | 2.34                     | 0.42              |
| 1:1:996:A:O4'     | 18:Q:10:LYS:HG2  | 2.19                     | 0.42              |
| 1:1:1058:U:C2     | 1:1:1059:G:C8    | 3.08                     | 0.42              |
| 1:1:1059:G:C2     | 1:1:1080:A:C2    | 3.08                     | 0.42              |
| 1:1:1315:C:O2'    | 1:1:1392:A:N3    | 2.49                     | 0.42              |
| 1:1:1584:U:C5'    | 1:1:1585:C:C6    | 3.02                     | 0.42              |
| 1:1:1746:A:H2'    | 1:1:1747:U:C6    | 2.55                     | 0.42              |
| 1:1:1817:G:O5'    | 4:C:156:ARG:NH2  | 2.52                     | 0.42              |
| 1:1:2121:G:H2'    | 1:1:2122:U:C6    | 2.54                     | 0.42              |
| 1:1:2189:U:O2'    | 1:1:2190:G:H5''  | 2.19                     | 0.42              |
| 1:1:2305:U:H5''   | 7:F:131:GLY:HA3  | 2.02                     | 0.42              |
| 1:1:2350:C:H2'    | 1:1:2351:G:O4'   | 2.19                     | 0.42              |
| 1:1:2484:G:OP1    | 13:L:44:ARG:NH1  | 2.48                     | 0.42              |
| 2:2:1227:A:C2     | 2:2:1228:C:C6    | 3.08                     | 0.42              |
| 3:3:2:G:H2'       | 3:3:3:C:C6       | 2.55                     | 0.42              |
| 7:F:17:MET:SD     | 7:F:22:TYR:HB2   | 2.58                     | 0.42              |
| 7:F:113:ASP:OD1   | 44:q:71:ARG:NH2  | 2.52                     | 0.42              |
| 9:H:91:PHE:N      | 9:H:91:PHE:CD1   | 2.84                     | 0.42              |
| 9:H:100:ALA:HA    | 9:H:103:VAL:HG12 | 2.01                     | 0.42              |
| 9:H:130:VAL:HG13  | 9:H:130:VAL:O    | 2.20                     | 0.42              |
| 33:f:117:LEU:HD11 | 33:f:137:ARG:HD2 | 2.01                     | 0.42              |
| 44:q:53:ILE:HG22  | 44:q:57:ARG:CZ   | 2.49                     | 0.42              |
| 54:z:19:G:O4'     | 54:z:20:5MU:OP2  | 2.38                     | 0.42              |
| 55:B:8:ILE:HG22   | 55:B:9:VAL:N     | 2.34                     | 0.42              |
| 1:1:643:A:N6      | 1:1:2369:A:C2    | 2.88                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:1:1011:G:OP2   | 17:P:66:ASN:ND2  | 2.49                     | 0.42              |
| 1:1:1802:A:H2'   | 1:1:1803:A:C8    | 2.55                     | 0.42              |
| 1:1:2147:A:N6    | 1:1:2148:G:H21   | 2.17                     | 0.42              |
| 1:1:2457:PSU:HN3 | 1:1:2494:G:H1    | 1.65                     | 0.42              |
| 2:2:8:A:C6       | 35:h:206:LYS:HD2 | 2.55                     | 0.42              |
| 5:D:153:GLY:O    | 5:D:154:LYS:HB3  | 2.18                     | 0.42              |
| 9:H:81:ALA:HA    | 9:H:147:VAL:HB   | 2.00                     | 0.42              |
| 9:H:138:VAL:O    | 9:H:138:VAL:CG2  | 2.66                     | 0.42              |
| 39:l:55:THR:HG23 | 39:l:56:LYS:HG2  | 2.02                     | 0.42              |
| 53:4:3:U:O2      | 53:4:3:U:O4'     | 2.37                     | 0.42              |
| 54:z:50:C:O2     | 54:z:52:A:C2     | 2.72                     | 0.42              |
| 1:1:142:A:H2'    | 1:1:143:C:C6     | 2.54                     | 0.42              |
| 1:1:270:A:H5'    | 1:1:271:G:H5''   | 2.02                     | 0.42              |
| 1:1:511:U:C2'    | 1:1:512:G:H5'    | 2.47                     | 0.42              |
| 2:2:41:G:H2'     | 2:2:42:G:H8      | 1.85                     | 0.42              |
| 2:2:594:U:H2'    | 2:2:595:A:O4'    | 2.19                     | 0.42              |
| 9:H:140:ALA:C    | 9:H:141:LYS:HD3  | 2.44                     | 0.42              |
| 31:d:31:HIS:N    | 31:d:31:HIS:CD2  | 2.87                     | 0.42              |
| 1:1:558:U:H2'    | 1:1:559:G:C8     | 2.55                     | 0.42              |
| 1:1:653:U:H3'    | 1:1:654:A:C8     | 2.55                     | 0.42              |
| 1:1:1111:A:N3    | 1:1:1112:G:H1'   | 2.34                     | 0.42              |
| 1:1:2101:A:H2'   | 1:1:2102:G:O4'   | 2.19                     | 0.42              |
| 1:1:2489:U:H2'   | 1:1:2490:G:O4'   | 2.20                     | 0.42              |
| 2:2:41:G:H2'     | 2:2:42:G:C8      | 2.54                     | 0.42              |
| 2:2:754:C:O5'    | 46:s:72:ARG:NH1  | 2.52                     | 0.42              |
| 9:H:42:LYS:O     | 9:H:42:LYS:HD3   | 2.20                     | 0.42              |
| 12:K:27:LEU:HD22 | 12:K:27:LEU:N    | 2.35                     | 0.42              |
| 38:k:31:MET:SD   | 38:k:36:LYS:HB2  | 2.60                     | 0.42              |
| 43:p:51:LYS:N    | 43:p:51:LYS:HD2  | 2.34                     | 0.42              |
| 54:z:8:5MU:O2    | 54:z:21:A:N1     | 2.52                     | 0.42              |
| 54:z:30:A:N1     | 54:z:42:5MU:O4   | 2.53                     | 0.42              |
| 54:z:70:C:C5'    | 54:z:70:C:C6     | 3.02                     | 0.42              |
| 54:z:80:G:H2'    | 54:z:81:C:O4'    | 2.19                     | 0.42              |
| 1:1:359:G:C6     | 1:1:360:U:C4     | 3.08                     | 0.42              |
| 1:1:897:C:H2'    | 1:1:898:C:C4'    | 2.49                     | 0.42              |
| 1:1:987:C:H2'    | 1:1:988:A:O4'    | 2.20                     | 0.42              |
| 1:1:1093:G:C2    | 1:1:1099:G:O6    | 2.73                     | 0.42              |
| 2:2:543:U:P      | 35:h:14:ARG:HH21 | 2.43                     | 0.42              |
| 2:2:1179:A:OP2   | 40:m:99:ARG:NH2  | 2.53                     | 0.42              |
| 2:2:1531:A:C6    | 2:2:1532:U:C4    | 3.08                     | 0.42              |
| 8:G:127:THR:HG22 | 8:G:128:GLN:N    | 2.35                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:H:80:ILE:HG12   | 9:H:102:ALA:CB    | 2.49                     | 0.42              |
| 16:O:110:ILE:HG21 | 16:O:110:ILE:HD13 | 1.73                     | 0.42              |
| 21:T:48:PRO:HG3   | 21:T:56:GLY:HA3   | 2.01                     | 0.42              |
| 25:X:59:GLU:HA    | 25:X:63:ALA:HB3   | 2.02                     | 0.42              |
| 31:d:26:HIS:CE1   | 31:d:48:ALA:HB2   | 2.55                     | 0.42              |
| 35:h:194:ASP:N    | 35:h:194:ASP:OD1  | 2.52                     | 0.42              |
| 38:k:113:ASP:HB2  | 38:k:119:ARG:HG3  | 2.02                     | 0.42              |
| 43:p:114:ARG:HG3  | 43:p:119:VAL:HB   | 2.01                     | 0.42              |
| 48:u:59:VAL:HG22  | 48:u:60:GLU:N     | 2.35                     | 0.42              |
| 52:y:62:ARG:NH2   | 52:y:63:GLU:OE2   | 2.52                     | 0.42              |
| 54:z:8:5MU:O2     | 54:z:21:A:C2      | 2.72                     | 0.42              |
| 1:1:248:G:H5'     | 1:1:250:G:N7      | 2.35                     | 0.42              |
| 1:1:299:A:N3      | 1:1:319:G:O2'     | 2.48                     | 0.42              |
| 1:1:356:G:C6      | 1:1:357:C:C4      | 3.07                     | 0.42              |
| 1:1:724:U:H2'     | 1:1:725:G:O4'     | 2.20                     | 0.42              |
| 1:1:1089:A:H2     | 1:1:1090:A:N6     | 2.18                     | 0.42              |
| 1:1:2881:U:H5'    | 14:M:90:ARG:NH2   | 2.34                     | 0.42              |
| 1:1:2900:A:H2'    | 1:1:2901:C:C6     | 2.55                     | 0.42              |
| 9:H:85:GLY:O      | 9:H:90:LEU:HB2    | 2.20                     | 0.42              |
| 9:H:93:SER:HB3    | 9:H:121:VAL:HG13  | 2.01                     | 0.42              |
| 9:H:146:VAL:HG13  | 9:H:146:VAL:O     | 2.19                     | 0.42              |
| 12:K:127:VAL:HG12 | 12:K:128:THR:O    | 2.20                     | 0.42              |
| 13:L:47:GLU:OE1   | 13:L:51:ARG:CZ    | 2.68                     | 0.42              |
| 17:P:97:ASP:OD2   | 18:Q:13:ARG:CZ    | 2.68                     | 0.42              |
| 20:S:68:LYS:O     | 20:S:75:GLY:N     | 2.52                     | 0.42              |
| 28:a:52:ARG:NH2   | 28:a:54:VAL:HG12  | 2.35                     | 0.42              |
| 30:c:42:LEU:HD23  | 30:c:43:THR:HG23  | 2.01                     | 0.42              |
| 34:g:115:LEU:O    | 34:g:118:ASP:OD1  | 2.38                     | 0.42              |
| 43:p:114:ARG:HG2  | 43:p:119:VAL:O    | 2.20                     | 0.42              |
| 51:x:79:LEU:HD23  | 51:x:79:LEU:HA    | 1.87                     | 0.42              |
| 54:z:49:G:C2      | 54:z:53:G:C6      | 3.08                     | 0.42              |
| 55:B:38:GLN:O     | 55:B:42:TYR:CB    | 2.68                     | 0.42              |
| 1:1:282:A:C6      | 1:1:359:G:C6      | 3.08                     | 0.41              |
| 1:1:1079:C:H2'    | 1:1:1080:A:H8     | 1.85                     | 0.41              |
| 1:1:1366:A:H2'    | 1:1:1367:A:O4'    | 2.20                     | 0.41              |
| 1:1:1607:C:H4'    | 1:1:1608:A:C5'    | 2.50                     | 0.41              |
| 1:1:2091:C:O3'    | 24:W:56:MET:HE1   | 2.20                     | 0.41              |
| 1:1:2195:U:H2'    | 1:1:2196:C:H6     | 1.85                     | 0.41              |
| 1:1:2311:A:O2'    | 1:1:2312:U:O4'    | 2.38                     | 0.41              |
| 1:1:2556:C:H2'    | 1:1:2557:G:O4'    | 2.20                     | 0.41              |
| 1:1:2708:G:H1'    | 14:M:71:ARG:NH1   | 2.34                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:C:240:PHE:CD2  | 4:C:240:PHE:O     | 2.73                     | 0.41              |
| 7:F:19:GLU:O     | 7:F:19:GLU:CG     | 2.68                     | 0.41              |
| 13:L:59:ARG:HD3  | 13:L:59:ARG:N     | 2.35                     | 0.41              |
| 25:X:44:LYS:O    | 25:X:48:ARG:CD    | 2.68                     | 0.41              |
| 40:m:21:ILE:HD13 | 40:m:63:LEU:HG    | 2.02                     | 0.41              |
| 54:z:19:G:C6     | 54:z:66:A:C2      | 3.08                     | 0.41              |
| 54:z:84:C:H5''   | 54:z:85:A:OP2     | 2.19                     | 0.41              |
| 1:1:747:5MU:O4   | 1:1:2014:A:C2     | 2.74                     | 0.41              |
| 1:1:1432:G:H2'   | 1:1:1433:A:C8     | 2.55                     | 0.41              |
| 1:1:2014:A:H2'   | 1:1:2015:A:C8     | 2.55                     | 0.41              |
| 2:2:381:C:H2'    | 2:2:382:A:O4'     | 2.20                     | 0.41              |
| 2:2:404:G:O2'    | 2:2:498:A:N1      | 2.47                     | 0.41              |
| 2:2:766:A:OP2    | 2:2:812:G:N2      | 2.54                     | 0.41              |
| 7:F:37:ASN:OD1   | 7:F:38:MET:N      | 2.53                     | 0.41              |
| 10:I:89:PHE:O    | 10:I:93:ILE:HG12  | 2.20                     | 0.41              |
| 13:L:66:ARG:HB2  | 13:L:101:VAL:O    | 2.21                     | 0.41              |
| 19:R:83:LYS:HB2  | 19:R:95:ARG:NH1   | 2.35                     | 0.41              |
| 20:S:68:LYS:N    | 20:S:75:GLY:O     | 2.49                     | 0.41              |
| 33:f:14:VAL:HG22 | 33:f:213:TYR:OH   | 2.20                     | 0.41              |
| 33:f:84:ALA:O    | 33:f:89:GLN:N     | 2.49                     | 0.41              |
| 33:f:207:ILE:O   | 33:f:211:THR:HG23 | 2.20                     | 0.41              |
| 35:h:100:ASN:OD1 | 35:h:111:ARG:NH1  | 2.53                     | 0.41              |
| 45:r:46:LEU:HD12 | 50:w:13:LEU:CB    | 2.50                     | 0.41              |
| 1:1:138:U:H1'    | 1:1:141:G:O6      | 2.21                     | 0.41              |
| 1:1:1452:G:O2'   | 1:1:2702:G:O6     | 2.33                     | 0.41              |
| 1:1:1722:A:H2'   | 1:1:1723:G:C8     | 2.55                     | 0.41              |
| 1:1:2144:G:N2    | 1:1:2148:G:O6     | 2.53                     | 0.41              |
| 1:1:2799:A:C2    | 1:1:2801:G:C4     | 3.08                     | 0.41              |
| 2:2:362:G:N2     | 2:2:365:U:OP2     | 2.52                     | 0.41              |
| 2:2:658:C:O4'    | 46:s:22:THR:OG1   | 2.38                     | 0.41              |
| 2:2:1002:G:C6    | 2:2:1039:G:C6     | 3.07                     | 0.41              |
| 8:G:170:ARG:HB2  | 8:G:170:ARG:NH2   | 2.35                     | 0.41              |
| 9:H:3:VAL:HG22   | 9:H:36:ALA:HB1    | 2.02                     | 0.41              |
| 9:H:15:LEU:HD11  | 9:H:55:GLU:OE2    | 2.20                     | 0.41              |
| 11:J:40:LYS:HD2  | 11:J:57:VAL:HG12  | 2.01                     | 0.41              |
| 23:V:18:ALA:O    | 23:V:20:ARG:HD2   | 2.20                     | 0.41              |
| 26:Y:6:LYS:HB2   | 26:Y:58:GLU:HB3   | 2.02                     | 0.41              |
| 40:m:22:LYS:O    | 40:m:61:LEU:HB3   | 2.20                     | 0.41              |
| 54:z:12:G:C2'    | 54:z:13:A:O5'     | 2.69                     | 0.41              |
| 54:z:71:5MU:C6   | 54:z:71:5MU:H5''  | 2.54                     | 0.41              |
| 1:1:20:C:OP1     | 17:P:22:LYS:NZ    | 2.52                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:1:157:C:H2'    | 1:1:158:U:O4'     | 2.20                     | 0.41              |
| 1:1:613:A:O4'    | 1:1:614:A:C8      | 2.73                     | 0.41              |
| 1:1:747:5MU:H1'  | 19:R:92:ARG:NH1   | 2.36                     | 0.41              |
| 1:1:1231:U:H2'   | 1:1:1232:G:H8     | 1.85                     | 0.41              |
| 1:1:1795:C:O2    | 4:C:253:LYS:HE2   | 2.20                     | 0.41              |
| 1:1:2102:G:C6    | 1:1:2188:U:C4     | 3.09                     | 0.41              |
| 1:1:2134:A:O2'   | 1:1:2159:G:C2'    | 2.68                     | 0.41              |
| 1:1:2698:U:H2'   | 1:1:2699:C:C6     | 2.55                     | 0.41              |
| 2:2:951:G:C6     | 2:2:1231:G:C6     | 3.09                     | 0.41              |
| 2:2:980:C:H2'    | 2:2:981:U:O4'     | 2.20                     | 0.41              |
| 2:2:1029:U:O2    | 2:2:1033:G:C2     | 2.74                     | 0.41              |
| 2:2:1118:U:H1'   | 2:2:1179:A:C5     | 2.55                     | 0.41              |
| 12:K:55:MET:SD   | 12:K:56:PRO:HD2   | 2.60                     | 0.41              |
| 15:N:111:ARG:NH2 | 15:N:117:PHE:OXT  | 2.54                     | 0.41              |
| 17:P:58:ARG:HA   | 17:P:61:TRP:CE3   | 2.54                     | 0.41              |
| 33:f:184:PHE:HD1 | 33:f:198:PHE:HB2  | 1.86                     | 0.41              |
| 33:f:207:ILE:O   | 33:f:210:VAL:HG22 | 2.21                     | 0.41              |
| 34:g:7:PRO:O     | 34:g:11:ARG:HD3   | 2.20                     | 0.41              |
| 34:g:86:LYS:O    | 34:g:89:LYS:HG2   | 2.20                     | 0.41              |
| 37:j:69:GLU:O    | 37:j:73:GLU:HG3   | 2.20                     | 0.41              |
| 1:1:848:C:H2'    | 1:1:849:A:C8      | 2.55                     | 0.41              |
| 2:2:579:A:O2'    | 46:s:54:ARG:NH1   | 2.43                     | 0.41              |
| 2:2:750:C:H1'    | 46:s:21:ASP:O     | 2.21                     | 0.41              |
| 2:2:1022:A:C6    | 2:2:1023:U:C2     | 3.08                     | 0.41              |
| 2:2:1060:U:H4'   | 41:n:53:ILE:HG13  | 2.03                     | 0.41              |
| 5:D:3:GLY:HA3    | 5:D:204:LYS:HG2   | 2.02                     | 0.41              |
| 6:E:118:LEU:HD11 | 6:E:188:MET:SD    | 2.61                     | 0.41              |
| 9:H:124:THR:OG1  | 9:H:128:HIS:CE1   | 2.74                     | 0.41              |
| 10:I:17:VAL:HG23 | 10:I:137:PRO:HB2  | 2.03                     | 0.41              |
| 21:T:98:SER:C    | 21:T:100:SER:H    | 2.28                     | 0.41              |
| 31:d:40:ARG:O    | 31:d:44:LEU:HG    | 2.21                     | 0.41              |
| 33:f:45:LYS:O    | 33:f:49:MET:SD    | 2.78                     | 0.41              |
| 1:1:322:A:P      | 6:E:162:ARG:HH11  | 2.43                     | 0.41              |
| 1:1:639:U:H2'    | 1:1:640:C:H6      | 1.85                     | 0.41              |
| 1:1:1528:A:C5    | 1:1:1529:G:H1'    | 2.56                     | 0.41              |
| 1:1:1922:G:C2'   | 1:1:1923:U:H5'    | 2.51                     | 0.41              |
| 2:2:218:U:H2'    | 2:2:219:U:O4'     | 2.20                     | 0.41              |
| 2:2:716:A:N3     | 42:o:119:ASN:O    | 2.54                     | 0.41              |
| 2:2:935:A:O2'    | 2:2:1383:C:N3     | 2.53                     | 0.41              |
| 20:S:93:LEU:HD23 | 20:S:94:ASP:N     | 2.35                     | 0.41              |
| 34:g:140:ASN:O   | 34:g:144:LEU:HD23 | 2.20                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 38:k:5:ARG:NH1   | 38:k:7:ILE:HA    | 2.35                     | 0.41              |
| 1:1:1827:U:H2'   | 1:1:1828:G:O4'   | 2.21                     | 0.41              |
| 1:1:2116:G:H1    | 1:1:2161:C:H5'   | 1.85                     | 0.41              |
| 2:2:66:A:H8      | 2:2:66:A:O5'     | 2.04                     | 0.41              |
| 2:2:983:A:OP1    | 45:r:6:MET:HE1   | 2.20                     | 0.41              |
| 2:2:1006:G:H2'   | 2:2:1007:U:H6    | 1.85                     | 0.41              |
| 24:W:27:ARG:NH1  | 24:W:29:PHE:CZ   | 2.88                     | 0.41              |
| 24:W:51:VAL:HG22 | 24:W:52:SER:O    | 2.20                     | 0.41              |
| 27:Z:65:ASN:OD1  | 27:Z:65:ASN:N    | 2.53                     | 0.41              |
| 35:h:13:ARG:NH2  | 35:h:38:PRO:HA   | 2.36                     | 0.41              |
| 44:q:2:ALA:O     | 44:q:9:ILE:N     | 2.54                     | 0.41              |
| 54:z:48:C:C2'    | 54:z:49:G:O5'    | 2.68                     | 0.41              |
| 1:1:11:C:C2'     | 1:1:12:U:H5'     | 2.50                     | 0.41              |
| 1:1:1386:C:H2'   | 1:1:1387:A:C8    | 2.56                     | 0.41              |
| 1:1:1469:A:OP2   | 1:1:1522:A:N6    | 2.49                     | 0.41              |
| 1:1:1671:U:O2'   | 1:1:1673:G:N7    | 2.45                     | 0.41              |
| 1:1:2162:G:H2'   | 1:1:2164:C:C4    | 2.56                     | 0.41              |
| 1:1:2266:A:H4'   | 1:1:2267:A:N3    | 2.35                     | 0.41              |
| 1:1:2291:U:H2'   | 1:1:2292:U:C6    | 2.56                     | 0.41              |
| 6:E:108:ILE:HD13 | 6:E:108:ILE:HG21 | 1.78                     | 0.41              |
| 6:E:122:GLU:O    | 6:E:189:THR:HG23 | 2.21                     | 0.41              |
| 10:I:114:LEU:O   | 10:I:118:MET:HG3 | 2.20                     | 0.41              |
| 20:S:11:LEU:O    | 25:X:29:ARG:NH1  | 2.49                     | 0.41              |
| 20:S:25:GLU:HG3  | 20:S:26:LYS:HG3  | 2.02                     | 0.41              |
| 32:e:16:ILE:HG12 | 32:e:25:VAL:HG22 | 2.01                     | 0.41              |
| 33:f:188:ASP:OD1 | 33:f:189:THR:N   | 2.49                     | 0.41              |
| 51:x:81:ALA:O    | 51:x:85:LYS:NZ   | 2.48                     | 0.41              |
| 54:z:32:A:C2'    | 54:z:33:U:H5'    | 2.50                     | 0.41              |
| 1:1:138:U:H2'    | 1:1:140:C:C4     | 2.55                     | 0.41              |
| 1:1:645:C:H2'    | 1:1:647:G:C5     | 2.56                     | 0.41              |
| 1:1:1048:A:N7    | 1:1:1111:A:C6    | 2.89                     | 0.41              |
| 1:1:1069:A:H4'   | 1:1:1070:A:H5''  | 2.02                     | 0.41              |
| 1:1:1176:U:OP1   | 1:1:1177:G:H4'   | 2.20                     | 0.41              |
| 1:1:2100:G:C6    | 1:1:2190:G:C6    | 3.09                     | 0.41              |
| 1:1:2570:G:H2'   | 1:1:2571:U:O4'   | 2.20                     | 0.41              |
| 1:1:2721:A:H2'   | 1:1:2722:G:O4'   | 2.21                     | 0.41              |
| 1:1:2885:G:O6    | 28:a:40:ARG:NH2  | 2.54                     | 0.41              |
| 2:2:208:U:H2'    | 2:2:210:C:N3     | 2.36                     | 0.41              |
| 2:2:209:U:H3'    | 2:2:210:C:O2     | 2.21                     | 0.41              |
| 2:2:407:U:H2'    | 2:2:408:A:C8     | 2.56                     | 0.41              |
| 2:2:460:A:H2'    | 2:2:461:A:C8     | 2.55                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:2:463:U:H3     | 2:2:469:C:N4     | 2.19                     | 0.41              |
| 2:2:767:A:H2'    | 2:2:768:A:O4'    | 2.21                     | 0.41              |
| 2:2:900:A:H2'    | 2:2:901:A:C8     | 2.56                     | 0.41              |
| 2:2:1279:G:H5''  | 41:n:9:ARG:NH2   | 2.36                     | 0.41              |
| 2:2:1315:U:O2    | 2:2:1360:A:H2    | 2.03                     | 0.41              |
| 4:C:232:HIS:HA   | 4:C:242:LYS:HD2  | 2.03                     | 0.41              |
| 5:D:89:GLU:C     | 5:D:90:PHE:CD1   | 2.99                     | 0.41              |
| 7:F:98:GLU:OE1   | 27:Z:9:TYR:OH    | 2.29                     | 0.41              |
| 8:G:44:LYS:CG    | 8:G:51:THR:OG1   | 2.69                     | 0.41              |
| 9:H:75:LEU:HD12  | 9:H:76:GLU:N     | 2.36                     | 0.41              |
| 9:H:110:VAL:HG12 | 9:H:111:ALA:N    | 2.35                     | 0.41              |
| 9:H:132:PHE:HB2  | 9:H:140:ALA:HB3  | 2.03                     | 0.41              |
| 28:a:3:VAL:HG22  | 28:a:4:GLN:H     | 1.86                     | 0.41              |
| 34:g:36:ASP:OD1  | 34:g:57:ILE:HG21 | 2.21                     | 0.41              |
| 35:h:50:ASP:O    | 35:h:54:GLN:HG3  | 2.21                     | 0.41              |
| 36:i:39:VAL:CG1  | 36:i:40:GLY:N    | 2.83                     | 0.41              |
| 36:i:112:ARG:O   | 36:i:116:GLU:HG3 | 2.21                     | 0.41              |
| 37:j:42:TRP:CZ3  | 37:j:102:MET:SD  | 3.14                     | 0.41              |
| 40:m:44:ALA:HA   | 40:m:47:VAL:HG22 | 2.02                     | 0.41              |
| 46:s:67:LEU:HD22 | 46:s:78:TYR:CE1  | 2.56                     | 0.41              |
| 47:t:57:ILE:O    | 47:t:61:VAL:HG23 | 2.21                     | 0.41              |
| 52:y:46:LYS:O    | 52:y:49:LYS:HG2  | 2.20                     | 0.41              |
| 54:z:12:G:H2'    | 54:z:13:A:O5'    | 2.20                     | 0.41              |
| 54:z:17:U:H4'    | 54:z:18:G:O5'    | 2.20                     | 0.41              |
| 54:z:59:C:O2'    | 54:z:60:G:H5'    | 2.21                     | 0.41              |
| 55:B:10:LYS:HG3  | 55:B:22:THR:N    | 2.36                     | 0.41              |
| 55:B:11:TRP:CZ2  | 55:B:20:PHE:CG   | 3.09                     | 0.41              |
| 1:1:615:U:O4     | 6:E:39:ALA:HB2   | 2.21                     | 0.41              |
| 1:1:1081:U:H2'   | 1:1:1082:U:H6    | 1.85                     | 0.41              |
| 1:1:1248:G:OP1   | 6:E:44:ARG:NH2   | 2.50                     | 0.41              |
| 1:1:2886:A:C4    | 28:a:40:ARG:NH2  | 2.89                     | 0.41              |
| 2:2:780:A:C2     | 2:2:801:U:C5     | 3.08                     | 0.41              |
| 2:2:1132:C:H2'   | 2:2:1133:G:C8    | 2.56                     | 0.41              |
| 2:2:1417:G:O2'   | 2:2:1483:A:N6    | 2.53                     | 0.41              |
| 9:H:89:LYS:C     | 9:H:91:PHE:N     | 2.77                     | 0.41              |
| 17:P:74:ILE:CD1  | 17:P:78:LYS:HB3  | 2.49                     | 0.41              |
| 27:Z:14:ALA:HA   | 27:Z:32:LEU:O    | 2.21                     | 0.41              |
| 35:h:156:LYS:O   | 35:h:160:GLU:HG2 | 2.20                     | 0.41              |
| 42:o:70:CYS:O    | 42:o:74:VAL:HG22 | 2.20                     | 0.41              |
| 44:q:55:THR:O    | 44:q:59:GLU:HG2  | 2.21                     | 0.41              |
| 46:s:21:ASP:C    | 46:s:22:THR:HG22 | 2.45                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:1:2111:U:C6    | 1:1:2118:U:H4'    | 2.56                     | 0.40              |
| 1:1:2111:U:H5    | 1:1:2118:U:OP2    | 2.03                     | 0.40              |
| 1:1:2161:C:O2'   | 1:1:2173:A:OP1    | 2.39                     | 0.40              |
| 2:2:190:A:N6     | 2:2:191:G:C2      | 2.89                     | 0.40              |
| 2:2:751:U:H2'    | 2:2:752:G:O4'     | 2.21                     | 0.40              |
| 5:D:1:MET:HE2    | 5:D:100:LEU:CD2   | 2.51                     | 0.40              |
| 8:G:54:PRO:HG2   | 8:G:62:TRP:CE2    | 2.56                     | 0.40              |
| 9:H:114:GLU:OE1  | 9:H:134:VAL:HG23  | 2.21                     | 0.40              |
| 19:R:7:HIS:CD2   | 19:R:10:ALA:HB2   | 2.56                     | 0.40              |
| 22:U:51:GLN:HB2  | 22:U:57:TYR:OH    | 2.21                     | 0.40              |
| 27:Z:59:ARG:HH21 | 27:Z:63:ARG:NH2   | 2.18                     | 0.40              |
| 32:e:30:GLU:HG3  | 32:e:32:LYS:H     | 1.86                     | 0.40              |
| 34:g:6:HIS:HB3   | 45:r:89:MET:SD    | 2.61                     | 0.40              |
| 37:j:38:ARG:NE   | 37:j:63:ASN:OD1   | 2.53                     | 0.40              |
| 54:z:12:G:H2'    | 54:z:13:A:O4'     | 2.21                     | 0.40              |
| 1:1:418:C:H2'    | 1:1:419:U:O4'     | 2.22                     | 0.40              |
| 1:1:833:A:H2'    | 1:1:834:G:C8      | 2.56                     | 0.40              |
| 1:1:2271:G:H5''  | 23:V:18:ALA:CB    | 2.51                     | 0.40              |
| 1:1:2313:C:H2'   | 1:1:2314:A:C8     | 2.56                     | 0.40              |
| 2:2:411:A:P      | 35:h:26:ARG:NH1   | 2.94                     | 0.40              |
| 2:2:868:C:H2'    | 2:2:869:G:O4'     | 2.21                     | 0.40              |
| 2:2:946:A:O2'    | 2:2:1333:A:N3     | 2.51                     | 0.40              |
| 4:C:79:GLU:N     | 4:C:93:LEU:O      | 2.48                     | 0.40              |
| 4:C:210:ALA:HA   | 4:C:213:TRP:CE3   | 2.56                     | 0.40              |
| 9:H:80:ILE:HD12  | 9:H:144:VAL:CG1   | 2.51                     | 0.40              |
| 9:H:115:VAL:HG22 | 9:H:132:PHE:CE1   | 2.57                     | 0.40              |
| 12:K:77:ILE:HG22 | 12:K:78:ARG:O     | 2.21                     | 0.40              |
| 12:K:92:LEU:O    | 12:K:96:LYS:HG3   | 2.22                     | 0.40              |
| 21:T:94:ARG:CB   | 21:T:103:ILE:HD12 | 2.51                     | 0.40              |
| 36:i:85:VAL:HG22 | 36:i:86:LYS:N     | 2.36                     | 0.40              |
| 37:j:20:GLY:O    | 37:j:24:ARG:HG3   | 2.21                     | 0.40              |
| 40:m:35:LEU:CD1  | 40:m:39:PHE:HD2   | 2.34                     | 0.40              |
| 48:u:22:VAL:HG22 | 48:u:45:HIS:CD2   | 2.56                     | 0.40              |
| 49:v:22:ASP:OD1  | 49:v:24:LYS:HE2   | 2.21                     | 0.40              |
| 51:x:68:HIS:CE1  | 51:x:70:ASN:OD1   | 2.75                     | 0.40              |
| 1:1:143:C:O2     | 1:1:143:C:H2'     | 2.21                     | 0.40              |
| 1:1:257:C:H2'    | 1:1:258:G:O4'     | 2.22                     | 0.40              |
| 1:1:674:G:H5''   | 6:E:71:GLY:N      | 2.36                     | 0.40              |
| 1:1:1009:A:N3    | 1:1:1153:C:O2'    | 2.50                     | 0.40              |
| 1:1:1174:U:H1'   | 1:1:1177:G:C2     | 2.57                     | 0.40              |
| 1:1:1276:A:O2'   | 14:M:16:HIS:NE2   | 2.45                     | 0.40              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:1:2128:G:N3    | 1:1:2173:A:H1'    | 2.36                     | 0.40              |
| 2:2:1391:U:H2'   | 2:2:1392:G:H8     | 1.86                     | 0.40              |
| 4:C:158:ALA:HB1  | 4:C:197:ASN:O     | 2.22                     | 0.40              |
| 18:Q:55:ASP:N    | 18:Q:55:ASP:OD1   | 2.47                     | 0.40              |
| 20:S:33:LYS:HG3  | 20:S:80:TRP:CE3   | 2.57                     | 0.40              |
| 33:f:213:TYR:O   | 33:f:217:VAL:HG23 | 2.21                     | 0.40              |
| 44:q:94:GLY:O    | 44:q:109:ARG:HB3  | 2.21                     | 0.40              |
| 48:u:12:VAL:HG23 | 48:u:57:ASP:O     | 2.21                     | 0.40              |
| 52:y:5:LYS:HD2   | 52:y:5:LYS:C      | 2.46                     | 0.40              |
| 1:1:388:G:O6     | 1:1:390:U:O2'     | 2.28                     | 0.40              |
| 1:1:2250:G:H5'   | 1:1:2250:G:N3     | 2.36                     | 0.40              |
| 1:1:2902:C:C2'   | 1:1:2903:U:H5''   | 2.51                     | 0.40              |
| 2:2:346:G:OP1    | 16:O:39:ARG:NH1   | 2.55                     | 0.40              |
| 2:2:579:A:H2'    | 2:2:580:C:C6      | 2.56                     | 0.40              |
| 2:2:972:C:O2'    | 41:n:57:VAL:HG23  | 2.21                     | 0.40              |
| 2:2:1333:A:H2'   | 2:2:1334:G:O4'    | 2.21                     | 0.40              |
| 3:3:42:C:C6      | 7:F:66:LEU:HB2    | 2.57                     | 0.40              |
| 13:L:75:GLU:HB2  | 13:L:90:GLU:OE2   | 2.22                     | 0.40              |
| 16:O:25:THR:HB   | 16:O:88:ARG:HB3   | 2.03                     | 0.40              |
| 41:n:99:GLN:OE1  | 41:n:99:GLN:HA    | 2.21                     | 0.40              |
| 1:1:93:G:N3      | 55:B:11:TRP:CZ2   | 2.90                     | 0.40              |
| 1:1:627:A:H5''   | 12:K:78:ARG:HH12  | 1.87                     | 0.40              |
| 1:1:932:U:O2'    | 1:1:934:U:O4      | 2.38                     | 0.40              |
| 1:1:1071:G:N2    | 1:1:1089:A:O2'    | 2.55                     | 0.40              |
| 1:1:1376:C:H2'   | 1:1:1377:G:O4'    | 2.21                     | 0.40              |
| 1:1:1716:U:H2'   | 1:1:1717:A:H8     | 1.87                     | 0.40              |
| 1:1:1856:U:H2'   | 1:1:1857:G:O4'    | 2.21                     | 0.40              |
| 1:1:2804:U:H2'   | 1:1:2805:C:C6     | 2.56                     | 0.40              |
| 2:2:213:G:C8     | 2:2:214:C:C5      | 3.09                     | 0.40              |
| 3:3:106:G:H2'    | 3:3:107:G:O4'     | 2.22                     | 0.40              |
| 8:G:16:ASP:HB3   | 8:G:27:LYS:HB2    | 2.03                     | 0.40              |
| 9:H:93:SER:CB    | 9:H:121:VAL:HG13  | 2.51                     | 0.40              |
| 33:f:69:PHE:HB3  | 33:f:80:VAL:CG2   | 2.52                     | 0.40              |
| 37:j:29:ILE:HG21 | 37:j:36:ILE:HD11  | 2.04                     | 0.40              |
| 49:v:14:THR:HG21 | 49:v:48:ARG:HG3   | 2.03                     | 0.40              |
| 50:w:3:ARG:HE    | 50:w:7:LYS:HD2    | 1.86                     | 0.40              |
| 54:z:17:U:H1'    | 54:z:18:G:OP2     | 2.22                     | 0.40              |
| 54:z:18:G:H1     | 54:z:64:5MU:H1'   | 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 |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 4   | C     | 269/271 (99%) | 256 (95%) | 13 (5%) | 0        | 100         | 100 |
| 5   | D     | 207/209 (99%) | 201 (97%) | 3 (1%)  | 3 (1%)   | 9           | 36  |
| 6   | E     | 199/201 (99%) | 197 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 7   | F     | 175/177 (99%) | 164 (94%) | 10 (6%) | 1 (1%)   | 21          | 56  |
| 8   | G     | 173/175 (99%) | 162 (94%) | 11 (6%) | 0        | 100         | 100 |
| 9   | H     | 147/149 (99%) | 135 (92%) | 10 (7%) | 2 (1%)   | 9           | 36  |
| 10  | I     | 140/142 (99%) | 137 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 11  | J     | 121/123 (98%) | 119 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 12  | K     | 142/144 (99%) | 138 (97%) | 4 (3%)  | 0        | 100         | 100 |
| 13  | L     | 134/136 (98%) | 130 (97%) | 4 (3%)  | 0        | 100         | 100 |
| 14  | M     | 117/119 (98%) | 114 (97%) | 3 (3%)  | 0        | 100         | 100 |
| 15  | N     | 114/116 (98%) | 111 (97%) | 3 (3%)  | 0        | 100         | 100 |
| 16  | O     | 112/114 (98%) | 109 (97%) | 3 (3%)  | 0        | 100         | 100 |
| 17  | P     | 115/117 (98%) | 114 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 18  | Q     | 101/103 (98%) | 94 (93%)  | 5 (5%)  | 2 (2%)   | 6           | 28  |
| 19  | R     | 108/110 (98%) | 107 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 20  | S     | 92/94 (98%)   | 91 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 21  | T     | 101/103 (98%) | 93 (92%)  | 8 (8%)  | 0        | 100         | 100 |
| 22  | U     | 92/94 (98%)   | 90 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 23  | V     | 82/84 (98%)   | 73 (89%)  | 7 (8%)  | 2 (2%)   | 4           | 24  |
| 24  | W     | 75/77 (97%)   | 74 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 25  | X     | 60/62 (97%)   | 59 (98%)  | 1 (2%)  | 0        | 100         | 100 |
| 26  | Y     | 56/58 (97%)   | 55 (98%)  | 1 (2%)  | 0        | 100         | 100 |
| 27  | Z     | 64/66 (97%)   | 59 (92%)  | 5 (8%)  | 0        | 100         | 100 |
| 28  | a     | 54/56 (96%)   | 52 (96%)  | 2 (4%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 29  | b     | 50/52 (96%)     | 50 (100%)  | 0        | 0        | 100         | 100 |
| 30  | c     | 44/46 (96%)     | 44 (100%)  | 0        | 0        | 100         | 100 |
| 31  | d     | 62/64 (97%)     | 58 (94%)   | 4 (6%)   | 0        | 100         | 100 |
| 32  | e     | 36/38 (95%)     | 35 (97%)   | 1 (3%)   | 0        | 100         | 100 |
| 33  | f     | 223/225 (99%)   | 211 (95%)  | 12 (5%)  | 0        | 100         | 100 |
| 34  | g     | 206/208 (99%)   | 197 (96%)  | 9 (4%)   | 0        | 100         | 100 |
| 35  | h     | 203/205 (99%)   | 200 (98%)  | 3 (2%)   | 0        | 100         | 100 |
| 36  | i     | 154/156 (99%)   | 144 (94%)  | 10 (6%)  | 0        | 100         | 100 |
| 37  | j     | 102/104 (98%)   | 99 (97%)   | 3 (3%)   | 0        | 100         | 100 |
| 38  | k     | 149/151 (99%)   | 145 (97%)  | 4 (3%)   | 0        | 100         | 100 |
| 39  | l     | 127/129 (98%)   | 125 (98%)  | 2 (2%)   | 0        | 100         | 100 |
| 40  | m     | 125/127 (98%)   | 117 (94%)  | 8 (6%)   | 0        | 100         | 100 |
| 41  | n     | 97/99 (98%)     | 92 (95%)   | 5 (5%)   | 0        | 100         | 100 |
| 42  | o     | 115/117 (98%)   | 109 (95%)  | 6 (5%)   | 0        | 100         | 100 |
| 43  | p     | 120/123 (98%)   | 114 (95%)  | 6 (5%)   | 0        | 100         | 100 |
| 44  | q     | 114/116 (98%)   | 109 (96%)  | 5 (4%)   | 0        | 100         | 100 |
| 45  | r     | 98/100 (98%)    | 97 (99%)   | 1 (1%)   | 0        | 100         | 100 |
| 46  | s     | 86/88 (98%)     | 84 (98%)   | 2 (2%)   | 0        | 100         | 100 |
| 47  | t     | 80/82 (98%)     | 78 (98%)   | 2 (2%)   | 0        | 100         | 100 |
| 48  | u     | 78/80 (98%)     | 75 (96%)   | 3 (4%)   | 0        | 100         | 100 |
| 49  | v     | 64/66 (97%)     | 64 (100%)  | 0        | 0        | 100         | 100 |
| 50  | w     | 81/83 (98%)     | 80 (99%)   | 1 (1%)   | 0        | 100         | 100 |
| 51  | x     | 84/86 (98%)     | 84 (100%)  | 0        | 0        | 100         | 100 |
| 52  | y     | 68/70 (97%)     | 66 (97%)   | 2 (3%)   | 0        | 100         | 100 |
| 55  | B     | 37/39 (95%)     | 29 (78%)   | 8 (22%)  | 0        | 100         | 100 |
| All | All   | 5653/5754 (98%) | 5440 (96%) | 203 (4%) | 10 (0%)  | 44          | 76  |

All (10) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | D     | 152 | PRO  |
| 5   | D     | 153 | GLY  |
| 5   | D     | 154 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9   | H     | 90  | LEU  |
| 23  | V     | 5   | LYS  |
| 23  | V     | 11  | ARG  |
| 18  | Q     | 52  | PRO  |
| 18  | Q     | 53  | PHE  |
| 9   | H     | 89  | LYS  |
| 7   | F     | 124 | GLY  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 4   | C     | 216/216 (100%) | 216 (100%) | 0        | 100         | 100 |
| 5   | D     | 164/164 (100%) | 163 (99%)  | 1 (1%)   | 78          | 88  |
| 6   | E     | 165/165 (100%) | 165 (100%) | 0        | 100         | 100 |
| 7   | F     | 148/148 (100%) | 148 (100%) | 0        | 100         | 100 |
| 8   | G     | 136/136 (100%) | 136 (100%) | 0        | 100         | 100 |
| 9   | H     | 114/114 (100%) | 113 (99%)  | 1 (1%)   | 70          | 85  |
| 10  | I     | 116/116 (100%) | 116 (100%) | 0        | 100         | 100 |
| 11  | J     | 104/104 (100%) | 104 (100%) | 0        | 100         | 100 |
| 12  | K     | 103/103 (100%) | 103 (100%) | 0        | 100         | 100 |
| 13  | L     | 109/109 (100%) | 109 (100%) | 0        | 100         | 100 |
| 14  | M     | 99/99 (100%)   | 99 (100%)  | 0        | 100         | 100 |
| 15  | N     | 86/86 (100%)   | 86 (100%)  | 0        | 100         | 100 |
| 16  | O     | 99/99 (100%)   | 99 (100%)  | 0        | 100         | 100 |
| 17  | P     | 89/89 (100%)   | 88 (99%)   | 1 (1%)   | 65          | 83  |
| 18  | Q     | 84/84 (100%)   | 84 (100%)  | 0        | 100         | 100 |
| 19  | R     | 93/93 (100%)   | 93 (100%)  | 0        | 100         | 100 |
| 20  | S     | 81/81 (100%)   | 81 (100%)  | 0        | 100         | 100 |
| 21  | T     | 84/84 (100%)   | 83 (99%)   | 1 (1%)   | 63          | 82  |

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| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 22  | U     | 78/78 (100%)   | 78 (100%)  | 0        | 100         | 100 |
| 23  | V     | 62/62 (100%)   | 62 (100%)  | 0        | 100         | 100 |
| 24  | W     | 67/67 (100%)   | 67 (100%)  | 0        | 100         | 100 |
| 25  | X     | 54/54 (100%)   | 54 (100%)  | 0        | 100         | 100 |
| 26  | Y     | 48/48 (100%)   | 48 (100%)  | 0        | 100         | 100 |
| 27  | Z     | 59/59 (100%)   | 59 (100%)  | 0        | 100         | 100 |
| 28  | a     | 47/47 (100%)   | 47 (100%)  | 0        | 100         | 100 |
| 29  | b     | 47/47 (100%)   | 47 (100%)  | 0        | 100         | 100 |
| 30  | c     | 38/38 (100%)   | 38 (100%)  | 0        | 100         | 100 |
| 31  | d     | 51/51 (100%)   | 49 (96%)   | 2 (4%)   | 28          | 62  |
| 32  | e     | 34/34 (100%)   | 34 (100%)  | 0        | 100         | 100 |
| 33  | f     | 187/187 (100%) | 187 (100%) | 0        | 100         | 100 |
| 34  | g     | 171/171 (100%) | 169 (99%)  | 2 (1%)   | 63          | 82  |
| 35  | h     | 172/172 (100%) | 172 (100%) | 0        | 100         | 100 |
| 36  | i     | 119/119 (100%) | 119 (100%) | 0        | 100         | 100 |
| 37  | j     | 91/91 (100%)   | 91 (100%)  | 0        | 100         | 100 |
| 38  | k     | 124/124 (100%) | 124 (100%) | 0        | 100         | 100 |
| 39  | l     | 104/104 (100%) | 104 (100%) | 0        | 100         | 100 |
| 40  | m     | 105/105 (100%) | 104 (99%)  | 1 (1%)   | 68          | 84  |
| 41  | n     | 86/86 (100%)   | 85 (99%)   | 1 (1%)   | 63          | 82  |
| 42  | o     | 90/90 (100%)   | 90 (100%)  | 0        | 100         | 100 |
| 43  | p     | 102/102 (100%) | 102 (100%) | 0        | 100         | 100 |
| 44  | q     | 94/94 (100%)   | 94 (100%)  | 0        | 100         | 100 |
| 45  | r     | 83/83 (100%)   | 83 (100%)  | 0        | 100         | 100 |
| 46  | s     | 76/76 (100%)   | 76 (100%)  | 0        | 100         | 100 |
| 47  | t     | 65/65 (100%)   | 65 (100%)  | 0        | 100         | 100 |
| 48  | u     | 74/74 (100%)   | 74 (100%)  | 0        | 100         | 100 |
| 49  | v     | 57/57 (100%)   | 57 (100%)  | 0        | 100         | 100 |
| 50  | w     | 72/72 (100%)   | 72 (100%)  | 0        | 100         | 100 |
| 51  | x     | 65/65 (100%)   | 65 (100%)  | 0        | 100         | 100 |
| 52  | y     | 60/60 (100%)   | 59 (98%)   | 1 (2%)   | 53          | 78  |

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| Mol | Chain | Analysed         | Rotameric   | Outliers | Percentiles |     |
|-----|-------|------------------|-------------|----------|-------------|-----|
| 55  | B     | 16/28 (57%)      | 16 (100%)   | 0        | 100         | 100 |
| All | All   | 4688/4700 (100%) | 4677 (100%) | 11 (0%)  | 85          | 92  |

All (11) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | D     | 151 | THR  |
| 9   | H     | 122 | LEU  |
| 17  | P     | 78  | LYS  |
| 21  | T     | 68  | SER  |
| 31  | d     | 31  | HIS  |
| 31  | d     | 51  | SER  |
| 34  | g     | 118 | ASP  |
| 34  | g     | 165 | THR  |
| 40  | m     | 25  | ASN  |
| 41  | n     | 87  | LEU  |
| 52  | y     | 13  | ASP  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | C     | 70  | ASN  |
| 4   | C     | 153 | GLN  |
| 4   | C     | 200 | HIS  |
| 4   | C     | 226 | ASN  |
| 4   | C     | 243 | HIS  |
| 5   | D     | 140 | HIS  |
| 6   | E     | 115 | GLN  |
| 9   | H     | 128 | HIS  |
| 10  | I     | 76  | HIS  |
| 12  | K     | 104 | GLN  |
| 13  | L     | 13  | HIS  |
| 13  | L     | 60  | GLN  |
| 14  | M     | 31  | HIS  |
| 15  | N     | 100 | HIS  |
| 16  | O     | 66  | ASN  |
| 19  | R     | 7   | HIS  |
| 19  | R     | 9   | HIS  |
| 22  | U     | 87  | GLN  |
| 24  | W     | 36  | HIS  |
| 29  | b     | 26  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 31  | d     | 31  | HIS  |
| 33  | f     | 18  | HIS  |
| 34  | g     | 8   | ASN  |
| 35  | h     | 198 | HIS  |
| 37  | j     | 52  | ASN  |
| 37  | j     | 94  | HIS  |
| 40  | m     | 110 | GLN  |
| 42  | o     | 22  | HIS  |
| 44  | q     | 8   | ASN  |
| 46  | s     | 50  | HIS  |
| 47  | t     | 63  | GLN  |
| 50  | w     | 69  | HIS  |
| 51  | x     | 20  | HIS  |
| 52  | y     | 64  | ASN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1   | 1     | 2902/2903 (99%) | 496 (17%)         | 10 (0%)         |
| 2   | 2     | 1532/1534 (99%) | 256 (16%)         | 5 (0%)          |
| 3   | 3     | 119/120 (99%)   | 16 (13%)          | 0               |
| 53  | 4     | 5/6 (83%)       | 1 (20%)           | 0               |
| 54  | z     | 84/85 (98%)     | 27 (32%)          | 0               |
| All | All   | 4642/4648 (99%) | 796 (17%)         | 15 (0%)         |

All (796) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 1     | 10  | A    |
| 1   | 1     | 15  | G    |
| 1   | 1     | 34  | U    |
| 1   | 1     | 35  | G    |
| 1   | 1     | 46  | G    |
| 1   | 1     | 51  | G    |
| 1   | 1     | 71  | A    |
| 1   | 1     | 74  | A    |
| 1   | 1     | 75  | G    |
| 1   | 1     | 80  | G    |
| 1   | 1     | 84  | A    |
| 1   | 1     | 85  | G    |
| 1   | 1     | 101 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 1     | 102 | U    |
| 1   | 1     | 110 | G    |
| 1   | 1     | 118 | A    |
| 1   | 1     | 119 | A    |
| 1   | 1     | 120 | U    |
| 1   | 1     | 122 | G    |
| 1   | 1     | 125 | A    |
| 1   | 1     | 138 | U    |
| 1   | 1     | 139 | U    |
| 1   | 1     | 140 | C    |
| 1   | 1     | 142 | A    |
| 1   | 1     | 163 | C    |
| 1   | 1     | 181 | A    |
| 1   | 1     | 196 | A    |
| 1   | 1     | 199 | A    |
| 1   | 1     | 215 | G    |
| 1   | 1     | 216 | A    |
| 1   | 1     | 221 | A    |
| 1   | 1     | 222 | A    |
| 1   | 1     | 225 | C    |
| 1   | 1     | 248 | G    |
| 1   | 1     | 249 | C    |
| 1   | 1     | 264 | C    |
| 1   | 1     | 265 | A    |
| 1   | 1     | 266 | G    |
| 1   | 1     | 272 | A    |
| 1   | 1     | 273 | G    |
| 1   | 1     | 275 | C    |
| 1   | 1     | 276 | U    |
| 1   | 1     | 285 | G    |
| 1   | 1     | 301 | G    |
| 1   | 1     | 311 | A    |
| 1   | 1     | 329 | G    |
| 1   | 1     | 330 | A    |
| 1   | 1     | 343 | C    |
| 1   | 1     | 353 | C    |
| 1   | 1     | 361 | G    |
| 1   | 1     | 371 | A    |
| 1   | 1     | 372 | G    |
| 1   | 1     | 373 | U    |
| 1   | 1     | 383 | C    |
| 1   | 1     | 386 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 1     | 396 | G    |
| 1   | 1     | 399 | U    |
| 1   | 1     | 405 | U    |
| 1   | 1     | 406 | G    |
| 1   | 1     | 411 | G    |
| 1   | 1     | 412 | A    |
| 1   | 1     | 424 | G    |
| 1   | 1     | 435 | C    |
| 1   | 1     | 457 | A    |
| 1   | 1     | 467 | G    |
| 1   | 1     | 481 | G    |
| 1   | 1     | 489 | G    |
| 1   | 1     | 491 | G    |
| 1   | 1     | 505 | A    |
| 1   | 1     | 509 | C    |
| 1   | 1     | 513 | A    |
| 1   | 1     | 532 | A    |
| 1   | 1     | 533 | G    |
| 1   | 1     | 543 | G    |
| 1   | 1     | 544 | C    |
| 1   | 1     | 546 | U    |
| 1   | 1     | 547 | A    |
| 1   | 1     | 548 | G    |
| 1   | 1     | 549 | G    |
| 1   | 1     | 551 | G    |
| 1   | 1     | 563 | A    |
| 1   | 1     | 573 | U    |
| 1   | 1     | 575 | A    |
| 1   | 1     | 603 | A    |
| 1   | 1     | 609 | A    |
| 1   | 1     | 612 | G    |
| 1   | 1     | 613 | A    |
| 1   | 1     | 614 | A    |
| 1   | 1     | 615 | U    |
| 1   | 1     | 616 | A    |
| 1   | 1     | 621 | A    |
| 1   | 1     | 627 | A    |
| 1   | 1     | 637 | A    |
| 1   | 1     | 645 | C    |
| 1   | 1     | 647 | G    |
| 1   | 1     | 654 | A    |
| 1   | 1     | 655 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 1     | 670 | A    |
| 1   | 1     | 685 | A    |
| 1   | 1     | 686 | U    |
| 1   | 1     | 702 | U    |
| 1   | 1     | 717 | C    |
| 1   | 1     | 726 | G    |
| 1   | 1     | 730 | A    |
| 1   | 1     | 747 | 5MU  |
| 1   | 1     | 764 | A    |
| 1   | 1     | 765 | C    |
| 1   | 1     | 775 | G    |
| 1   | 1     | 776 | G    |
| 1   | 1     | 782 | A    |
| 1   | 1     | 784 | G    |
| 1   | 1     | 785 | G    |
| 1   | 1     | 792 | A    |
| 1   | 1     | 800 | A    |
| 1   | 1     | 805 | G    |
| 1   | 1     | 812 | C    |
| 1   | 1     | 819 | A    |
| 1   | 1     | 827 | U    |
| 1   | 1     | 828 | U    |
| 1   | 1     | 845 | A    |
| 1   | 1     | 846 | U    |
| 1   | 1     | 858 | G    |
| 1   | 1     | 859 | G    |
| 1   | 1     | 866 | A    |
| 1   | 1     | 869 | G    |
| 1   | 1     | 878 | A    |
| 1   | 1     | 880 | G    |
| 1   | 1     | 882 | G    |
| 1   | 1     | 884 | U    |
| 1   | 1     | 885 | C    |
| 1   | 1     | 887 | A    |
| 1   | 1     | 891 | G    |
| 1   | 1     | 892 | A    |
| 1   | 1     | 893 | C    |
| 1   | 1     | 895 | U    |
| 1   | 1     | 896 | A    |
| 1   | 1     | 897 | C    |
| 1   | 1     | 898 | C    |
| 1   | 1     | 907 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 1     | 910  | A    |
| 1   | 1     | 931  | U    |
| 1   | 1     | 932  | U    |
| 1   | 1     | 941  | A    |
| 1   | 1     | 946  | C    |
| 1   | 1     | 961  | C    |
| 1   | 1     | 973  | A    |
| 1   | 1     | 974  | G    |
| 1   | 1     | 983  | A    |
| 1   | 1     | 989  | G    |
| 1   | 1     | 995  | C    |
| 1   | 1     | 996  | A    |
| 1   | 1     | 999  | U    |
| 1   | 1     | 1005 | C    |
| 1   | 1     | 1012 | U    |
| 1   | 1     | 1013 | C    |
| 1   | 1     | 1022 | G    |
| 1   | 1     | 1023 | U    |
| 1   | 1     | 1025 | G    |
| 1   | 1     | 1026 | G    |
| 1   | 1     | 1033 | U    |
| 1   | 1     | 1043 | C    |
| 1   | 1     | 1046 | A    |
| 1   | 1     | 1047 | G    |
| 1   | 1     | 1057 | A    |
| 1   | 1     | 1060 | U    |
| 1   | 1     | 1061 | U    |
| 1   | 1     | 1062 | G    |
| 1   | 1     | 1064 | C    |
| 1   | 1     | 1065 | U    |
| 1   | 1     | 1066 | U    |
| 1   | 1     | 1067 | A    |
| 1   | 1     | 1068 | G    |
| 1   | 1     | 1070 | A    |
| 1   | 1     | 1071 | G    |
| 1   | 1     | 1073 | A    |
| 1   | 1     | 1084 | A    |
| 1   | 1     | 1085 | A    |
| 1   | 1     | 1087 | G    |
| 1   | 1     | 1088 | A    |
| 1   | 1     | 1090 | A    |
| 1   | 1     | 1096 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 1     | 1101 | U    |
| 1   | 1     | 1110 | G    |
| 1   | 1     | 1111 | A    |
| 1   | 1     | 1112 | G    |
| 1   | 1     | 1119 | U    |
| 1   | 1     | 1122 | G    |
| 1   | 1     | 1128 | G    |
| 1   | 1     | 1130 | U    |
| 1   | 1     | 1131 | G    |
| 1   | 1     | 1132 | U    |
| 1   | 1     | 1133 | A    |
| 1   | 1     | 1134 | A    |
| 1   | 1     | 1135 | C    |
| 1   | 1     | 1136 | G    |
| 1   | 1     | 1139 | G    |
| 1   | 1     | 1142 | A    |
| 1   | 1     | 1156 | A    |
| 1   | 1     | 1169 | A    |
| 1   | 1     | 1170 | C    |
| 1   | 1     | 1171 | G    |
| 1   | 1     | 1173 | U    |
| 1   | 1     | 1175 | A    |
| 1   | 1     | 1176 | U    |
| 1   | 1     | 1177 | G    |
| 1   | 1     | 1178 | C    |
| 1   | 1     | 1179 | G    |
| 1   | 1     | 1182 | G    |
| 1   | 1     | 1186 | G    |
| 1   | 1     | 1206 | G    |
| 1   | 1     | 1212 | G    |
| 1   | 1     | 1218 | G    |
| 1   | 1     | 1236 | G    |
| 1   | 1     | 1238 | G    |
| 1   | 1     | 1247 | A    |
| 1   | 1     | 1250 | G    |
| 1   | 1     | 1253 | A    |
| 1   | 1     | 1256 | G    |
| 1   | 1     | 1266 | G    |
| 1   | 1     | 1271 | G    |
| 1   | 1     | 1272 | A    |
| 1   | 1     | 1300 | G    |
| 1   | 1     | 1301 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 1     | 1321 | A    |
| 1   | 1     | 1324 | G    |
| 1   | 1     | 1325 | U    |
| 1   | 1     | 1329 | U    |
| 1   | 1     | 1341 | G    |
| 1   | 1     | 1345 | C    |
| 1   | 1     | 1352 | U    |
| 1   | 1     | 1365 | A    |
| 1   | 1     | 1368 | G    |
| 1   | 1     | 1379 | U    |
| 1   | 1     | 1380 | G    |
| 1   | 1     | 1383 | A    |
| 1   | 1     | 1386 | C    |
| 1   | 1     | 1408 | G    |
| 1   | 1     | 1417 | C    |
| 1   | 1     | 1419 | A    |
| 1   | 1     | 1427 | A    |
| 1   | 1     | 1428 | C    |
| 1   | 1     | 1437 | C    |
| 1   | 1     | 1460 | U    |
| 1   | 1     | 1468 | U    |
| 1   | 1     | 1476 | U    |
| 1   | 1     | 1482 | G    |
| 1   | 1     | 1490 | A    |
| 1   | 1     | 1493 | C    |
| 1   | 1     | 1494 | A    |
| 1   | 1     | 1503 | A    |
| 1   | 1     | 1504 | A    |
| 1   | 1     | 1508 | A    |
| 1   | 1     | 1509 | A    |
| 1   | 1     | 1510 | G    |
| 1   | 1     | 1515 | A    |
| 1   | 1     | 1524 | G    |
| 1   | 1     | 1529 | G    |
| 1   | 1     | 1530 | G    |
| 1   | 1     | 1532 | A    |
| 1   | 1     | 1535 | A    |
| 1   | 1     | 1536 | C    |
| 1   | 1     | 1537 | G    |
| 1   | 1     | 1554 | U    |
| 1   | 1     | 1559 | U    |
| 1   | 1     | 1566 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 1     | 1569 | A    |
| 1   | 1     | 1578 | U    |
| 1   | 1     | 1580 | A    |
| 1   | 1     | 1583 | A    |
| 1   | 1     | 1587 | G    |
| 1   | 1     | 1589 | U    |
| 1   | 1     | 1590 | A    |
| 1   | 1     | 1608 | A    |
| 1   | 1     | 1618 | 6MZ  |
| 1   | 1     | 1634 | A    |
| 1   | 1     | 1647 | U    |
| 1   | 1     | 1648 | U    |
| 1   | 1     | 1649 | G    |
| 1   | 1     | 1651 | G    |
| 1   | 1     | 1674 | G    |
| 1   | 1     | 1715 | G    |
| 1   | 1     | 1729 | U    |
| 1   | 1     | 1730 | C    |
| 1   | 1     | 1732 | C    |
| 1   | 1     | 1738 | G    |
| 1   | 1     | 1756 | G    |
| 1   | 1     | 1764 | C    |
| 1   | 1     | 1773 | A    |
| 1   | 1     | 1782 | U    |
| 1   | 1     | 1791 | A    |
| 1   | 1     | 1800 | C    |
| 1   | 1     | 1801 | A    |
| 1   | 1     | 1808 | A    |
| 1   | 1     | 1811 | G    |
| 1   | 1     | 1816 | C    |
| 1   | 1     | 1829 | A    |
| 1   | 1     | 1833 | C    |
| 1   | 1     | 1835 | 2MG  |
| 1   | 1     | 1847 | A    |
| 1   | 1     | 1848 | A    |
| 1   | 1     | 1858 | A    |
| 1   | 1     | 1865 | U    |
| 1   | 1     | 1868 | C    |
| 1   | 1     | 1869 | G    |
| 1   | 1     | 1870 | C    |
| 1   | 1     | 1871 | A    |
| 1   | 1     | 1872 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 1     | 1873 | G    |
| 1   | 1     | 1896 | G    |
| 1   | 1     | 1906 | G    |
| 1   | 1     | 1907 | G    |
| 1   | 1     | 1912 | A    |
| 1   | 1     | 1914 | C    |
| 1   | 1     | 1923 | U    |
| 1   | 1     | 1924 | C    |
| 1   | 1     | 1929 | G    |
| 1   | 1     | 1930 | G    |
| 1   | 1     | 1936 | A    |
| 1   | 1     | 1937 | A    |
| 1   | 1     | 1938 | A    |
| 1   | 1     | 1955 | U    |
| 1   | 1     | 1967 | C    |
| 1   | 1     | 1970 | A    |
| 1   | 1     | 1971 | U    |
| 1   | 1     | 1972 | G    |
| 1   | 1     | 1991 | U    |
| 1   | 1     | 1992 | G    |
| 1   | 1     | 1993 | U    |
| 1   | 1     | 1997 | C    |
| 1   | 1     | 2002 | G    |
| 1   | 1     | 2022 | U    |
| 1   | 1     | 2023 | C    |
| 1   | 1     | 2030 | 6MZ  |
| 1   | 1     | 2031 | A    |
| 1   | 1     | 2033 | A    |
| 1   | 1     | 2043 | C    |
| 1   | 1     | 2052 | A    |
| 1   | 1     | 2055 | C    |
| 1   | 1     | 2056 | G    |
| 1   | 1     | 2060 | A    |
| 1   | 1     | 2061 | G    |
| 1   | 1     | 2062 | A    |
| 1   | 1     | 2069 | G7M  |
| 1   | 1     | 2093 | G    |
| 1   | 1     | 2095 | A    |
| 1   | 1     | 2100 | G    |
| 1   | 1     | 2102 | G    |
| 1   | 1     | 2107 | G    |
| 1   | 1     | 2110 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 1     | 2112 | G    |
| 1   | 1     | 2113 | U    |
| 1   | 1     | 2115 | G    |
| 1   | 1     | 2116 | G    |
| 1   | 1     | 2117 | A    |
| 1   | 1     | 2118 | U    |
| 1   | 1     | 2119 | A    |
| 1   | 1     | 2121 | G    |
| 1   | 1     | 2122 | U    |
| 1   | 1     | 2125 | G    |
| 1   | 1     | 2131 | U    |
| 1   | 1     | 2132 | U    |
| 1   | 1     | 2133 | G    |
| 1   | 1     | 2134 | A    |
| 1   | 1     | 2139 | U    |
| 1   | 1     | 2140 | G    |
| 1   | 1     | 2142 | A    |
| 1   | 1     | 2145 | C    |
| 1   | 1     | 2146 | C    |
| 1   | 1     | 2147 | A    |
| 1   | 1     | 2158 | A    |
| 1   | 1     | 2159 | G    |
| 1   | 1     | 2162 | G    |
| 1   | 1     | 2163 | A    |
| 1   | 1     | 2164 | C    |
| 1   | 1     | 2165 | C    |
| 1   | 1     | 2169 | A    |
| 1   | 1     | 2171 | A    |
| 1   | 1     | 2172 | U    |
| 1   | 1     | 2173 | A    |
| 1   | 1     | 2178 | C    |
| 1   | 1     | 2183 | A    |
| 1   | 1     | 2189 | U    |
| 1   | 1     | 2190 | G    |
| 1   | 1     | 2191 | A    |
| 1   | 1     | 2194 | U    |
| 1   | 1     | 2198 | A    |
| 1   | 1     | 2204 | G    |
| 1   | 1     | 2211 | A    |
| 1   | 1     | 2225 | A    |
| 1   | 1     | 2229 | U    |
| 1   | 1     | 2238 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 1     | 2239 | G    |
| 1   | 1     | 2243 | U    |
| 1   | 1     | 2250 | G    |
| 1   | 1     | 2278 | A    |
| 1   | 1     | 2283 | C    |
| 1   | 1     | 2286 | G    |
| 1   | 1     | 2287 | A    |
| 1   | 1     | 2288 | A    |
| 1   | 1     | 2305 | U    |
| 1   | 1     | 2309 | A    |
| 1   | 1     | 2319 | G    |
| 1   | 1     | 2322 | A    |
| 1   | 1     | 2325 | G    |
| 1   | 1     | 2327 | A    |
| 1   | 1     | 2333 | A    |
| 1   | 1     | 2334 | U    |
| 1   | 1     | 2336 | A    |
| 1   | 1     | 2345 | G    |
| 1   | 1     | 2347 | C    |
| 1   | 1     | 2350 | C    |
| 1   | 1     | 2357 | G    |
| 1   | 1     | 2361 | G    |
| 1   | 1     | 2376 | A    |
| 1   | 1     | 2383 | G    |
| 1   | 1     | 2385 | C    |
| 1   | 1     | 2402 | U    |
| 1   | 1     | 2403 | C    |
| 1   | 1     | 2406 | A    |
| 1   | 1     | 2423 | U    |
| 1   | 1     | 2424 | C    |
| 1   | 1     | 2425 | A    |
| 1   | 1     | 2429 | G    |
| 1   | 1     | 2430 | A    |
| 1   | 1     | 2431 | U    |
| 1   | 1     | 2435 | A    |
| 1   | 1     | 2441 | U    |
| 1   | 1     | 2445 | 2MG  |
| 1   | 1     | 2448 | A    |
| 1   | 1     | 2470 | G    |
| 1   | 1     | 2476 | A    |
| 1   | 1     | 2478 | A    |
| 1   | 1     | 2480 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 1     | 2491 | U    |
| 1   | 1     | 2498 | OMC  |
| 1   | 1     | 2502 | G    |
| 1   | 1     | 2504 | PSU  |
| 1   | 1     | 2505 | G    |
| 1   | 1     | 2506 | U    |
| 1   | 1     | 2507 | C    |
| 1   | 1     | 2513 | A    |
| 1   | 1     | 2518 | A    |
| 1   | 1     | 2520 | C    |
| 1   | 1     | 2529 | G    |
| 1   | 1     | 2535 | G    |
| 1   | 1     | 2547 | A    |
| 1   | 1     | 2554 | U    |
| 1   | 1     | 2566 | A    |
| 1   | 1     | 2567 | G    |
| 1   | 1     | 2572 | A    |
| 1   | 1     | 2573 | C    |
| 1   | 1     | 2586 | U    |
| 1   | 1     | 2602 | A    |
| 1   | 1     | 2609 | U    |
| 1   | 1     | 2613 | U    |
| 1   | 1     | 2629 | U    |
| 1   | 1     | 2646 | C    |
| 1   | 1     | 2663 | G    |
| 1   | 1     | 2689 | U    |
| 1   | 1     | 2690 | U    |
| 1   | 1     | 2714 | G    |
| 1   | 1     | 2716 | C    |
| 1   | 1     | 2718 | G    |
| 1   | 1     | 2725 | A    |
| 1   | 1     | 2726 | A    |
| 1   | 1     | 2733 | A    |
| 1   | 1     | 2744 | G    |
| 1   | 1     | 2748 | A    |
| 1   | 1     | 2751 | G    |
| 1   | 1     | 2757 | A    |
| 1   | 1     | 2765 | A    |
| 1   | 1     | 2777 | G    |
| 1   | 1     | 2778 | A    |
| 1   | 1     | 2791 | G    |
| 1   | 1     | 2793 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 1     | 2797 | U    |
| 1   | 1     | 2799 | A    |
| 1   | 1     | 2811 | G    |
| 1   | 1     | 2818 | U    |
| 1   | 1     | 2820 | A    |
| 1   | 1     | 2823 | A    |
| 1   | 1     | 2825 | G    |
| 1   | 1     | 2833 | U    |
| 1   | 1     | 2835 | A    |
| 1   | 1     | 2836 | U    |
| 1   | 1     | 2861 | U    |
| 1   | 1     | 2867 | G    |
| 1   | 1     | 2872 | A    |
| 1   | 1     | 2873 | A    |
| 1   | 1     | 2879 | A    |
| 1   | 1     | 2880 | C    |
| 1   | 1     | 2883 | A    |
| 1   | 1     | 2884 | U    |
| 1   | 1     | 2885 | G    |
| 1   | 1     | 2891 | U    |
| 1   | 1     | 2898 | U    |
| 2   | 2     | 7    | A    |
| 2   | 2     | 8    | A    |
| 2   | 2     | 9    | G    |
| 2   | 2     | 22   | G    |
| 2   | 2     | 32   | A    |
| 2   | 2     | 39   | G    |
| 2   | 2     | 47   | C    |
| 2   | 2     | 48   | C    |
| 2   | 2     | 50   | A    |
| 2   | 2     | 51   | A    |
| 2   | 2     | 52   | C    |
| 2   | 2     | 54   | C    |
| 2   | 2     | 66   | A    |
| 2   | 2     | 68   | G    |
| 2   | 2     | 69   | G    |
| 2   | 2     | 70   | U    |
| 2   | 2     | 72   | A    |
| 2   | 2     | 73   | C    |
| 2   | 2     | 74   | A    |
| 2   | 2     | 75   | G    |
| 2   | 2     | 76   | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | 2     | 81  | A    |
| 2   | 2     | 83  | C    |
| 2   | 2     | 84  | U    |
| 2   | 2     | 85  | U    |
| 2   | 2     | 86  | G    |
| 2   | 2     | 87  | C    |
| 2   | 2     | 92  | U    |
| 2   | 2     | 120 | A    |
| 2   | 2     | 121 | U    |
| 2   | 2     | 130 | A    |
| 2   | 2     | 131 | A    |
| 2   | 2     | 141 | G    |
| 2   | 2     | 144 | G    |
| 2   | 2     | 149 | A    |
| 2   | 2     | 160 | A    |
| 2   | 2     | 163 | C    |
| 2   | 2     | 164 | G    |
| 2   | 2     | 177 | G    |
| 2   | 2     | 181 | A    |
| 2   | 2     | 182 | A    |
| 2   | 2     | 197 | A    |
| 2   | 2     | 204 | G    |
| 2   | 2     | 210 | C    |
| 2   | 2     | 211 | G    |
| 2   | 2     | 212 | G    |
| 2   | 2     | 226 | G    |
| 2   | 2     | 245 | U    |
| 2   | 2     | 247 | G    |
| 2   | 2     | 251 | G    |
| 2   | 2     | 266 | G    |
| 2   | 2     | 267 | C    |
| 2   | 2     | 279 | A    |
| 2   | 2     | 289 | G    |
| 2   | 2     | 306 | A    |
| 2   | 2     | 319 | G    |
| 2   | 2     | 321 | A    |
| 2   | 2     | 328 | C    |
| 2   | 2     | 332 | G    |
| 2   | 2     | 347 | G    |
| 2   | 2     | 352 | C    |
| 2   | 2     | 354 | G    |
| 2   | 2     | 362 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | 2     | 367 | U    |
| 2   | 2     | 372 | C    |
| 2   | 2     | 384 | G    |
| 2   | 2     | 392 | C    |
| 2   | 2     | 398 | U    |
| 2   | 2     | 406 | G    |
| 2   | 2     | 412 | A    |
| 2   | 2     | 413 | G    |
| 2   | 2     | 414 | A    |
| 2   | 2     | 421 | U    |
| 2   | 2     | 422 | C    |
| 2   | 2     | 424 | G    |
| 2   | 2     | 429 | U    |
| 2   | 2     | 436 | C    |
| 2   | 2     | 439 | U    |
| 2   | 2     | 457 | G    |
| 2   | 2     | 458 | U    |
| 2   | 2     | 463 | U    |
| 2   | 2     | 464 | U    |
| 2   | 2     | 467 | U    |
| 2   | 2     | 468 | A    |
| 2   | 2     | 476 | U    |
| 2   | 2     | 478 | A    |
| 2   | 2     | 479 | U    |
| 2   | 2     | 481 | G    |
| 2   | 2     | 484 | G    |
| 2   | 2     | 485 | U    |
| 2   | 2     | 486 | U    |
| 2   | 2     | 496 | A    |
| 2   | 2     | 499 | A    |
| 2   | 2     | 510 | A    |
| 2   | 2     | 511 | C    |
| 2   | 2     | 517 | G    |
| 2   | 2     | 518 | C    |
| 2   | 2     | 521 | G    |
| 2   | 2     | 527 | G7M  |
| 2   | 2     | 531 | U    |
| 2   | 2     | 532 | A    |
| 2   | 2     | 533 | A    |
| 2   | 2     | 547 | A    |
| 2   | 2     | 559 | A    |
| 2   | 2     | 564 | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | 2     | 568 | G    |
| 2   | 2     | 572 | A    |
| 2   | 2     | 573 | A    |
| 2   | 2     | 576 | C    |
| 2   | 2     | 577 | G    |
| 2   | 2     | 596 | A    |
| 2   | 2     | 605 | U    |
| 2   | 2     | 633 | G    |
| 2   | 2     | 650 | G    |
| 2   | 2     | 653 | U    |
| 2   | 2     | 660 | C    |
| 2   | 2     | 665 | A    |
| 2   | 2     | 700 | G    |
| 2   | 2     | 701 | U    |
| 2   | 2     | 702 | A    |
| 2   | 2     | 703 | G    |
| 2   | 2     | 718 | A    |
| 2   | 2     | 721 | G    |
| 2   | 2     | 723 | U    |
| 2   | 2     | 724 | G    |
| 2   | 2     | 731 | G    |
| 2   | 2     | 734 | G    |
| 2   | 2     | 747 | A    |
| 2   | 2     | 748 | G    |
| 2   | 2     | 753 | A    |
| 2   | 2     | 755 | G    |
| 2   | 2     | 777 | A    |
| 2   | 2     | 787 | A    |
| 2   | 2     | 793 | U    |
| 2   | 2     | 794 | A    |
| 2   | 2     | 815 | A    |
| 2   | 2     | 817 | C    |
| 2   | 2     | 821 | G    |
| 2   | 2     | 828 | U    |
| 2   | 2     | 829 | G    |
| 2   | 2     | 832 | G    |
| 2   | 2     | 841 | C    |
| 2   | 2     | 843 | U    |
| 2   | 2     | 844 | G    |
| 2   | 2     | 845 | A    |
| 2   | 2     | 846 | G    |
| 2   | 2     | 884 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | 2     | 885  | G    |
| 2   | 2     | 887  | G    |
| 2   | 2     | 914  | A    |
| 2   | 2     | 934  | C    |
| 2   | 2     | 935  | A    |
| 2   | 2     | 960  | U    |
| 2   | 2     | 965  | U    |
| 2   | 2     | 966  | 2MG  |
| 2   | 2     | 967  | 5MC  |
| 2   | 2     | 969  | A    |
| 2   | 2     | 971  | G    |
| 2   | 2     | 972  | C    |
| 2   | 2     | 974  | A    |
| 2   | 2     | 975  | A    |
| 2   | 2     | 976  | G    |
| 2   | 2     | 977  | A    |
| 2   | 2     | 982  | U    |
| 2   | 2     | 993  | G    |
| 2   | 2     | 994  | A    |
| 2   | 2     | 996  | A    |
| 2   | 2     | 1004 | A    |
| 2   | 2     | 1009 | U    |
| 2   | 2     | 1019 | A    |
| 2   | 2     | 1020 | G    |
| 2   | 2     | 1022 | A    |
| 2   | 2     | 1025 | U    |
| 2   | 2     | 1026 | G    |
| 2   | 2     | 1028 | C    |
| 2   | 2     | 1030 | U    |
| 2   | 2     | 1031 | C    |
| 2   | 2     | 1032 | G    |
| 2   | 2     | 1034 | G    |
| 2   | 2     | 1043 | G    |
| 2   | 2     | 1046 | A    |
| 2   | 2     | 1065 | U    |
| 2   | 2     | 1085 | U    |
| 2   | 2     | 1089 | G    |
| 2   | 2     | 1094 | G    |
| 2   | 2     | 1095 | U    |
| 2   | 2     | 1101 | A    |
| 2   | 2     | 1104 | G    |
| 2   | 2     | 1108 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | 2     | 1124 | G    |
| 2   | 2     | 1125 | U    |
| 2   | 2     | 1132 | C    |
| 2   | 2     | 1136 | C    |
| 2   | 2     | 1137 | C    |
| 2   | 2     | 1139 | G    |
| 2   | 2     | 1140 | C    |
| 2   | 2     | 1141 | C    |
| 2   | 2     | 1143 | G    |
| 2   | 2     | 1146 | A    |
| 2   | 2     | 1151 | A    |
| 2   | 2     | 1152 | A    |
| 2   | 2     | 1158 | C    |
| 2   | 2     | 1159 | U    |
| 2   | 2     | 1160 | G    |
| 2   | 2     | 1167 | A    |
| 2   | 2     | 1169 | A    |
| 2   | 2     | 1175 | G    |
| 2   | 2     | 1176 | A    |
| 2   | 2     | 1184 | G    |
| 2   | 2     | 1196 | A    |
| 2   | 2     | 1197 | A    |
| 2   | 2     | 1212 | U    |
| 2   | 2     | 1213 | A    |
| 2   | 2     | 1215 | G    |
| 2   | 2     | 1227 | A    |
| 2   | 2     | 1228 | C    |
| 2   | 2     | 1238 | A    |
| 2   | 2     | 1239 | A    |
| 2   | 2     | 1257 | A    |
| 2   | 2     | 1258 | G    |
| 2   | 2     | 1260 | G    |
| 2   | 2     | 1261 | A    |
| 2   | 2     | 1275 | A    |
| 2   | 2     | 1279 | G    |
| 2   | 2     | 1280 | A    |
| 2   | 2     | 1286 | U    |
| 2   | 2     | 1287 | A    |
| 2   | 2     | 1297 | G    |
| 2   | 2     | 1299 | A    |
| 2   | 2     | 1302 | C    |
| 2   | 2     | 1305 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | 2     | 1312 | G    |
| 2   | 2     | 1317 | C    |
| 2   | 2     | 1320 | C    |
| 2   | 2     | 1335 | U    |
| 2   | 2     | 1336 | C    |
| 2   | 2     | 1340 | A    |
| 2   | 2     | 1346 | A    |
| 2   | 2     | 1353 | G    |
| 2   | 2     | 1363 | A    |
| 2   | 2     | 1364 | U    |
| 2   | 2     | 1370 | G    |
| 2   | 2     | 1379 | G    |
| 2   | 2     | 1381 | U    |
| 2   | 2     | 1419 | G    |
| 2   | 2     | 1446 | A    |
| 2   | 2     | 1494 | G    |
| 2   | 2     | 1497 | G    |
| 2   | 2     | 1499 | A    |
| 2   | 2     | 1503 | A    |
| 2   | 2     | 1506 | U    |
| 2   | 2     | 1517 | G    |
| 2   | 2     | 1519 | MA6  |
| 2   | 2     | 1529 | G    |
| 2   | 2     | 1530 | G    |
| 2   | 2     | 1534 | A    |
| 3   | 3     | 2    | G    |
| 3   | 3     | 9    | G    |
| 3   | 3     | 13   | G    |
| 3   | 3     | 24   | G    |
| 3   | 3     | 31   | C    |
| 3   | 3     | 35   | C    |
| 3   | 3     | 36   | C    |
| 3   | 3     | 45   | A    |
| 3   | 3     | 51   | G    |
| 3   | 3     | 56   | G    |
| 3   | 3     | 66   | A    |
| 3   | 3     | 88   | C    |
| 3   | 3     | 89   | U    |
| 3   | 3     | 90   | C    |
| 3   | 3     | 99   | A    |
| 3   | 3     | 109  | A    |
| 53  | 4     | 6    | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 54  | z     | 7   | G    |
| 54  | z     | 8   | 5MU  |
| 54  | z     | 14  | A    |
| 54  | z     | 16  | U    |
| 54  | z     | 17  | U    |
| 54  | z     | 18  | G    |
| 54  | z     | 19  | G    |
| 54  | z     | 20  | 5MU  |
| 54  | z     | 21  | A    |
| 54  | z     | 22  | G    |
| 54  | z     | 23  | A    |
| 54  | z     | 24  | C    |
| 54  | z     | 46  | G    |
| 54  | z     | 49  | G    |
| 54  | z     | 57  | 5MU  |
| 54  | z     | 58  | G    |
| 54  | z     | 62  | G    |
| 54  | z     | 63  | 5MU  |
| 54  | z     | 64  | 5MU  |
| 54  | z     | 67  | A    |
| 54  | z     | 68  | G    |
| 54  | z     | 69  | 5MU  |
| 54  | z     | 70  | C    |
| 54  | z     | 71  | 5MU  |
| 54  | z     | 72  | C    |
| 54  | z     | 76  | 5MU  |
| 54  | z     | 85  | A    |

All (15) RNA pucker outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 1     | 372  | G    |
| 1   | 1     | 404  | A    |
| 1   | 1     | 613  | A    |
| 1   | 1     | 784  | G    |
| 1   | 1     | 891  | G    |
| 1   | 1     | 894  | U    |
| 1   | 1     | 1379 | U    |
| 1   | 1     | 1475 | G    |
| 1   | 1     | 2189 | U    |
| 1   | 1     | 2756 | U    |
| 2   | 2     | 85   | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | 2     | 86   | G    |
| 2   | 2     | 516  | PSU  |
| 2   | 2     | 1109 | C    |
| 2   | 2     | 1145 | A    |

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

46 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 |
| 54  | 5MU  | z     | 42   | 54,2  | 19,22,23     | 4.34 | 7 (36%)  | 28,32,35    | 3.84  | 11 (39%) |
| 54  | 5MU  | z     | 69   | 54    | 19,22,23     | 6.60 | 6 (31%)  | 28,32,35    | 28.78 | 14 (50%) |
| 43  | 0TD  | p     | 89   | 43    | 7,9,10       | 1.49 | 1 (14%)  | 6,11,13     | 1.92  | 2 (33%)  |
| 1   | OMU  | 1     | 2552 | 1     | 19,22,23     | 2.74 | 6 (31%)  | 26,31,34    | 1.67  | 6 (23%)  |
| 2   | 4OC  | 2     | 1402 | 2     | 20,23,24     | 2.69 | 8 (40%)  | 26,32,35    | 1.08  | 1 (3%)   |
| 54  | 5MU  | z     | 39   | 54    | 19,22,23     | 1.44 | 5 (26%)  | 28,32,35    | 2.17  | 9 (32%)  |
| 1   | PSU  | 1     | 1917 | 1     | 18,21,22     | 1.01 | 1 (5%)   | 22,30,33    | 2.13  | 5 (22%)  |
| 2   | 5MC  | 2     | 1407 | 2     | 18,22,23     | 3.12 | 7 (38%)  | 26,32,35    | 0.90  | 1 (3%)   |
| 54  | 5MU  | z     | 40   | 54    | 19,22,23     | 1.38 | 5 (26%)  | 28,32,35    | 2.27  | 11 (39%) |
| 2   | 5MC  | 2     | 967  | 2     | 18,22,23     | 3.27 | 7 (38%)  | 26,32,35    | 1.12  | 2 (7%)   |
| 1   | PSU  | 1     | 2457 | 1     | 18,21,22     | 1.18 | 2 (11%)  | 22,30,33    | 2.20  | 5 (22%)  |
| 54  | 5MU  | z     | 20   | 54,56 | 19,22,23     | 4.78 | 7 (36%)  | 28,32,35    | 3.73  | 9 (32%)  |
| 1   | 5MU  | 1     | 747  | 1     | 19,22,23     | 4.50 | 7 (36%)  | 28,32,35    | 3.78  | 9 (32%)  |
| 1   | 1MG  | 1     | 745  | 1     | 22,26,27     | 2.72 | 7 (31%)  | 33,39,42    | 2.29  | 8 (24%)  |
| 1   | 6MZ  | 1     | 1618 | 1     | 22,25,26     | 2.52 | 6 (27%)  | 30,36,39    | 3.29  | 12 (40%) |
| 54  | 5MU  | z     | 8    | 54    | 19,22,23     | 4.51 | 7 (36%)  | 28,32,35    | 3.93  | 9 (32%)  |
| 1   | 6MZ  | 1     | 2030 | 1     | 22,25,26     | 2.52 | 6 (27%)  | 30,36,39    | 3.33  | 12 (40%) |
| 1   | 2MA  | 1     | 2503 | 56,1  | 22,25,26     | 3.43 | 10 (45%) | 33,37,40    | 2.18  | 9 (27%)  |
| 1   | 2MG  | 1     | 1835 | 1     | 23,26,27     | 2.54 | 8 (34%)  | 32,38,41    | 2.09  | 8 (25%)  |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 1   | 3TD  | 1     | 1915 | 1    | 18,22,23     | 4.04 | 7 (38%)  | 22,32,35    | 1.54 | 3 (13%)  |
| 1   | PSU  | 1     | 1911 | 1    | 18,21,22     | 0.90 | 0        | 22,30,33    | 1.87 | 3 (13%)  |
| 1   | PSU  | 1     | 2580 | 56,1 | 18,21,22     | 1.14 | 1 (5%)   | 22,30,33    | 2.23 | 6 (27%)  |
| 1   | 5MU  | 1     | 1939 | 56,1 | 19,22,23     | 4.39 | 7 (36%)  | 28,32,35    | 3.71 | 10 (35%) |
| 1   | 5MC  | 1     | 1962 | 1    | 18,22,23     | 3.04 | 7 (38%)  | 26,32,35    | 1.26 | 5 (19%)  |
| 1   | G7M  | 1     | 2069 | 1    | 23,26,27     | 2.68 | 9 (39%)  | 35,39,42    | 2.31 | 12 (34%) |
| 2   | 2MG  | 2     | 1207 | 2    | 23,26,27     | 2.59 | 8 (34%)  | 32,38,41    | 2.04 | 9 (28%)  |
| 54  | 5MU  | z     | 63   | 54   | 19,22,23     | 1.45 | 6 (31%)  | 28,32,35    | 2.45 | 13 (46%) |
| 54  | 5MU  | z     | 57   | 54   | 19,22,23     | 4.54 | 7 (36%)  | 28,32,35    | 3.71 | 9 (32%)  |
| 2   | MA6  | 2     | 1518 | 2    | 23,26,27     | 1.63 | 6 (26%)  | 34,38,41    | 3.25 | 11 (32%) |
| 2   | 2MG  | 2     | 1516 | 2    | 23,26,27     | 2.58 | 8 (34%)  | 32,38,41    | 2.09 | 10 (31%) |
| 1   | OMC  | 1     | 2498 | 56,1 | 19,22,23     | 2.51 | 6 (31%)  | 26,31,34    | 0.96 | 0        |
| 1   | PSU  | 1     | 955  | 1    | 18,21,22     | 1.08 | 1 (5%)   | 22,30,33    | 1.99 | 5 (22%)  |
| 1   | 2MG  | 1     | 2445 | 1    | 23,26,27     | 2.56 | 8 (34%)  | 32,38,41    | 1.87 | 9 (28%)  |
| 1   | PSU  | 1     | 2605 | 1    | 18,21,22     | 1.05 | 1 (5%)   | 22,30,33    | 1.92 | 4 (18%)  |
| 1   | PSU  | 1     | 2504 | 1    | 18,21,22     | 0.98 | 1 (5%)   | 22,30,33    | 1.85 | 4 (18%)  |
| 2   | 2MG  | 2     | 966  | 2    | 23,26,27     | 2.77 | 7 (30%)  | 32,38,41    | 2.10 | 8 (25%)  |
| 54  | 5MU  | z     | 71   | 54   | 19,22,23     | 1.34 | 5 (26%)  | 28,32,35    | 2.21 | 9 (32%)  |
| 2   | UR3  | 2     | 1498 | 2    | 19,22,23     | 2.41 | 6 (31%)  | 26,32,35    | 1.04 | 2 (7%)   |
| 2   | MA6  | 2     | 1519 | 2    | 23,26,27     | 1.65 | 6 (26%)  | 34,38,41    | 3.36 | 11 (32%) |
| 54  | 5MU  | z     | 64   | 54   | 19,22,23     | 1.44 | 6 (31%)  | 28,32,35    | 2.32 | 7 (25%)  |
| 2   | PSU  | 2     | 516  | 56,2 | 18,21,22     | 0.97 | 1 (5%)   | 22,30,33    | 1.88 | 3 (13%)  |
| 54  | 5MU  | z     | 55   | 54   | 19,22,23     | 4.68 | 7 (36%)  | 28,32,35    | 3.48 | 9 (32%)  |
| 2   | G7M  | 2     | 527  | 2    | 23,26,27     | 2.72 | 9 (39%)  | 35,39,42    | 2.22 | 11 (31%) |
| 1   | OMG  | 1     | 2251 | 54,1 | 23,26,27     | 2.07 | 6 (26%)  | 33,38,41    | 1.70 | 8 (24%)  |
| 54  | 5MU  | z     | 76   | 54   | 19,22,23     | 1.43 | 6 (31%)  | 28,32,35    | 2.14 | 9 (32%)  |
| 1   | PSU  | 1     | 746  | 56,1 | 18,21,22     | 1.04 | 2 (11%)  | 22,30,33    | 1.74 | 3 (13%)  |

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   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 54  | 5MU  | z     | 42  | 54,2 | -       | 0/7/25/26 | 0/2/2/2 |
| 54  | 5MU  | z     | 69  | 54   | -       | 2/7/25/26 | 1/2/2/2 |

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| Mol | Type | Chain | Res  | Link  | Chirals | Torsions   | Rings   |
|-----|------|-------|------|-------|---------|------------|---------|
| 43  | 0TD  | p     | 89   | 43    | -       | 3/7/12/14  | -       |
| 1   | OMU  | 1     | 2552 | 1     | -       | 0/9/27/28  | 0/2/2/2 |
| 2   | 4OC  | 2     | 1402 | 2     | -       | 2/9/29/30  | 0/2/2/2 |
| 54  | 5MU  | z     | 39   | 54    | -       | 4/7/25/26  | 0/2/2/2 |
| 1   | PSU  | 1     | 1917 | 1     | -       | 0/7/25/26  | 0/2/2/2 |
| 2   | 5MC  | 2     | 1407 | 2     | -       | 0/7/25/26  | 0/2/2/2 |
| 54  | 5MU  | z     | 40   | 54    | -       | 2/7/25/26  | 0/2/2/2 |
| 2   | 5MC  | 2     | 967  | 2     | -       | 2/7/25/26  | 0/2/2/2 |
| 1   | PSU  | 1     | 2457 | 1     | -       | 0/7/25/26  | 0/2/2/2 |
| 54  | 5MU  | z     | 20   | 54,56 | -       | 4/7/25/26  | 0/2/2/2 |
| 1   | 5MU  | 1     | 747  | 1     | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | 1MG  | 1     | 745  | 1     | -       | 0/7/25/26  | 0/3/3/3 |
| 1   | 6MZ  | 1     | 1618 | 1     | -       | 3/9/27/28  | 0/3/3/3 |
| 54  | 5MU  | z     | 8    | 54    | -       | 2/7/25/26  | 0/2/2/2 |
| 1   | 6MZ  | 1     | 2030 | 1     | -       | 2/9/27/28  | 0/3/3/3 |
| 1   | 2MA  | 1     | 2503 | 56,1  | -       | 2/7/25/26  | 0/3/3/3 |
| 1   | 2MG  | 1     | 1835 | 1     | -       | 2/9/27/28  | 0/3/3/3 |
| 1   | 3TD  | 1     | 1915 | 1     | -       | 3/7/25/26  | 0/2/2/2 |
| 1   | PSU  | 1     | 1911 | 1     | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | PSU  | 1     | 2580 | 56,1  | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | 5MU  | 1     | 1939 | 56,1  | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | 5MC  | 1     | 1962 | 1     | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | G7M  | 1     | 2069 | 1     | -       | 1/7/25/26  | 0/3/3/3 |
| 2   | 2MG  | 2     | 1207 | 2     | -       | 0/9/27/28  | 0/3/3/3 |
| 54  | 5MU  | z     | 63   | 54    | -       | 2/7/25/26  | 0/2/2/2 |
| 54  | 5MU  | z     | 57   | 54    | -       | 2/7/25/26  | 0/2/2/2 |
| 2   | MA6  | 2     | 1518 | 2     | -       | 3/11/29/30 | 0/3/3/3 |
| 2   | 2MG  | 2     | 1516 | 2     | -       | 0/9/27/28  | 0/3/3/3 |
| 1   | OMC  | 1     | 2498 | 56,1  | -       | 0/9/27/28  | 0/2/2/2 |
| 1   | PSU  | 1     | 955  | 1     | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | 2MG  | 1     | 2445 | 1     | -       | 2/9/27/28  | 0/3/3/3 |
| 1   | PSU  | 1     | 2605 | 1     | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | PSU  | 1     | 2504 | 1     | -       | 2/7/25/26  | 0/2/2/2 |
| 2   | 2MG  | 2     | 966  | 2     | -       | 0/9/27/28  | 0/3/3/3 |
| 54  | 5MU  | z     | 71   | 54    | -       | 3/7/25/26  | 0/2/2/2 |
| 2   | UR3  | 2     | 1498 | 2     | -       | 1/7/25/26  | 0/2/2/2 |
| 2   | MA6  | 2     | 1519 | 2     | -       | 5/11/29/30 | 0/3/3/3 |
| 54  | 5MU  | z     | 64   | 54    | -       | 2/7/25/26  | 0/2/2/2 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|------|------|---------|-----------|---------|
| 2   | PSU  | 2     | 516  | 56,2 | -       | 2/7/25/26 | 0/2/2/2 |
| 54  | 5MU  | z     | 55   | 54   | -       | 0/7/25/26 | 0/2/2/2 |
| 2   | G7M  | 2     | 527  | 2    | -       | 3/7/25/26 | 0/3/3/3 |
| 1   | OMG  | 1     | 2251 | 54,1 | -       | 0/9/27/28 | 0/3/3/3 |
| 54  | 5MU  | z     | 76   | 54   | -       | 2/7/25/26 | 0/2/2/2 |
| 1   | PSU  | 1     | 746  | 56,1 | -       | 1/7/25/26 | 0/2/2/2 |

All (257) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 54  | z     | 69   | 5MU  | C6-C5 | 23.78 | 1.73        | 1.34     |
| 1   | 1     | 1915 | 3TD  | C6-C5 | 11.71 | 1.49        | 1.35     |
| 54  | z     | 57   | 5MU  | C2-N1 | 11.02 | 1.56        | 1.38     |
| 54  | z     | 20   | 5MU  | C2-N1 | 10.76 | 1.55        | 1.38     |
| 1   | 1     | 2503 | 2MA  | C4-N3 | 10.57 | 1.47        | 1.34     |
| 54  | z     | 20   | 5MU  | C6-N1 | 10.47 | 1.55        | 1.38     |
| 54  | z     | 42   | 5MU  | C2-N1 | 10.46 | 1.55        | 1.38     |
| 54  | z     | 55   | 5MU  | C2-N1 | 10.34 | 1.55        | 1.38     |
| 54  | z     | 20   | 5MU  | C4-C5 | 10.30 | 1.61        | 1.44     |
| 54  | z     | 55   | 5MU  | C6-N1 | 10.22 | 1.55        | 1.38     |
| 1   | 1     | 747  | 5MU  | C2-N1 | 10.12 | 1.54        | 1.38     |
| 1   | 1     | 1939 | 5MU  | C2-N1 | 9.97  | 1.54        | 1.38     |
| 54  | z     | 69   | 5MU  | C4-C5 | -9.95 | 1.28        | 1.44     |
| 54  | z     | 8    | 5MU  | C2-N1 | 9.91  | 1.54        | 1.38     |
| 1   | 1     | 747  | 5MU  | C6-N1 | 9.67  | 1.54        | 1.38     |
| 54  | z     | 55   | 5MU  | C4-C5 | 9.54  | 1.60        | 1.44     |
| 1   | 1     | 1618 | 6MZ  | C6-N6 | 9.41  | 1.44        | 1.34     |
| 54  | z     | 8    | 5MU  | C6-N1 | 9.25  | 1.53        | 1.38     |
| 54  | z     | 57   | 5MU  | C6-N1 | 9.21  | 1.53        | 1.38     |
| 54  | z     | 8    | 5MU  | C4-C5 | 9.20  | 1.60        | 1.44     |
| 54  | z     | 69   | 5MU  | C6-N1 | 9.20  | 1.53        | 1.38     |
| 1   | 1     | 1939 | 5MU  | C6-N1 | 9.01  | 1.53        | 1.38     |
| 1   | 1     | 1915 | 3TD  | C2-N1 | 8.95  | 1.48        | 1.37     |
| 1   | 1     | 2030 | 6MZ  | C6-N6 | 8.94  | 1.43        | 1.34     |
| 1   | 1     | 1939 | 5MU  | C4-C5 | 8.85  | 1.59        | 1.44     |
| 1   | 1     | 747  | 5MU  | C4-C5 | 8.50  | 1.58        | 1.44     |
| 54  | z     | 42   | 5MU  | C6-N1 | 8.50  | 1.52        | 1.38     |
| 54  | z     | 42   | 5MU  | C4-N3 | -8.42 | 1.23        | 1.38     |
| 54  | z     | 57   | 5MU  | C4-C5 | 8.37  | 1.58        | 1.44     |
| 2   | 2     | 1407 | 5MC  | C6-C5 | 8.23  | 1.48        | 1.34     |
| 54  | z     | 57   | 5MU  | C4-N3 | -8.16 | 1.23        | 1.38     |
| 54  | z     | 42   | 5MU  | C4-C5 | 8.05  | 1.58        | 1.44     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 1   | 1     | 747  | 5MU  | C4-N3 | -7.99 | 1.24        | 1.38     |
| 2   | 2     | 967  | 5MC  | C6-C5 | 7.97  | 1.47        | 1.34     |
| 1   | 1     | 1939 | 5MU  | C4-N3 | -7.86 | 1.24        | 1.38     |
| 54  | z     | 8    | 5MU  | C4-N3 | -7.86 | 1.24        | 1.38     |
| 2   | 2     | 966  | 2MG  | C2-N3 | 7.68  | 1.46        | 1.31     |
| 54  | z     | 55   | 5MU  | C4-N3 | -7.64 | 1.24        | 1.38     |
| 1   | 1     | 745  | 1MG  | C2-N2 | 7.49  | 1.47        | 1.34     |
| 2   | 2     | 527  | G7M  | C5-N7 | -7.20 | 1.30        | 1.39     |
| 1   | 1     | 2069 | G7M  | C5-N7 | -7.17 | 1.30        | 1.39     |
| 1   | 1     | 1962 | 5MC  | C6-C5 | 7.07  | 1.46        | 1.34     |
| 54  | z     | 69   | 5MU  | C4-N3 | 6.96  | 1.51        | 1.38     |
| 54  | z     | 20   | 5MU  | C4-N3 | -6.96 | 1.25        | 1.38     |
| 1   | 1     | 1835 | 2MG  | C2-N3 | 6.91  | 1.45        | 1.31     |
| 2   | 2     | 1207 | 2MG  | C2-N3 | 6.76  | 1.44        | 1.31     |
| 2   | 2     | 1516 | 2MG  | C2-N3 | 6.59  | 1.44        | 1.31     |
| 1   | 1     | 2445 | 2MG  | C2-N3 | 6.47  | 1.44        | 1.31     |
| 2   | 2     | 966  | 2MG  | C4-N3 | 6.34  | 1.49        | 1.34     |
| 2   | 2     | 1402 | 4OC  | C4-N3 | 6.27  | 1.43        | 1.32     |
| 1   | 1     | 1962 | 5MC  | C4-N3 | 6.24  | 1.44        | 1.34     |
| 2   | 2     | 967  | 5MC  | C4-N3 | 6.19  | 1.44        | 1.34     |
| 1   | 1     | 2552 | OMU  | C2-N3 | 6.10  | 1.48        | 1.38     |
| 54  | z     | 55   | 5MU  | C6-C5 | 6.04  | 1.44        | 1.34     |
| 54  | z     | 20   | 5MU  | C6-C5 | 5.96  | 1.44        | 1.34     |
| 2   | 2     | 1498 | UR3  | C6-C5 | 5.95  | 1.48        | 1.35     |
| 2   | 2     | 967  | 5MC  | C2-N3 | 5.85  | 1.48        | 1.36     |
| 1   | 1     | 2552 | OMU  | C2-N1 | 5.76  | 1.47        | 1.38     |
| 2   | 2     | 1207 | 2MG  | C4-N3 | 5.74  | 1.47        | 1.34     |
| 2   | 2     | 527  | G7M  | C4-N3 | 5.74  | 1.47        | 1.34     |
| 1   | 1     | 1915 | 3TD  | C6-N1 | 5.70  | 1.45        | 1.36     |
| 1   | 1     | 2503 | 2MA  | C2-N3 | 5.62  | 1.44        | 1.34     |
| 1   | 1     | 1835 | 2MG  | C4-N3 | 5.61  | 1.47        | 1.34     |
| 1   | 1     | 2498 | OMC  | C2-N3 | 5.50  | 1.47        | 1.36     |
| 1   | 1     | 745  | 1MG  | C4-N3 | 5.39  | 1.47        | 1.34     |
| 2   | 2     | 1516 | 2MG  | C4-N3 | 5.38  | 1.47        | 1.34     |
| 1   | 1     | 2445 | 2MG  | C4-N3 | 5.37  | 1.47        | 1.34     |
| 1   | 1     | 2069 | G7M  | C4-N3 | 5.33  | 1.46        | 1.34     |
| 1   | 1     | 1962 | 5MC  | C2-N3 | 5.32  | 1.47        | 1.36     |
| 1   | 1     | 747  | 5MU  | C6-C5 | 5.30  | 1.43        | 1.34     |
| 54  | z     | 8    | 5MU  | C6-C5 | 5.22  | 1.43        | 1.34     |
| 2   | 2     | 1402 | 4OC  | C2-N3 | 5.22  | 1.46        | 1.36     |
| 1   | 1     | 2552 | OMU  | C6-C5 | 5.20  | 1.47        | 1.35     |
| 2   | 2     | 1407 | 5MC  | C4-N3 | 5.17  | 1.42        | 1.34     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 2   | 2     | 1407 | 5MC  | C2-N3 | 5.08  | 1.46        | 1.36     |
| 54  | z     | 57   | 5MU  | C6-C5 | 5.08  | 1.42        | 1.34     |
| 2   | 2     | 1402 | 4OC  | C6-C5 | 5.07  | 1.46        | 1.35     |
| 2   | 2     | 966  | 2MG  | C2-N2 | 5.04  | 1.44        | 1.33     |
| 2   | 2     | 527  | G7M  | C2-N3 | 5.02  | 1.45        | 1.33     |
| 1   | 1     | 2251 | OMG  | C4-N3 | 4.93  | 1.46        | 1.34     |
| 2   | 2     | 1498 | UR3  | C2-N1 | 4.92  | 1.45        | 1.38     |
| 1   | 1     | 2503 | 2MA  | C6-N1 | 4.84  | 1.42        | 1.35     |
| 1   | 1     | 2498 | OMC  | C6-C5 | 4.74  | 1.46        | 1.35     |
| 2   | 2     | 1207 | 2MG  | C2-N2 | 4.66  | 1.43        | 1.33     |
| 1   | 1     | 1915 | 3TD  | C2-N3 | 4.60  | 1.48        | 1.38     |
| 1   | 1     | 1939 | 5MU  | C6-C5 | 4.57  | 1.42        | 1.34     |
| 2   | 2     | 527  | G7M  | C2-N2 | 4.46  | 1.44        | 1.34     |
| 1   | 1     | 2503 | 2MA  | C2-N1 | 4.45  | 1.41        | 1.34     |
| 1   | 1     | 2251 | OMG  | C2-N3 | 4.45  | 1.43        | 1.33     |
| 1   | 1     | 2069 | G7M  | C2-N3 | 4.34  | 1.43        | 1.33     |
| 1   | 1     | 2445 | 2MG  | C2-N2 | 4.32  | 1.43        | 1.33     |
| 1   | 1     | 2498 | OMC  | C4-N3 | 4.27  | 1.43        | 1.34     |
| 1   | 1     | 745  | 1MG  | C5-N7 | -4.23 | 1.30        | 1.39     |
| 1   | 1     | 745  | 1MG  | C2-N3 | 4.17  | 1.41        | 1.34     |
| 2   | 2     | 967  | 5MC  | C4-N4 | 4.17  | 1.44        | 1.34     |
| 1   | 1     | 2503 | 2MA  | C6-N6 | -4.12 | 1.23        | 1.34     |
| 2   | 2     | 1519 | MA6  | C5-C4 | -4.11 | 1.31        | 1.39     |
| 2   | 2     | 1516 | 2MG  | C2-N2 | 4.08  | 1.42        | 1.33     |
| 1   | 1     | 1835 | 2MG  | C2-N2 | 4.07  | 1.42        | 1.33     |
| 54  | z     | 42   | 5MU  | C6-C5 | 4.05  | 1.41        | 1.34     |
| 2   | 2     | 1498 | UR3  | C2-N3 | 4.05  | 1.46        | 1.39     |
| 2   | 2     | 1516 | 2MG  | C2-N1 | 4.02  | 1.43        | 1.36     |
| 1   | 1     | 2498 | OMC  | C4-N4 | 4.00  | 1.43        | 1.33     |
| 54  | z     | 69   | 5MU  | C2-N1 | 3.99  | 1.44        | 1.38     |
| 2   | 2     | 1407 | 5MC  | C6-N1 | 3.97  | 1.44        | 1.38     |
| 1   | 1     | 745  | 1MG  | O6-C6 | -3.95 | 1.14        | 1.23     |
| 1   | 1     | 2030 | 6MZ  | C5-N7 | -3.91 | 1.31        | 1.39     |
| 1   | 1     | 2069 | G7M  | C2-N2 | 3.90  | 1.43        | 1.34     |
| 1   | 1     | 2552 | OMU  | C4-N3 | 3.85  | 1.45        | 1.38     |
| 1   | 1     | 2503 | 2MA  | C5-C6 | 3.77  | 1.51        | 1.41     |
| 2   | 2     | 966  | 2MG  | C5-N7 | -3.77 | 1.31        | 1.39     |
| 1   | 1     | 2445 | 2MG  | C5-N7 | -3.76 | 1.31        | 1.39     |
| 2   | 2     | 1402 | 4OC  | C4-N4 | 3.76  | 1.43        | 1.35     |
| 2   | 2     | 1207 | 2MG  | C2-N1 | 3.75  | 1.42        | 1.36     |
| 1   | 1     | 1835 | 2MG  | C5-N7 | -3.75 | 1.31        | 1.39     |
| 1   | 1     | 1962 | 5MC  | C4-N4 | 3.74  | 1.43        | 1.34     |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 1   | 1     | 2030 | 6MZ  | C5-C4  | -3.73 | 1.32        | 1.39     |
| 2   | 2     | 1407 | 5MC  | C4-N4  | 3.70  | 1.43        | 1.34     |
| 1   | 1     | 1962 | 5MC  | C2-N1  | 3.66  | 1.47        | 1.40     |
| 2   | 2     | 1518 | MA6  | C5-C4  | -3.63 | 1.32        | 1.39     |
| 2   | 2     | 966  | 2MG  | C2-N1  | 3.60  | 1.42        | 1.36     |
| 1   | 1     | 1618 | 6MZ  | C5-N7  | -3.60 | 1.32        | 1.39     |
| 1   | 1     | 2251 | OMG  | C5-N7  | -3.60 | 1.32        | 1.39     |
| 54  | z     | 42   | 5MU  | O4-C4  | -3.55 | 1.16        | 1.23     |
| 2   | 2     | 1516 | 2MG  | C5-N7  | -3.53 | 1.32        | 1.39     |
| 1   | 1     | 747  | 5MU  | O4-C4  | -3.53 | 1.16        | 1.23     |
| 2   | 2     | 967  | 5MC  | C2-N1  | 3.50  | 1.47        | 1.40     |
| 1   | 1     | 2503 | 2MA  | C4-N9  | -3.49 | 1.29        | 1.37     |
| 54  | z     | 8    | 5MU  | O4-C4  | -3.48 | 1.17        | 1.23     |
| 1   | 1     | 1618 | 6MZ  | C5-C4  | -3.45 | 1.32        | 1.39     |
| 1   | 1     | 2498 | OMC  | C2-N1  | 3.41  | 1.47        | 1.40     |
| 2   | 2     | 967  | 5MC  | C6-N1  | 3.39  | 1.43        | 1.38     |
| 54  | z     | 8    | 5MU  | O2-C2  | -3.39 | 1.16        | 1.23     |
| 1   | 1     | 2445 | 2MG  | C2-N1  | 3.34  | 1.42        | 1.36     |
| 2   | 2     | 1402 | 4OC  | C2-N1  | 3.31  | 1.47        | 1.40     |
| 2   | 2     | 1407 | 5MC  | O2-C2  | -3.29 | 1.17        | 1.23     |
| 2   | 2     | 1407 | 5MC  | C2-N1  | 3.27  | 1.47        | 1.40     |
| 2   | 2     | 1518 | MA6  | C8-N9  | -3.25 | 1.31        | 1.37     |
| 54  | z     | 57   | 5MU  | O4-C4  | -3.23 | 1.17        | 1.23     |
| 1   | 1     | 1835 | 2MG  | C2-N1  | 3.23  | 1.41        | 1.36     |
| 2   | 2     | 1498 | UR3  | C3U-N3 | -3.18 | 1.41        | 1.47     |
| 2   | 2     | 967  | 5MC  | O2-C2  | -3.18 | 1.17        | 1.23     |
| 1   | 1     | 2503 | 2MA  | C5-N7  | -3.18 | 1.33        | 1.39     |
| 1   | 1     | 1962 | 5MC  | O2-C2  | -3.18 | 1.17        | 1.23     |
| 1   | 1     | 1939 | 5MU  | O4-C4  | -3.16 | 1.17        | 1.23     |
| 1   | 1     | 2251 | OMG  | O6-C6  | -3.15 | 1.17        | 1.23     |
| 1   | 1     | 745  | 1MG  | C4-N9  | -3.15 | 1.29        | 1.38     |
| 1   | 1     | 2498 | OMC  | O2-C2  | -3.12 | 1.17        | 1.23     |
| 2   | 2     | 1402 | 4OC  | O2-C2  | -3.11 | 1.17        | 1.23     |
| 2   | 2     | 1207 | 2MG  | C5-N7  | -3.10 | 1.33        | 1.39     |
| 1   | 1     | 2251 | OMG  | C4-N9  | -3.04 | 1.30        | 1.38     |
| 2   | 2     | 1516 | 2MG  | C4-N9  | -3.02 | 1.30        | 1.38     |
| 2   | 2     | 1518 | MA6  | C5-N7  | -3.00 | 1.33        | 1.39     |
| 1   | 1     | 2030 | 6MZ  | C8-N9  | -2.99 | 1.32        | 1.37     |
| 1   | 1     | 2069 | G7M  | C4-N9  | -2.99 | 1.30        | 1.38     |
| 54  | z     | 55   | 5MU  | O4-C4  | -2.96 | 1.18        | 1.23     |
| 54  | z     | 20   | 5MU  | O4-C4  | -2.96 | 1.18        | 1.23     |
| 1   | 1     | 2069 | G7M  | CN7-N7 | -2.95 | 1.41        | 1.46     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 1   | 1     | 2445 | 2MG  | C4-N9 | -2.95 | 1.30        | 1.38     |
| 2   | 2     | 1519 | MA6  | C8-N9 | -2.94 | 1.32        | 1.37     |
| 1   | 1     | 1962 | 5MC  | C6-N1 | 2.94  | 1.43        | 1.38     |
| 2   | 2     | 527  | G7M  | C5-C6 | 2.93  | 1.51        | 1.43     |
| 1   | 1     | 2552 | OMU  | O4-C4 | -2.92 | 1.18        | 1.24     |
| 2   | 2     | 1519 | MA6  | C5-N7 | -2.90 | 1.33        | 1.39     |
| 1   | 1     | 2445 | 2MG  | O6-C6 | -2.88 | 1.18        | 1.23     |
| 1   | 1     | 2069 | G7M  | C5-C6 | 2.88  | 1.51        | 1.43     |
| 1   | 1     | 1939 | 5MU  | O2-C2 | -2.87 | 1.17        | 1.23     |
| 2   | 2     | 1518 | MA6  | C6-N6 | 2.85  | 1.45        | 1.36     |
| 1   | 1     | 1835 | 2MG  | O6-C6 | -2.85 | 1.18        | 1.23     |
| 1   | 1     | 2069 | G7M  | O6-C6 | -2.85 | 1.18        | 1.23     |
| 2   | 2     | 527  | G7M  | O6-C6 | -2.83 | 1.18        | 1.23     |
| 2   | 2     | 966  | 2MG  | O6-C6 | -2.83 | 1.18        | 1.23     |
| 1   | 1     | 2552 | OMU  | O2-C2 | -2.82 | 1.17        | 1.23     |
| 2   | 2     | 1402 | 4OC  | C5-C4 | 2.81  | 1.46        | 1.40     |
| 1   | 1     | 1618 | 6MZ  | C6-N1 | -2.80 | 1.30        | 1.35     |
| 1   | 1     | 747  | 5MU  | O2-C2 | -2.77 | 1.18        | 1.23     |
| 54  | z     | 64   | 5MU  | C4-N3 | -2.76 | 1.33        | 1.38     |
| 54  | z     | 57   | 5MU  | O2-C2 | -2.75 | 1.18        | 1.23     |
| 54  | z     | 39   | 5MU  | C4-N3 | -2.72 | 1.33        | 1.38     |
| 54  | z     | 39   | 5MU  | C6-C5 | 2.70  | 1.39        | 1.34     |
| 54  | z     | 42   | 5MU  | O2-C2 | -2.68 | 1.18        | 1.23     |
| 54  | z     | 76   | 5MU  | C4-N3 | -2.68 | 1.33        | 1.38     |
| 54  | z     | 69   | 5MU  | O2-C2 | -2.66 | 1.18        | 1.23     |
| 1   | 1     | 2030 | 6MZ  | C5-C6 | -2.65 | 1.35        | 1.41     |
| 2   | 2     | 1207 | 2MG  | O6-C6 | -2.65 | 1.18        | 1.23     |
| 54  | z     | 63   | 5MU  | C4-N3 | -2.63 | 1.34        | 1.38     |
| 1   | 1     | 2030 | 6MZ  | C6-N1 | -2.62 | 1.30        | 1.35     |
| 2   | 2     | 1516 | 2MG  | O6-C6 | -2.61 | 1.18        | 1.23     |
| 1   | 1     | 1915 | 3TD  | O4-C4 | -2.60 | 1.17        | 1.23     |
| 54  | z     | 55   | 5MU  | O2-C2 | -2.59 | 1.18        | 1.23     |
| 54  | z     | 64   | 5MU  | C6-C5 | 2.57  | 1.38        | 1.34     |
| 54  | z     | 76   | 5MU  | C6-C5 | 2.55  | 1.38        | 1.34     |
| 54  | z     | 63   | 5MU  | C6-C5 | 2.55  | 1.38        | 1.34     |
| 2   | 2     | 1498 | UR3  | O2-C2 | -2.55 | 1.17        | 1.22     |
| 1   | 1     | 745  | 1MG  | C5-C6 | 2.54  | 1.52        | 1.45     |
| 1   | 1     | 2580 | PSU  | C4-C5 | -2.53 | 1.36        | 1.44     |
| 2   | 2     | 1207 | 2MG  | C4-N9 | -2.52 | 1.31        | 1.38     |
| 2   | 2     | 1519 | MA6  | C6-N6 | 2.51  | 1.44        | 1.36     |
| 54  | z     | 63   | 5MU  | C4-C5 | 2.51  | 1.48        | 1.44     |
| 1   | 1     | 1915 | 3TD  | O2-C2 | -2.48 | 1.18        | 1.23     |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 54  | z     | 76   | 5MU  | C4-C5  | 2.48  | 1.48        | 1.44     |
| 54  | z     | 64   | 5MU  | C6-N1  | -2.48 | 1.33        | 1.38     |
| 2   | 2     | 1519 | MA6  | C4-N9  | -2.48 | 1.32        | 1.37     |
| 54  | z     | 39   | 5MU  | C2-N1  | 2.48  | 1.42        | 1.38     |
| 54  | z     | 71   | 5MU  | C4-N3  | -2.47 | 1.34        | 1.38     |
| 54  | z     | 40   | 5MU  | C6-C5  | 2.45  | 1.38        | 1.34     |
| 54  | z     | 40   | 5MU  | C4-N3  | -2.43 | 1.34        | 1.38     |
| 2   | 2     | 516  | PSU  | C4-C5  | -2.41 | 1.37        | 1.44     |
| 54  | z     | 40   | 5MU  | C6-N1  | -2.39 | 1.34        | 1.38     |
| 54  | z     | 76   | 5MU  | C6-N1  | -2.39 | 1.34        | 1.38     |
| 2   | 2     | 527  | G7M  | CN7-N7 | -2.39 | 1.42        | 1.46     |
| 1   | 1     | 2503 | 2MA  | C8-N9  | -2.38 | 1.33        | 1.37     |
| 54  | z     | 40   | 5MU  | C4-C5  | 2.38  | 1.48        | 1.44     |
| 1   | 1     | 2457 | PSU  | C4-C5  | -2.37 | 1.37        | 1.44     |
| 54  | z     | 20   | 5MU  | O2-C2  | -2.34 | 1.18        | 1.23     |
| 1   | 1     | 2503 | 2MA  | C5-C4  | -2.34 | 1.34        | 1.39     |
| 2   | 2     | 527  | G7M  | C4-N9  | -2.33 | 1.32        | 1.38     |
| 54  | z     | 71   | 5MU  | C6-C5  | 2.32  | 1.38        | 1.34     |
| 1   | 1     | 955  | PSU  | C4-C5  | -2.32 | 1.37        | 1.44     |
| 2   | 2     | 1207 | 2MG  | C5-C6  | 2.32  | 1.53        | 1.44     |
| 54  | z     | 64   | 5MU  | C4-C5  | 2.30  | 1.48        | 1.44     |
| 2   | 2     | 1498 | UR3  | C6-N1  | 2.30  | 1.43        | 1.38     |
| 1   | 1     | 1618 | 6MZ  | C5-C6  | -2.30 | 1.36        | 1.41     |
| 54  | z     | 39   | 5MU  | C4-C5  | 2.29  | 1.48        | 1.44     |
| 54  | z     | 71   | 5MU  | C2-N1  | 2.29  | 1.42        | 1.38     |
| 2   | 2     | 1516 | 2MG  | C5-C6  | 2.29  | 1.52        | 1.44     |
| 1   | 1     | 2251 | OMG  | C2-N2  | 2.28  | 1.39        | 1.34     |
| 1   | 1     | 1835 | 2MG  | C4-N9  | -2.27 | 1.32        | 1.38     |
| 54  | z     | 40   | 5MU  | C2-N1  | 2.27  | 1.42        | 1.38     |
| 54  | z     | 39   | 5MU  | C6-N1  | -2.25 | 1.34        | 1.38     |
| 54  | z     | 63   | 5MU  | C6-N1  | -2.24 | 1.34        | 1.38     |
| 1   | 1     | 1618 | 6MZ  | C8-N9  | -2.24 | 1.33        | 1.37     |
| 1   | 1     | 1917 | PSU  | C4-C5  | -2.24 | 1.37        | 1.44     |
| 2   | 2     | 1519 | MA6  | C5-C6  | -2.23 | 1.35        | 1.41     |
| 43  | p     | 89   | 0TD  | CSB-SB | -2.20 | 1.75        | 1.79     |
| 2   | 2     | 1402 | 4OC  | C6-N1  | 2.20  | 1.43        | 1.38     |
| 54  | z     | 64   | 5MU  | C2-N1  | 2.20  | 1.42        | 1.38     |
| 54  | z     | 71   | 5MU  | C6-N1  | -2.19 | 1.34        | 1.38     |
| 1   | 1     | 1835 | 2MG  | C5-C6  | 2.14  | 1.52        | 1.44     |
| 1   | 1     | 2605 | PSU  | C4-C5  | -2.14 | 1.38        | 1.44     |
| 54  | z     | 76   | 5MU  | C2-N3  | -2.12 | 1.34        | 1.38     |
| 54  | z     | 63   | 5MU  | C2-N1  | 2.12  | 1.41        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 54  | z     | 63   | 5MU  | C2-N3   | -2.12 | 1.34        | 1.38     |
| 2   | 2     | 527  | G7M  | C2-N1   | 2.11  | 1.42        | 1.37     |
| 1   | 1     | 746  | PSU  | C4-C5   | -2.10 | 1.38        | 1.44     |
| 54  | z     | 64   | 5MU  | C2-N3   | -2.10 | 1.34        | 1.38     |
| 54  | z     | 76   | 5MU  | C2-N1   | 2.09  | 1.41        | 1.38     |
| 1   | 1     | 746  | PSU  | C6-C5   | 2.08  | 1.37        | 1.35     |
| 1   | 1     | 2504 | PSU  | C4-C5   | -2.08 | 1.38        | 1.44     |
| 2   | 2     | 1518 | MA6  | C4-N9   | -2.07 | 1.33        | 1.37     |
| 2   | 2     | 1518 | MA6  | C5-C6   | -2.06 | 1.36        | 1.41     |
| 54  | z     | 71   | 5MU  | C4-C5   | 2.06  | 1.48        | 1.44     |
| 1   | 1     | 2457 | PSU  | C6-N1   | -2.05 | 1.32        | 1.36     |
| 1   | 1     | 2445 | 2MG  | CM2-N2  | -2.05 | 1.41        | 1.45     |
| 2   | 2     | 966  | 2MG  | C5-C6   | 2.04  | 1.52        | 1.44     |
| 1   | 1     | 1915 | 3TD  | O4'-C1' | -2.02 | 1.41        | 1.43     |
| 1   | 1     | 2069 | G7M  | C6-N1   | 2.01  | 1.42        | 1.38     |

All (336) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms     | Z       | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|---------|-------------|----------|
| 54  | z     | 69   | 5MU  | C6-C5-C4  | -115.15 | 21.76       | 118.03   |
| 54  | z     | 69   | 5MU  | C5-C4-N3  | -87.09  | 40.98       | 115.31   |
| 54  | z     | 69   | 5MU  | C6-N1-C2  | -29.10  | 91.84       | 121.30   |
| 54  | z     | 69   | 5MU  | O4-C4-C5  | -25.79  | 95.01       | 124.90   |
| 54  | z     | 69   | 5MU  | N3-C2-N1  | -18.31  | 90.58       | 114.89   |
| 2   | 2     | 1519 | MA6  | N1-C6-N6  | -14.08  | 101.68      | 117.08   |
| 2   | 2     | 1518 | MA6  | N1-C6-N6  | -13.42  | 102.42      | 117.08   |
| 54  | z     | 20   | 5MU  | C5-C4-N3  | 12.87   | 126.29      | 115.31   |
| 1   | 1     | 747  | 5MU  | C5-C4-N3  | 12.70   | 126.15      | 115.31   |
| 54  | z     | 8    | 5MU  | C5-C4-N3  | 12.60   | 126.06      | 115.31   |
| 54  | z     | 42   | 5MU  | C5-C4-N3  | 12.09   | 125.63      | 115.31   |
| 54  | z     | 55   | 5MU  | C5-C4-N3  | 11.91   | 125.48      | 115.31   |
| 54  | z     | 57   | 5MU  | C5-C4-N3  | 11.68   | 125.28      | 115.31   |
| 1   | 1     | 1939 | 5MU  | C5-C4-N3  | 11.44   | 125.08      | 115.31   |
| 54  | z     | 69   | 5MU  | C1'-N1-C2 | 10.72   | 136.98      | 117.57   |
| 54  | z     | 57   | 5MU  | C5-C6-N1  | -10.51  | 112.52      | 123.34   |
| 54  | z     | 42   | 5MU  | C5-C6-N1  | -10.27  | 112.77      | 123.34   |
| 1   | 1     | 747  | 5MU  | C5-C6-N1  | -9.96   | 113.09      | 123.34   |
| 1   | 1     | 1939 | 5MU  | C5-C6-N1  | -9.82   | 113.24      | 123.34   |
| 54  | z     | 8    | 5MU  | C5-C6-N1  | -9.67   | 113.39      | 123.34   |
| 54  | z     | 69   | 5MU  | O2-C2-N1  | 9.36    | 135.23      | 122.79   |
| 54  | z     | 55   | 5MU  | C5-C6-N1  | -8.98   | 114.10      | 123.34   |
| 1   | 1     | 1618 | 6MZ  | C1'-N9-C8 | 8.92    | 147.28      | 127.14   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 54  | z     | 20   | 5MU  | C5-C6-N1  | -8.81 | 114.28      | 123.34   |
| 1   | 1     | 1618 | 6MZ  | C4-N9-C1' | -8.63 | 106.04      | 126.59   |
| 1   | 1     | 2030 | 6MZ  | C4-N9-C1' | -8.44 | 106.49      | 126.59   |
| 54  | z     | 69   | 5MU  | O4-C4-N3  | 8.28  | 135.99      | 120.12   |
| 1   | 1     | 2030 | 6MZ  | C1'-N9-C8 | 8.27  | 145.82      | 127.14   |
| 54  | z     | 69   | 5MU  | C5M-C5-C6 | 7.90  | 133.40      | 122.85   |
| 1   | 1     | 745  | 1MG  | C1'-N9-C4 | -6.87 | 106.11      | 126.50   |
| 54  | z     | 69   | 5MU  | O2-C2-N3  | 6.80  | 134.17      | 121.50   |
| 1   | 1     | 1618 | 6MZ  | C5-C4-N3  | -6.76 | 117.93      | 126.75   |
| 1   | 1     | 2030 | 6MZ  | C5-C4-N3  | -6.67 | 118.05      | 126.75   |
| 54  | z     | 20   | 5MU  | C5M-C5-C4 | 6.62  | 126.06      | 118.77   |
| 2   | 2     | 1518 | MA6  | C5-C6-N6  | 6.48  | 136.59      | 125.30   |
| 54  | z     | 69   | 5MU  | C5M-C5-C4 | -6.47 | 111.65      | 118.77   |
| 2   | 2     | 1519 | MA6  | C5-C6-N6  | 6.42  | 136.49      | 125.30   |
| 1   | 1     | 745  | 1MG  | C1'-N9-C8 | 6.15  | 144.20      | 126.70   |
| 1   | 1     | 2069 | G7M  | CN7-N7-C5 | 6.15  | 134.41      | 126.77   |
| 1   | 1     | 747  | 5MU  | O4-C4-C5  | -6.13 | 117.79      | 124.90   |
| 54  | z     | 69   | 5MU  | C1'-N1-C6 | 6.03  | 131.16      | 121.12   |
| 54  | z     | 8    | 5MU  | C4-N3-C2  | -6.02 | 119.56      | 127.35   |
| 54  | z     | 42   | 5MU  | O4-C4-C5  | -6.02 | 117.93      | 124.90   |
| 1   | 1     | 2503 | 2MA  | C1'-N9-C8 | -5.96 | 113.67      | 127.14   |
| 1   | 1     | 2457 | PSU  | C4-N3-C2  | -5.93 | 117.80      | 126.34   |
| 2   | 2     | 966  | 2MG  | C2-N3-C4  | 5.93  | 119.39      | 112.04   |
| 2   | 2     | 966  | 2MG  | C5-C4-N3  | -5.80 | 119.05      | 128.46   |
| 1   | 1     | 2069 | G7M  | CN7-N7-C8 | -5.77 | 115.93      | 124.84   |
| 1   | 1     | 2503 | 2MA  | N9-C8-N7  | -5.70 | 106.11      | 113.91   |
| 54  | z     | 57   | 5MU  | O4-C4-C5  | -5.69 | 118.31      | 124.90   |
| 1   | 1     | 2457 | PSU  | N1-C2-N3  | 5.65  | 121.53      | 115.13   |
| 2   | 2     | 1519 | MA6  | N1-C2-N3  | -5.64 | 119.77      | 128.60   |
| 2   | 2     | 1207 | 2MG  | C2-N3-C4  | 5.64  | 119.03      | 112.04   |
| 1   | 1     | 2030 | 6MZ  | C4-C5-C6  | 5.62  | 121.16      | 116.81   |
| 1   | 1     | 1835 | 2MG  | C5-C4-N3  | -5.58 | 119.41      | 128.46   |
| 1   | 1     | 747  | 5MU  | C4-N3-C2  | -5.58 | 120.13      | 127.35   |
| 54  | z     | 57   | 5MU  | C4-N3-C2  | -5.56 | 120.15      | 127.35   |
| 1   | 1     | 1939 | 5MU  | C5M-C5-C6 | -5.50 | 115.50      | 122.85   |
| 1   | 1     | 1835 | 2MG  | C2-N3-C4  | 5.50  | 118.85      | 112.04   |
| 54  | z     | 42   | 5MU  | C4-N3-C2  | -5.47 | 120.28      | 127.35   |
| 54  | z     | 8    | 5MU  | O4-C4-C5  | -5.44 | 118.60      | 124.90   |
| 54  | z     | 64   | 5MU  | C4-N3-C2  | -5.39 | 120.37      | 127.35   |
| 1   | 1     | 2580 | PSU  | C4-N3-C2  | -5.39 | 118.58      | 126.34   |
| 1   | 1     | 1917 | PSU  | C4-N3-C2  | -5.39 | 118.58      | 126.34   |
| 54  | z     | 69   | 5MU  | C5-C6-N1  | -5.36 | 117.83      | 123.34   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 2   | 2     | 516  | PSU  | C4-N3-C2  | -5.35 | 118.63      | 126.34   |
| 1   | 1     | 2580 | PSU  | N1-C2-N3  | 5.31  | 121.14      | 115.13   |
| 2   | 2     | 1516 | 2MG  | C2-N3-C4  | 5.27  | 118.57      | 112.04   |
| 1   | 1     | 2605 | PSU  | C4-N3-C2  | -5.25 | 118.77      | 126.34   |
| 54  | z     | 63   | 5MU  | C4-N3-C2  | -5.25 | 120.56      | 127.35   |
| 1   | 1     | 1939 | 5MU  | C4-N3-C2  | -5.23 | 120.58      | 127.35   |
| 54  | z     | 76   | 5MU  | C4-N3-C2  | -5.22 | 120.60      | 127.35   |
| 1   | 1     | 1618 | 6MZ  | C4-C5-C6  | 5.19  | 120.83      | 116.81   |
| 54  | z     | 8    | 5MU  | N3-C2-N1  | 5.19  | 121.78      | 114.89   |
| 1   | 1     | 1911 | PSU  | C4-N3-C2  | -5.13 | 118.94      | 126.34   |
| 54  | z     | 71   | 5MU  | C4-N3-C2  | -5.11 | 120.73      | 127.35   |
| 1   | 1     | 1917 | PSU  | N1-C2-N3  | 5.11  | 120.92      | 115.13   |
| 54  | z     | 8    | 5MU  | C5M-C5-C4 | 5.11  | 124.39      | 118.77   |
| 54  | z     | 39   | 5MU  | N3-C2-N1  | 5.09  | 121.64      | 114.89   |
| 1   | 1     | 1939 | 5MU  | C5M-C5-C4 | 5.06  | 124.33      | 118.77   |
| 1   | 1     | 746  | PSU  | C4-N3-C2  | -5.04 | 119.08      | 126.34   |
| 1   | 1     | 1939 | 5MU  | O4-C4-C5  | -5.04 | 119.06      | 124.90   |
| 1   | 1     | 2030 | 6MZ  | N3-C4-N9  | 5.02  | 135.35      | 127.08   |
| 54  | z     | 8    | 5MU  | C5M-C5-C6 | -5.00 | 116.17      | 122.85   |
| 54  | z     | 20   | 5MU  | C5M-C5-C6 | -4.99 | 116.18      | 122.85   |
| 1   | 1     | 2504 | PSU  | C4-N3-C2  | -4.99 | 119.15      | 126.34   |
| 1   | 1     | 955  | PSU  | C4-N3-C2  | -4.98 | 119.16      | 126.34   |
| 54  | z     | 64   | 5MU  | N3-C2-N1  | 4.97  | 121.49      | 114.89   |
| 2   | 2     | 1518 | MA6  | C5-C4-N3  | -4.95 | 120.29      | 126.75   |
| 1   | 1     | 2503 | 2MA  | C4-N9-C8  | 4.94  | 111.08      | 105.73   |
| 1   | 1     | 955  | PSU  | N1-C2-N3  | 4.92  | 120.71      | 115.13   |
| 1   | 1     | 2445 | 2MG  | C2-N3-C4  | 4.92  | 118.14      | 112.04   |
| 54  | z     | 39   | 5MU  | C4-N3-C2  | -4.91 | 120.99      | 127.35   |
| 2   | 2     | 1519 | MA6  | C5-C4-N3  | -4.90 | 120.36      | 126.75   |
| 54  | z     | 40   | 5MU  | C4-N3-C2  | -4.90 | 121.01      | 127.35   |
| 2   | 2     | 527  | G7M  | CN7-N7-C5 | 4.85  | 132.79      | 126.77   |
| 2   | 2     | 1518 | MA6  | N1-C2-N3  | -4.84 | 121.03      | 128.60   |
| 1   | 1     | 2552 | OMU  | C4-N3-C2  | -4.83 | 120.21      | 126.58   |
| 2   | 2     | 1516 | 2MG  | C2-N1-C6  | -4.82 | 118.93      | 124.48   |
| 1   | 1     | 1835 | 2MG  | C2-N1-C6  | -4.81 | 118.94      | 124.48   |
| 54  | z     | 76   | 5MU  | N3-C2-N1  | 4.81  | 121.27      | 114.89   |
| 54  | z     | 20   | 5MU  | O4-C4-C5  | -4.79 | 119.35      | 124.90   |
| 54  | z     | 57   | 5MU  | N3-C2-N1  | 4.78  | 121.23      | 114.89   |
| 54  | z     | 42   | 5MU  | C5M-C5-C6 | -4.77 | 116.48      | 122.85   |
| 2   | 2     | 1207 | 2MG  | C5-C4-N3  | -4.76 | 120.74      | 128.46   |
| 54  | z     | 63   | 5MU  | N3-C2-N1  | 4.75  | 121.20      | 114.89   |
| 54  | z     | 71   | 5MU  | N3-C2-N1  | 4.71  | 121.14      | 114.89   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 54  | z     | 71   | 5MU  | C5-C4-N3  | 4.69  | 119.32      | 115.31   |
| 1   | 1     | 2605 | PSU  | N1-C2-N3  | 4.69  | 120.44      | 115.13   |
| 2   | 2     | 1516 | 2MG  | C5-C4-N3  | -4.66 | 120.90      | 128.46   |
| 54  | z     | 63   | 5MU  | C5-C4-N3  | 4.65  | 119.28      | 115.31   |
| 1   | 1     | 747  | 5MU  | N3-C2-N1  | 4.63  | 121.03      | 114.89   |
| 1   | 1     | 1911 | PSU  | N1-C2-N3  | 4.60  | 120.35      | 115.13   |
| 1   | 1     | 2251 | OMG  | C5-C4-N3  | -4.60 | 120.99      | 128.46   |
| 54  | z     | 55   | 5MU  | C5M-C5-C4 | 4.59  | 123.82      | 118.77   |
| 54  | z     | 40   | 5MU  | N3-C2-N1  | 4.59  | 120.98      | 114.89   |
| 54  | z     | 20   | 5MU  | C4-N3-C2  | -4.58 | 121.42      | 127.35   |
| 1   | 1     | 2504 | PSU  | N1-C2-N3  | 4.56  | 120.30      | 115.13   |
| 1   | 1     | 1939 | 5MU  | N3-C2-N1  | 4.56  | 120.94      | 114.89   |
| 1   | 1     | 2445 | 2MG  | C5-C4-N3  | -4.53 | 121.11      | 128.46   |
| 1   | 1     | 2030 | 6MZ  | N1-C2-N3  | -4.50 | 121.56      | 128.60   |
| 54  | z     | 71   | 5MU  | O4-C4-C5  | -4.50 | 119.69      | 124.90   |
| 54  | z     | 76   | 5MU  | C5-C4-N3  | 4.50  | 119.15      | 115.31   |
| 54  | z     | 64   | 5MU  | C5-C4-N3  | 4.46  | 119.12      | 115.31   |
| 54  | z     | 55   | 5MU  | C4-N3-C2  | -4.45 | 121.59      | 127.35   |
| 2   | 2     | 527  | G7M  | CN7-N7-C8 | -4.42 | 118.01      | 124.84   |
| 54  | z     | 55   | 5MU  | O4-C4-C5  | -4.42 | 119.78      | 124.90   |
| 2   | 2     | 1519 | MA6  | N9-C8-N7  | -4.41 | 107.88      | 113.91   |
| 1   | 1     | 1618 | 6MZ  | N1-C2-N3  | -4.40 | 121.72      | 128.60   |
| 1   | 1     | 1915 | 3TD  | N1-C2-N3  | 4.38  | 119.59      | 116.14   |
| 1   | 1     | 746  | PSU  | N1-C2-N3  | 4.37  | 120.08      | 115.13   |
| 2   | 2     | 1207 | 2MG  | C2-N1-C6  | -4.35 | 119.47      | 124.48   |
| 2   | 2     | 516  | PSU  | N1-C2-N3  | 4.34  | 120.05      | 115.13   |
| 2   | 2     | 527  | G7M  | C5-C4-N3  | -4.25 | 119.99      | 128.15   |
| 1   | 1     | 1618 | 6MZ  | N3-C4-N9  | 4.23  | 134.06      | 127.08   |
| 1   | 1     | 745  | 1MG  | C5-C4-N3  | -4.23 | 121.60      | 128.46   |
| 54  | z     | 64   | 5MU  | C5-C6-N1  | -4.22 | 118.99      | 123.34   |
| 2   | 2     | 966  | 2MG  | C2-N1-C6  | -4.21 | 119.63      | 124.48   |
| 54  | z     | 55   | 5MU  | N3-C2-N1  | 4.21  | 120.47      | 114.89   |
| 1   | 1     | 745  | 1MG  | CM1-N1-C2 | -4.16 | 116.40      | 120.72   |
| 1   | 1     | 2580 | PSU  | O2-C2-N1  | -4.15 | 118.22      | 122.79   |
| 54  | z     | 42   | 5MU  | N3-C2-N1  | 4.14  | 120.39      | 114.89   |
| 2   | 2     | 527  | G7M  | C1'-N9-C8 | -4.08 | 112.98      | 126.74   |
| 54  | z     | 8    | 5MU  | O2-C2-N1  | -4.07 | 117.38      | 122.79   |
| 54  | z     | 40   | 5MU  | C5-C4-N3  | 4.06  | 118.78      | 115.31   |
| 2   | 2     | 1518 | MA6  | N9-C8-N7  | -4.04 | 108.38      | 113.91   |
| 54  | z     | 63   | 5MU  | C5-C6-N1  | -4.01 | 119.21      | 123.34   |
| 2   | 2     | 527  | G7M  | C2-N3-C4  | 4.01  | 119.44      | 112.30   |
| 54  | z     | 55   | 5MU  | C5M-C5-C6 | -4.00 | 117.51      | 122.85   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 54  | z     | 39   | 5MU  | C5-C4-N3   | 3.99  | 118.71      | 115.31   |
| 2   | 2     | 966  | 2MG  | N9-C4-N3   | 3.98  | 133.94      | 125.94   |
| 2   | 2     | 527  | G7M  | C1'-N9-C4  | 3.95  | 138.24      | 126.50   |
| 54  | z     | 76   | 5MU  | C5-C6-N1   | -3.93 | 119.29      | 123.34   |
| 54  | z     | 64   | 5MU  | O4-C4-C5   | -3.85 | 120.44      | 124.90   |
| 54  | z     | 57   | 5MU  | C6-C5-C4   | 3.82  | 121.22      | 118.03   |
| 54  | z     | 63   | 5MU  | O4-C4-C5   | -3.81 | 120.48      | 124.90   |
| 54  | z     | 69   | 5MU  | C4-N3-C2   | -3.77 | 122.47      | 127.35   |
| 54  | z     | 63   | 5MU  | C2'-C1'-N1 | -3.77 | 102.54      | 113.22   |
| 1   | 1     | 2069 | G7M  | C2-N3-C4   | 3.76  | 118.99      | 112.30   |
| 54  | z     | 40   | 5MU  | O4-C4-C5   | -3.73 | 120.58      | 124.90   |
| 1   | 1     | 2069 | G7M  | O6-C6-C5   | -3.72 | 119.67      | 128.06   |
| 54  | z     | 42   | 5MU  | C5M-C5-C4  | 3.71  | 122.85      | 118.77   |
| 1   | 1     | 1618 | 6MZ  | C2-N3-C4   | 3.70  | 120.50      | 111.75   |
| 1   | 1     | 2445 | 2MG  | C2-N1-C6   | -3.70 | 120.23      | 124.48   |
| 1   | 1     | 1835 | 2MG  | CM2-N2-C2  | -3.68 | 115.72      | 123.86   |
| 1   | 1     | 2030 | 6MZ  | N9-C8-N7   | -3.67 | 108.89      | 113.91   |
| 43  | p     | 89   | 0TD  | OD2-CG-CB  | 3.66  | 121.06      | 113.15   |
| 2   | 2     | 1518 | MA6  | N3-C4-N9   | 3.65  | 133.10      | 127.08   |
| 1   | 1     | 2503 | 2MA  | C4-N9-C1'  | 3.61  | 135.19      | 126.59   |
| 1   | 1     | 2503 | 2MA  | C5-C4-N3   | -3.58 | 123.17      | 127.19   |
| 1   | 1     | 2030 | 6MZ  | C2-N3-C4   | 3.57  | 120.19      | 111.75   |
| 54  | z     | 39   | 5MU  | O4-C4-C5   | -3.57 | 120.76      | 124.90   |
| 2   | 2     | 527  | G7M  | C5-C6-N1   | 3.56  | 119.23      | 111.79   |
| 54  | z     | 76   | 5MU  | O4-C4-C5   | -3.55 | 120.78      | 124.90   |
| 2   | 2     | 1519 | MA6  | C2-N3-C4   | 3.55  | 120.14      | 111.75   |
| 1   | 1     | 2552 | OMU  | N3-C2-N1   | 3.55  | 119.60      | 114.89   |
| 2   | 2     | 1519 | MA6  | N3-C4-N9   | 3.53  | 132.90      | 127.08   |
| 1   | 1     | 2030 | 6MZ  | C9-N6-C6   | -3.53 | 119.83      | 122.87   |
| 1   | 1     | 1917 | PSU  | C6-C5-C4   | 3.50  | 120.65      | 118.20   |
| 1   | 1     | 2069 | G7M  | C1'-N9-C8  | -3.50 | 114.93      | 126.74   |
| 2   | 2     | 1518 | MA6  | C4-C5-C6   | 3.48  | 119.77      | 115.88   |
| 1   | 1     | 2580 | PSU  | C6-C5-C4   | 3.48  | 120.63      | 118.20   |
| 1   | 1     | 2457 | PSU  | O2-C2-N1   | -3.47 | 118.97      | 122.79   |
| 2   | 2     | 527  | G7M  | O6-C6-C5   | -3.46 | 120.26      | 128.06   |
| 1   | 1     | 1835 | 2MG  | N9-C4-N3   | 3.45  | 132.87      | 125.94   |
| 54  | z     | 20   | 5MU  | N3-C2-N1   | 3.44  | 119.45      | 114.89   |
| 1   | 1     | 2251 | OMG  | C2-N1-C6   | -3.43 | 118.85      | 125.10   |
| 1   | 1     | 747  | 5MU  | C5M-C5-C6  | -3.42 | 118.28      | 122.85   |
| 1   | 1     | 2069 | G7M  | C5-C4-N3   | -3.41 | 121.62      | 128.15   |
| 1   | 1     | 1915 | 3TD  | C4-N3-C2   | -3.39 | 120.93      | 124.61   |
| 1   | 1     | 1917 | PSU  | O2-C2-N1   | -3.32 | 119.13      | 122.79   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | 1     | 747  | 5MU  | O2-C2-N1    | -3.32 | 118.38      | 122.79   |
| 1   | 1     | 2069 | G7M  | C5-C6-N1    | 3.29  | 118.66      | 111.79   |
| 54  | z     | 40   | 5MU  | C5-C6-N1    | -3.28 | 119.97      | 123.34   |
| 54  | z     | 57   | 5MU  | C5M-C5-C6   | -3.25 | 118.50      | 122.85   |
| 1   | 1     | 745  | 1MG  | N9-C8-N7    | -3.24 | 107.28      | 113.39   |
| 2   | 2     | 1516 | 2MG  | CM2-N2-C2   | -3.21 | 116.76      | 123.86   |
| 2   | 2     | 1519 | MA6  | C4-N9-C8    | 3.21  | 109.20      | 105.73   |
| 2   | 2     | 527  | G7M  | N9-C4-N3    | 3.21  | 132.38      | 125.94   |
| 54  | z     | 42   | 5MU  | C6-C5-C4    | 3.16  | 120.67      | 118.03   |
| 54  | z     | 39   | 5MU  | C5-C6-N1    | -3.11 | 120.14      | 123.34   |
| 1   | 1     | 955  | PSU  | O2-C2-N1    | -3.11 | 119.37      | 122.79   |
| 1   | 1     | 2251 | OMG  | C2-N3-C4    | 3.10  | 117.83      | 112.30   |
| 1   | 1     | 1618 | 6MZ  | N9-C8-N7    | -3.10 | 109.67      | 113.91   |
| 54  | z     | 39   | 5MU  | C1'-N1-C2   | 3.09  | 123.17      | 117.57   |
| 2   | 2     | 1407 | 5MC  | C5-C6-N1    | -3.09 | 120.16      | 123.34   |
| 2   | 2     | 1518 | MA6  | C2-N3-C4    | 3.08  | 119.03      | 111.75   |
| 2   | 2     | 1498 | UR3  | C4-N3-C2    | -3.07 | 121.67      | 124.56   |
| 1   | 1     | 2251 | OMG  | N9-C8-N7    | -3.07 | 107.61      | 113.39   |
| 54  | z     | 64   | 5MU  | C2'-C1'-N1  | -3.04 | 104.62      | 113.22   |
| 1   | 1     | 1911 | PSU  | O2-C2-N1    | -3.04 | 119.45      | 122.79   |
| 2   | 2     | 1518 | MA6  | C2-N1-C6    | 3.02  | 118.90      | 111.75   |
| 54  | z     | 20   | 5MU  | O4-C4-N3    | -3.01 | 114.35      | 120.12   |
| 1   | 1     | 2030 | 6MZ  | C6-C5-N7    | -2.99 | 129.15      | 132.39   |
| 2   | 2     | 1519 | MA6  | C2-N1-C6    | 2.99  | 118.82      | 111.75   |
| 1   | 1     | 2030 | 6MZ  | C5-C6-N1    | 2.98  | 121.38      | 118.20   |
| 1   | 1     | 2069 | G7M  | C1'-N9-C4   | 2.98  | 135.36      | 126.50   |
| 54  | z     | 40   | 5MU  | C1'-N1-C2   | 2.98  | 122.96      | 117.57   |
| 1   | 1     | 1618 | 6MZ  | C5-C6-N1    | 2.97  | 121.37      | 118.20   |
| 2   | 2     | 1402 | 4OC  | CM4-N4-C4   | -2.96 | 116.66      | 122.45   |
| 1   | 1     | 2552 | OMU  | O4-C4-C5    | -2.96 | 119.95      | 125.16   |
| 54  | z     | 63   | 5MU  | O3'-C3'-C2' | 2.96  | 121.39      | 111.82   |
| 2   | 2     | 1518 | MA6  | C4-N9-C8    | 2.95  | 108.92      | 105.73   |
| 1   | 1     | 747  | 5MU  | C5M-C5-C4   | 2.94  | 122.01      | 118.77   |
| 1   | 1     | 2503 | 2MA  | N3-C2-N1    | -2.89 | 120.41      | 125.72   |
| 54  | z     | 40   | 5MU  | O4'-C1'-N1  | 2.88  | 114.96      | 108.36   |
| 54  | z     | 40   | 5MU  | C1'-N1-C6   | -2.87 | 116.34      | 121.12   |
| 54  | z     | 71   | 5MU  | C5-C6-N1    | -2.87 | 120.39      | 123.34   |
| 2   | 2     | 1207 | 2MG  | N9-C8-N7    | -2.86 | 108.01      | 113.39   |
| 2   | 2     | 527  | G7M  | C2-N1-C6    | -2.86 | 119.89      | 125.10   |
| 54  | z     | 63   | 5MU  | O3'-C3'-C4' | 2.86  | 119.31      | 111.05   |
| 2   | 2     | 1519 | MA6  | C4-C5-C6    | 2.86  | 119.08      | 115.88   |
| 1   | 1     | 2503 | 2MA  | C5-N7-C8    | 2.85  | 107.56      | 103.51   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | 1     | 745  | 1MG  | N9-C4-N3    | 2.81  | 131.57      | 125.94   |
| 54  | z     | 55   | 5MU  | O4-C4-N3    | -2.80 | 114.74      | 120.12   |
| 1   | 1     | 2504 | PSU  | O2-C2-N1    | -2.80 | 119.71      | 122.79   |
| 1   | 1     | 1939 | 5MU  | O2-C2-N1    | -2.78 | 119.09      | 122.79   |
| 1   | 1     | 2552 | OMU  | C5-C4-N3    | 2.76  | 118.97      | 114.84   |
| 54  | z     | 55   | 5MU  | O2-C2-N1    | -2.74 | 119.14      | 122.79   |
| 2   | 2     | 1516 | 2MG  | C1'-N9-C4   | -2.74 | 118.37      | 126.50   |
| 1   | 1     | 745  | 1MG  | CM1-N1-C6   | 2.73  | 121.88      | 117.69   |
| 1   | 1     | 2445 | 2MG  | N9-C4-N3    | 2.73  | 131.43      | 125.94   |
| 1   | 1     | 2445 | 2MG  | N9-C8-N7    | -2.72 | 108.27      | 113.39   |
| 1   | 1     | 2552 | OMU  | CM2-O2'-C2' | -2.72 | 107.39      | 114.52   |
| 54  | z     | 40   | 5MU  | C5M-C5-C4   | 2.70  | 121.74      | 118.77   |
| 1   | 1     | 746  | PSU  | O2-C2-N1    | -2.69 | 119.83      | 122.79   |
| 2   | 2     | 1516 | 2MG  | N9-C8-N7    | -2.66 | 108.38      | 113.39   |
| 1   | 1     | 745  | 1MG  | C2-N3-C4    | 2.66  | 117.95      | 111.98   |
| 2   | 2     | 1207 | 2MG  | CM2-N2-C2   | -2.64 | 118.02      | 123.86   |
| 54  | z     | 42   | 5MU  | C1'-N1-C2   | 2.64  | 122.34      | 117.57   |
| 1   | 1     | 2069 | G7M  | C2-N1-C6    | -2.63 | 120.30      | 125.10   |
| 54  | z     | 63   | 5MU  | O2-C2-N1    | -2.62 | 119.31      | 122.79   |
| 2   | 2     | 1498 | UR3  | C3U-N3-C4   | 2.61  | 121.61      | 117.89   |
| 2   | 2     | 1207 | 2MG  | N9-C4-N3    | 2.60  | 131.17      | 125.94   |
| 2   | 2     | 966  | 2MG  | C5-C6-N1    | 2.60  | 119.79      | 113.19   |
| 54  | z     | 40   | 5MU  | C2'-C1'-N1  | -2.60 | 105.86      | 113.22   |
| 1   | 1     | 1962 | 5MC  | CM5-C5-C6   | -2.59 | 119.39      | 122.85   |
| 1   | 1     | 1618 | 6MZ  | C9-N6-C6    | -2.58 | 120.65      | 122.87   |
| 1   | 1     | 1939 | 5MU  | C6-C5-C4    | 2.55  | 120.16      | 118.03   |
| 1   | 1     | 2030 | 6MZ  | C5-N7-C8    | 2.54  | 107.12      | 103.51   |
| 2   | 2     | 1207 | 2MG  | C5-C6-N1    | 2.53  | 119.61      | 113.19   |
| 54  | z     | 71   | 5MU  | C5'-C4'-C3' | -2.53 | 105.72      | 115.18   |
| 2   | 2     | 966  | 2MG  | O6-C6-C5    | -2.52 | 119.92      | 126.60   |
| 1   | 1     | 955  | PSU  | C6-N1-C2    | -2.52 | 120.11      | 122.68   |
| 2   | 2     | 516  | PSU  | O2-C2-N1    | -2.52 | 120.02      | 122.79   |
| 1   | 1     | 2457 | PSU  | C6-N1-C2    | -2.51 | 120.12      | 122.68   |
| 54  | z     | 8    | 5MU  | O4-C4-N3    | -2.49 | 115.34      | 120.12   |
| 54  | z     | 39   | 5MU  | O4'-C1'-N1  | 2.49  | 114.06      | 108.36   |
| 54  | z     | 63   | 5MU  | O4'-C4'-C3' | -2.48 | 100.21      | 105.11   |
| 1   | 1     | 2251 | OMG  | N9-C4-N3    | 2.47  | 130.90      | 125.94   |
| 54  | z     | 39   | 5MU  | C1'-N1-C6   | -2.47 | 117.02      | 121.12   |
| 1   | 1     | 1962 | 5MC  | C5-C4-N4    | -2.47 | 117.79      | 121.48   |
| 2   | 2     | 966  | 2MG  | N9-C8-N7    | -2.46 | 108.76      | 113.39   |
| 2   | 2     | 1516 | 2MG  | O6-C6-C5    | -2.46 | 120.08      | 126.60   |
| 1   | 1     | 2069 | G7M  | N9-C8-N7    | -2.45 | 106.16      | 112.21   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | 1     | 1835 | 2MG  | C5-C6-N1    | 2.44  | 119.38      | 113.19   |
| 2   | 2     | 1516 | 2MG  | C1'-N9-C8   | 2.44  | 133.63      | 126.70   |
| 54  | z     | 20   | 5MU  | O2-C2-N1    | -2.43 | 119.56      | 122.79   |
| 43  | p     | 89   | 0TD  | OD1-CG-CB   | -2.42 | 117.37      | 122.44   |
| 1   | 1     | 2503 | 2MA  | N3-C4-N9    | 2.42  | 130.34      | 126.99   |
| 2   | 2     | 1207 | 2MG  | C1'-N9-C4   | -2.41 | 119.33      | 126.50   |
| 1   | 1     | 1962 | 5MC  | C1'-N1-C6   | -2.39 | 117.14      | 121.12   |
| 54  | z     | 57   | 5MU  | C1'-N1-C2   | 2.39  | 121.90      | 117.57   |
| 1   | 1     | 1962 | 5MC  | C5-C6-N1    | -2.39 | 120.88      | 123.34   |
| 54  | z     | 40   | 5MU  | C5M-C5-C6   | -2.38 | 119.68      | 122.85   |
| 1   | 1     | 2504 | PSU  | C6-C5-C4    | 2.36  | 119.85      | 118.20   |
| 1   | 1     | 955  | PSU  | C6-C5-C4    | 2.36  | 119.85      | 118.20   |
| 1   | 1     | 2445 | 2MG  | O6-C6-C5    | -2.35 | 120.35      | 126.60   |
| 2   | 2     | 1516 | 2MG  | C5-C6-N1    | 2.34  | 119.14      | 113.19   |
| 2   | 2     | 1516 | 2MG  | N9-C4-N3    | 2.33  | 130.63      | 125.94   |
| 1   | 1     | 2580 | PSU  | O4'-C1'-C2' | 2.33  | 108.43      | 105.14   |
| 1   | 1     | 2069 | G7M  | N2-C2-N1    | 2.31  | 121.64      | 116.71   |
| 54  | z     | 76   | 5MU  | O2-C2-N1    | -2.31 | 119.72      | 122.79   |
| 1   | 1     | 2069 | G7M  | N9-C4-N3    | 2.30  | 130.57      | 125.94   |
| 54  | z     | 76   | 5MU  | C2'-C1'-N1  | -2.28 | 106.75      | 113.22   |
| 54  | z     | 63   | 5MU  | C5M-C5-C4   | 2.28  | 121.28      | 118.77   |
| 54  | z     | 63   | 5MU  | C3'-C2'-C1' | -2.27 | 97.11       | 101.43   |
| 1   | 1     | 2445 | 2MG  | CM2-N2-C2   | -2.27 | 118.85      | 123.86   |
| 54  | z     | 71   | 5MU  | C2'-C3'-C4' | 2.27  | 107.05      | 102.64   |
| 1   | 1     | 2445 | 2MG  | C1'-N9-C4   | -2.27 | 119.77      | 126.50   |
| 1   | 1     | 1618 | 6MZ  | C6-C5-N7    | -2.27 | 129.94      | 132.39   |
| 1   | 1     | 2503 | 2MA  | CM2-C2-N1   | 2.27  | 120.69      | 117.15   |
| 1   | 1     | 2605 | PSU  | C6-C5-C4    | 2.26  | 119.78      | 118.20   |
| 1   | 1     | 2580 | PSU  | C6-N1-C2    | -2.25 | 120.38      | 122.68   |
| 54  | z     | 42   | 5MU  | C1'-N1-C6   | -2.25 | 117.38      | 121.12   |
| 54  | z     | 76   | 5MU  | C5M-C5-C4   | 2.24  | 121.23      | 118.77   |
| 1   | 1     | 1939 | 5MU  | O4-C4-N3    | -2.22 | 115.86      | 120.12   |
| 1   | 1     | 2251 | OMG  | C5-C6-N1    | 2.22  | 118.83      | 113.19   |
| 54  | z     | 39   | 5MU  | O2-C2-N3    | -2.22 | 117.37      | 121.50   |
| 1   | 1     | 2445 | 2MG  | C5-C6-N1    | 2.22  | 118.82      | 113.19   |
| 2   | 2     | 1518 | MA6  | C5-N7-C8    | 2.21  | 106.64      | 103.51   |
| 1   | 1     | 2552 | OMU  | O2-C2-N1    | -2.20 | 119.86      | 122.79   |
| 1   | 1     | 1835 | 2MG  | O6-C6-C5    | -2.19 | 120.80      | 126.60   |
| 1   | 1     | 1618 | 6MZ  | C5-N7-C8    | 2.18  | 106.61      | 103.51   |
| 2   | 2     | 527  | G7M  | N9-C8-N7    | -2.17 | 106.84      | 112.21   |
| 1   | 1     | 2605 | PSU  | O2-C2-N1    | -2.17 | 120.40      | 122.79   |
| 1   | 1     | 1835 | 2MG  | N9-C8-N7    | -2.16 | 109.33      | 113.39   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | 1     | 2251 | OMG  | O6-C6-C5    | -2.15 | 120.89      | 126.60   |
| 54  | z     | 71   | 5MU  | O2-C2-N1    | -2.15 | 119.93      | 122.79   |
| 1   | 1     | 2457 | PSU  | O4'-C1'-C2' | 2.14  | 108.16      | 105.14   |
| 1   | 1     | 1915 | 3TD  | C6-C5-C4    | 2.14  | 119.70      | 118.22   |
| 2   | 2     | 1519 | MA6  | C5-N7-C8    | 2.13  | 106.54      | 103.51   |
| 54  | z     | 57   | 5MU  | O2-C2-N1    | -2.13 | 119.95      | 122.79   |
| 1   | 1     | 747  | 5MU  | O4-C4-N3    | -2.12 | 116.05      | 120.12   |
| 2   | 2     | 1207 | 2MG  | O6-C6-C5    | -2.12 | 120.98      | 126.60   |
| 1   | 1     | 1917 | PSU  | C6-N1-C2    | -2.10 | 120.53      | 122.68   |
| 1   | 1     | 2251 | OMG  | CM2-O2'-C2' | -2.10 | 109.01      | 114.52   |
| 2   | 2     | 967  | 5MC  | CM5-C5-C6   | -2.05 | 120.11      | 122.85   |
| 54  | z     | 71   | 5MU  | C5M-C5-C4   | 2.04  | 121.01      | 118.77   |
| 2   | 2     | 967  | 5MC  | C5-C6-N1    | -2.04 | 121.24      | 123.34   |
| 2   | 2     | 966  | 2MG  | N1-C2-N3    | -2.03 | 120.81      | 123.95   |
| 54  | z     | 42   | 5MU  | O2-C2-N1    | -2.01 | 120.11      | 122.79   |
| 54  | z     | 64   | 5MU  | O4'-C1'-N1  | 2.01  | 112.95      | 108.36   |
| 1   | 1     | 1962 | 5MC  | C1'-N1-C2   | 2.01  | 122.90      | 118.42   |
| 54  | z     | 76   | 5MU  | C5M-C5-C6   | -2.00 | 120.17      | 122.85   |
| 54  | z     | 63   | 5MU  | C5M-C5-C6   | -2.00 | 120.17      | 122.85   |

There are no chirality outliers.

All (64) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 2   | 2     | 516  | PSU  | O4'-C1'-C5-C4   |
| 2   | 2     | 516  | PSU  | O4'-C1'-C5-C6   |
| 2   | 2     | 527  | G7M  | C3'-C4'-C5'-O5' |
| 2   | 2     | 967  | 5MC  | O4'-C4'-C5'-O5' |
| 2   | 2     | 967  | 5MC  | C3'-C4'-C5'-O5' |
| 2   | 2     | 1518 | MA6  | C5-C6-N6-C9     |
| 2   | 2     | 1518 | MA6  | C5-C6-N6-C10    |
| 2   | 2     | 1519 | MA6  | O4'-C4'-C5'-O5' |
| 2   | 2     | 1519 | MA6  | C5-C6-N6-C9     |
| 2   | 2     | 1519 | MA6  | C5-C6-N6-C10    |
| 1   | 1     | 1618 | 6MZ  | N1-C6-N6-C9     |
| 1   | 1     | 1618 | 6MZ  | O4'-C4'-C5'-O5' |
| 1   | 1     | 1618 | 6MZ  | C3'-C4'-C5'-O5' |
| 1   | 1     | 1915 | 3TD  | C2'-C1'-C5-C4   |
| 1   | 1     | 1915 | 3TD  | O4'-C1'-C5-C4   |
| 1   | 1     | 1915 | 3TD  | O4'-C1'-C5-C6   |
| 1   | 1     | 2445 | 2MG  | C3'-C4'-C5'-O5' |
| 1   | 1     | 2504 | PSU  | O4'-C4'-C5'-O5' |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 54  | z     | 8    | 5MU  | O4'-C4'-C5'-O5' |
| 54  | z     | 39   | 5MU  | O4'-C1'-N1-C2   |
| 54  | z     | 39   | 5MU  | O4'-C1'-N1-C6   |
| 54  | z     | 40   | 5MU  | O4'-C1'-N1-C2   |
| 54  | z     | 40   | 5MU  | O4'-C1'-N1-C6   |
| 54  | z     | 64   | 5MU  | O4'-C1'-N1-C2   |
| 54  | z     | 64   | 5MU  | O4'-C1'-N1-C6   |
| 1   | 1     | 2030 | 6MZ  | O4'-C4'-C5'-O5' |
| 1   | 1     | 2030 | 6MZ  | C3'-C4'-C5'-O5' |
| 1   | 1     | 2504 | PSU  | C3'-C4'-C5'-O5' |
| 54  | z     | 8    | 5MU  | C3'-C4'-C5'-O5' |
| 54  | z     | 57   | 5MU  | C3'-C4'-C5'-O5' |
| 54  | z     | 57   | 5MU  | O4'-C4'-C5'-O5' |
| 54  | z     | 63   | 5MU  | C3'-C4'-C5'-O5' |
| 54  | z     | 69   | 5MU  | C3'-C4'-C5'-O5' |
| 54  | z     | 69   | 5MU  | O4'-C4'-C5'-O5' |
| 54  | z     | 71   | 5MU  | C3'-C4'-C5'-O5' |
| 54  | z     | 71   | 5MU  | O4'-C4'-C5'-O5' |
| 2   | 2     | 527  | G7M  | O4'-C4'-C5'-O5' |
| 2   | 2     | 1519 | MA6  | C3'-C4'-C5'-O5' |
| 54  | z     | 20   | 5MU  | O4'-C4'-C5'-O5' |
| 2   | 2     | 1518 | MA6  | N1-C6-N6-C10    |
| 2   | 2     | 1519 | MA6  | N1-C6-N6-C10    |
| 1   | 1     | 1835 | 2MG  | C3'-C4'-C5'-O5' |
| 1   | 1     | 1835 | 2MG  | O4'-C4'-C5'-O5' |
| 54  | z     | 20   | 5MU  | C3'-C4'-C5'-O5' |
| 2   | 2     | 1402 | 4OC  | O4'-C4'-C5'-O5' |
| 54  | z     | 39   | 5MU  | O4'-C4'-C5'-O5' |
| 54  | z     | 63   | 5MU  | O4'-C4'-C5'-O5' |
| 1   | 1     | 2445 | 2MG  | O4'-C4'-C5'-O5' |
| 1   | 1     | 2503 | 2MA  | O4'-C4'-C5'-O5' |
| 43  | p     | 89   | 0TD  | CG-CB-SB-CSB    |
| 2   | 2     | 527  | G7M  | C4'-C5'-O5'-P   |
| 43  | p     | 89   | 0TD  | SB-CB-CG-OD1    |
| 54  | z     | 71   | 5MU  | C4'-C5'-O5'-P   |
| 54  | z     | 76   | 5MU  | O4'-C4'-C5'-O5' |
| 54  | z     | 39   | 5MU  | C3'-C4'-C5'-O5' |
| 1   | 1     | 2503 | 2MA  | C3'-C4'-C5'-O5' |
| 54  | z     | 76   | 5MU  | C3'-C4'-C5'-O5' |
| 43  | p     | 89   | 0TD  | SB-CB-CG-OD2    |
| 54  | z     | 20   | 5MU  | C2'-C1'-N1-C2   |
| 2   | 2     | 1402 | 4OC  | C3'-C4'-C5'-O5' |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 2   | 2     | 1498 | UR3  | O4'-C4'-C5'-O5' |
| 1   | 1     | 746  | PSU  | O4'-C1'-C5-C6   |
| 1   | 1     | 2069 | G7M  | O4'-C4'-C5'-O5' |
| 54  | z     | 20   | 5MU  | C4'-C5'-O5'-P   |

All (1) ring outliers are listed below:

| Mol | Chain | Res | Type | Atoms             |
|-----|-------|-----|------|-------------------|
| 54  | z     | 69  | 5MU  | C2-C4-C5-C6-N1-N3 |

27 monomers are involved in 52 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 54  | z     | 42   | 5MU  | 1       | 0            |
| 54  | z     | 69   | 5MU  | 2       | 0            |
| 1   | 1     | 2552 | OMU  | 1       | 0            |
| 2   | 2     | 1402 | 4OC  | 1       | 0            |
| 54  | z     | 39   | 5MU  | 2       | 0            |
| 54  | z     | 40   | 5MU  | 1       | 0            |
| 1   | 1     | 2457 | PSU  | 1       | 0            |
| 54  | z     | 20   | 5MU  | 4       | 0            |
| 1   | 1     | 747  | 5MU  | 4       | 0            |
| 1   | 1     | 745  | 1MG  | 1       | 0            |
| 54  | z     | 8    | 5MU  | 3       | 0            |
| 1   | 1     | 2030 | 6MZ  | 2       | 0            |
| 1   | 1     | 2503 | 2MA  | 1       | 0            |
| 1   | 1     | 1915 | 3TD  | 2       | 0            |
| 1   | 1     | 2580 | PSU  | 1       | 0            |
| 1   | 1     | 1962 | 5MC  | 1       | 0            |
| 54  | z     | 63   | 5MU  | 2       | 0            |
| 2   | 2     | 1518 | MA6  | 4       | 0            |
| 2   | 2     | 1516 | 2MG  | 1       | 0            |
| 1   | 1     | 2498 | OMC  | 3       | 0            |
| 1   | 1     | 2445 | 2MG  | 2       | 0            |
| 54  | z     | 71   | 5MU  | 7       | 0            |
| 2   | 2     | 1519 | MA6  | 5       | 0            |
| 54  | z     | 64   | 5MU  | 1       | 0            |
| 2   | 2     | 516  | PSU  | 1       | 0            |
| 54  | z     | 55   | 5MU  | 2       | 0            |
| 54  | z     | 76   | 5MU  | 1       | 0            |

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 424 ligands modelled in this entry, 424 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

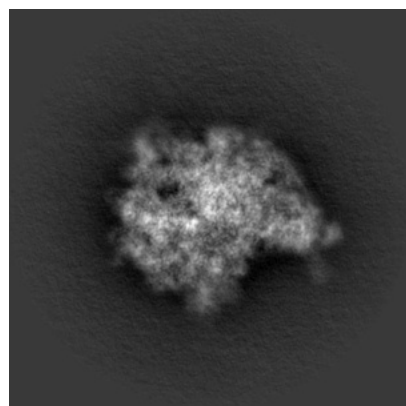
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12930. These allow visual inspection of the internal detail of the map and identification of artifacts.

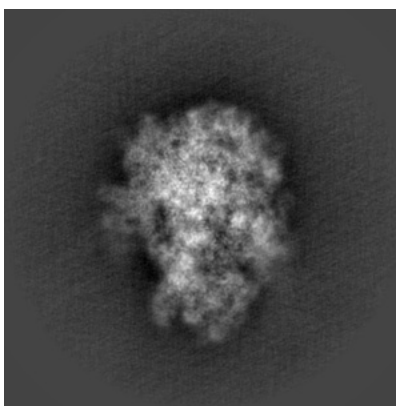
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

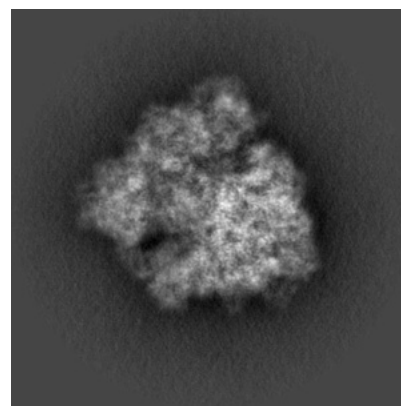
#### 6.1.1 Primary map



X

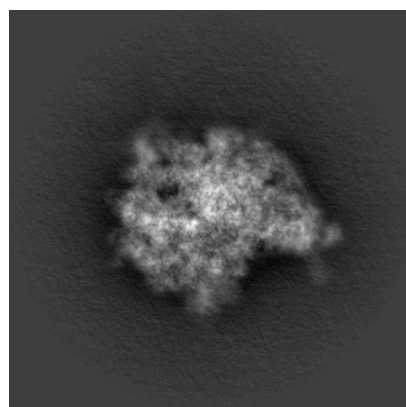


Y

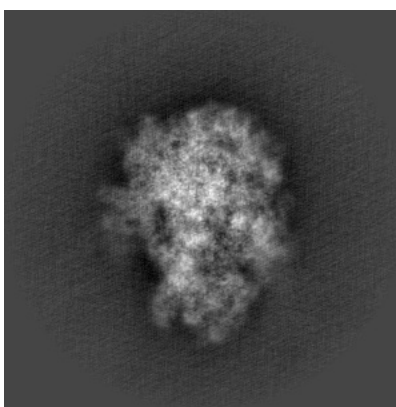


Z

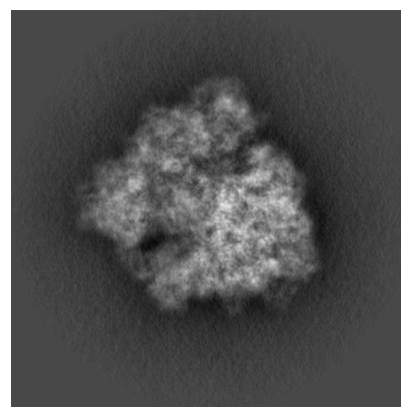
#### 6.1.2 Raw map



X



Y

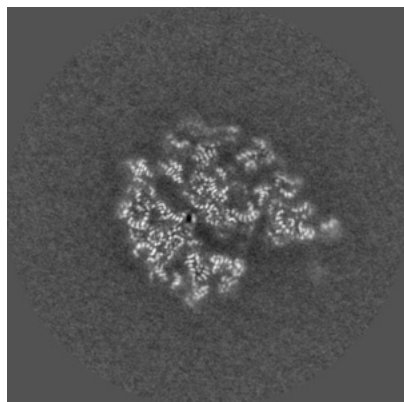


Z

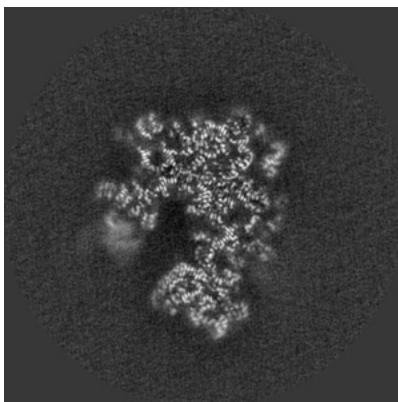
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

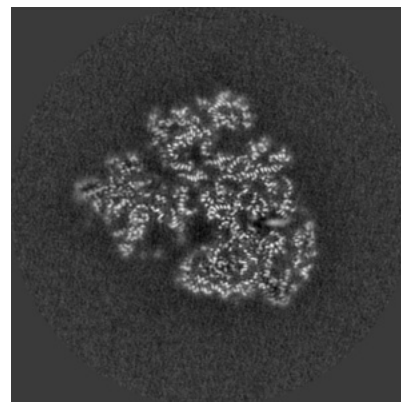
### 6.2.1 Primary map



X Index: 200

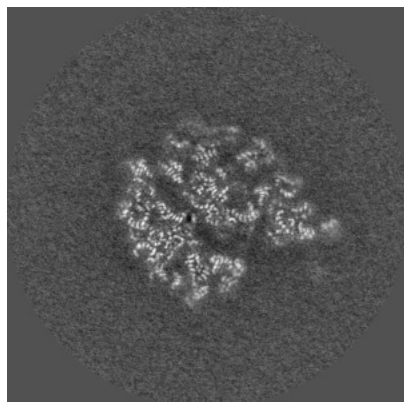


Y Index: 200

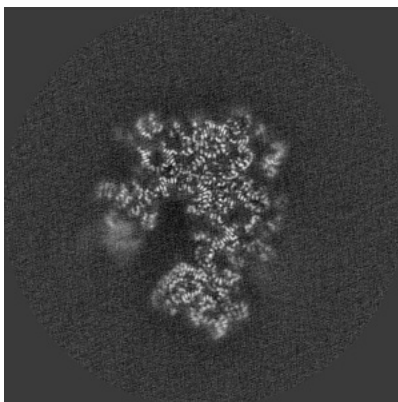


Z Index: 200

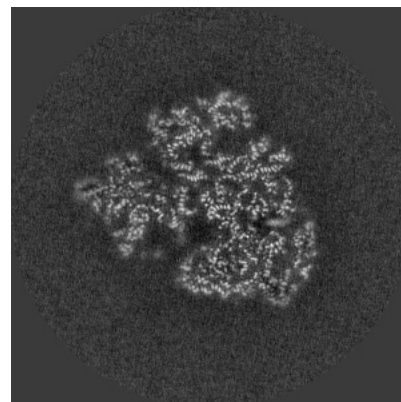
### 6.2.2 Raw map



X Index: 200



Y Index: 200

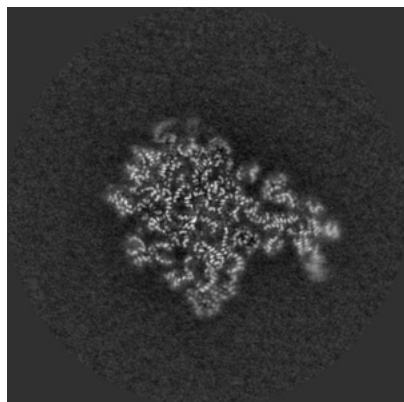


Z Index: 200

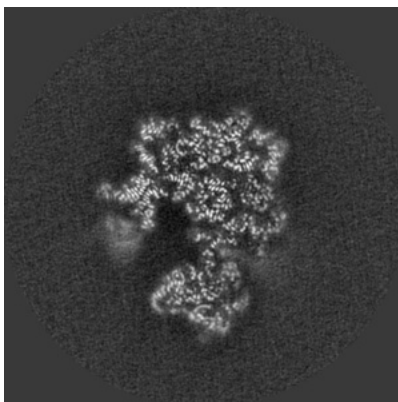
The images above show central slices of the map in three orthogonal directions.

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

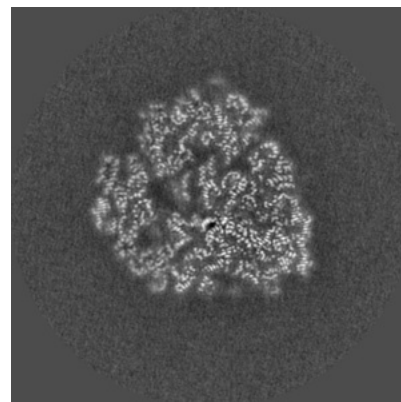
### 6.3.1 Primary map



X Index: 215

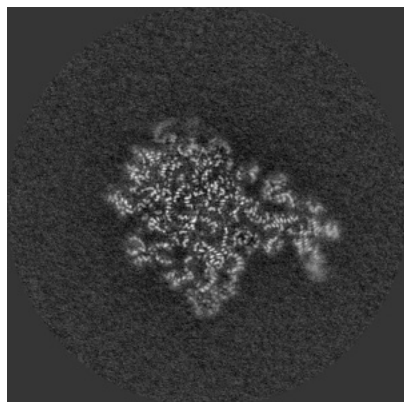


Y Index: 205

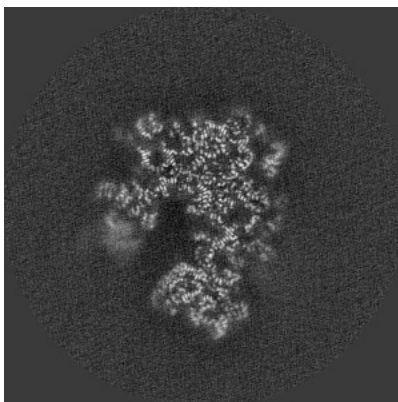


Z Index: 188

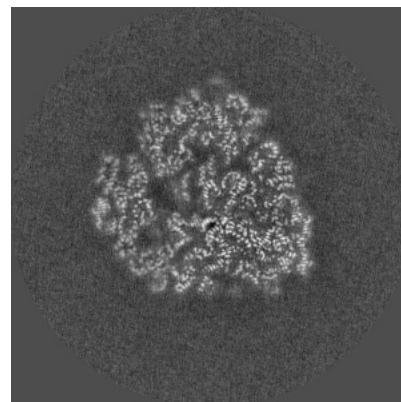
### 6.3.2 Raw map



X Index: 215



Y Index: 200



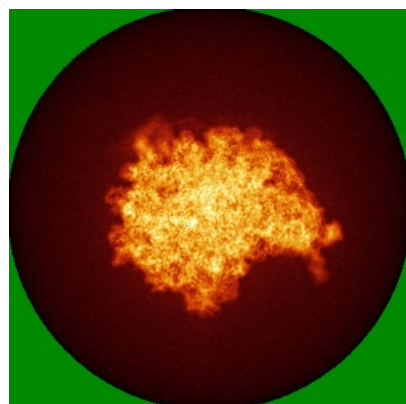
Z Index: 188

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

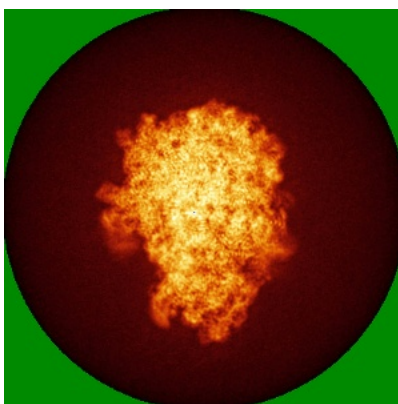


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

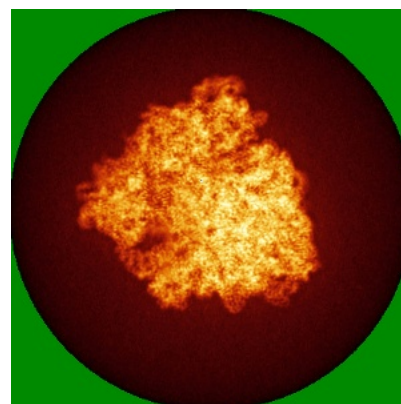
### 6.4.1 Primary map



X

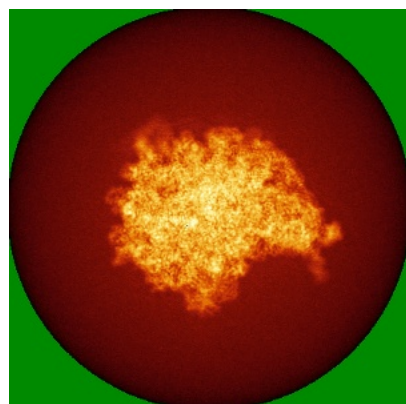


Y

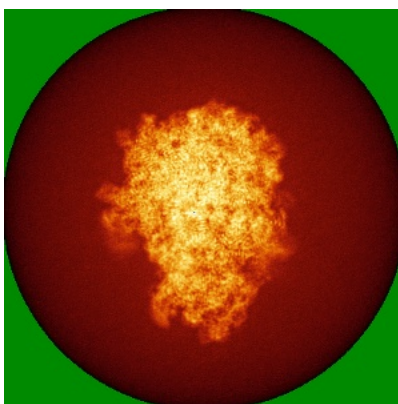


Z

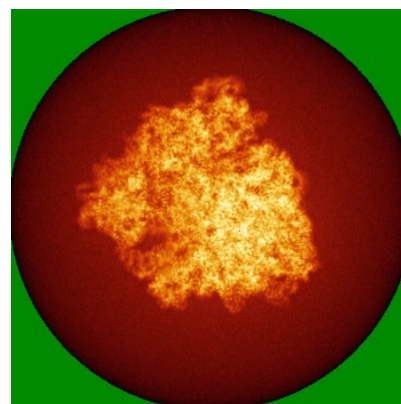
### 6.4.2 Raw map



X



Y

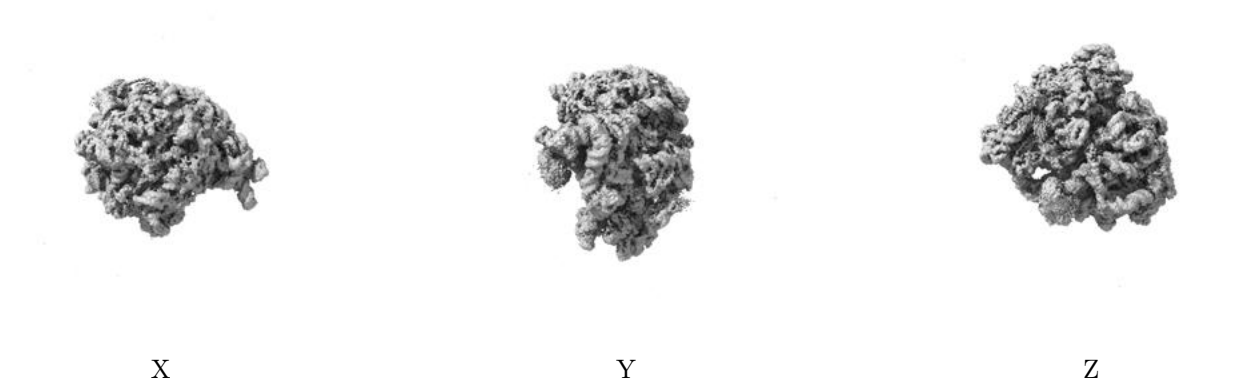


Z

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.

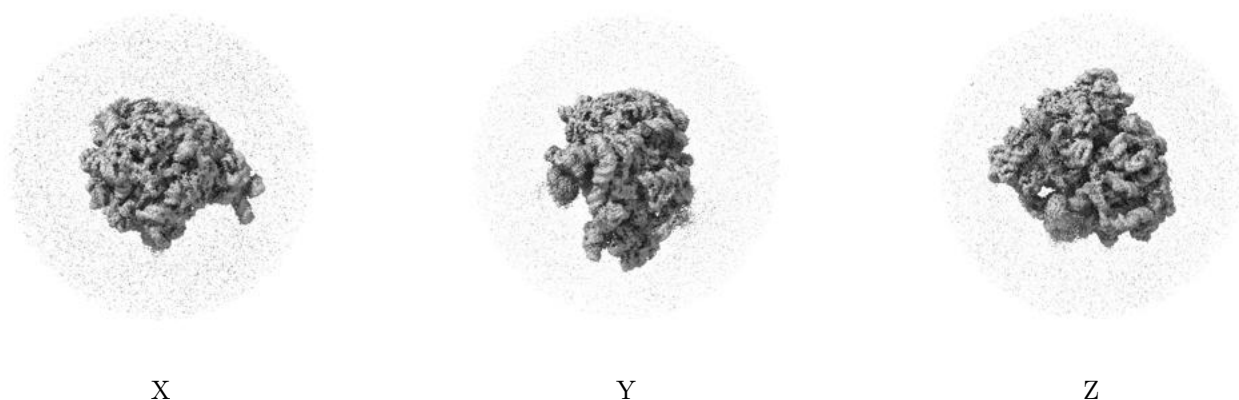
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. 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.

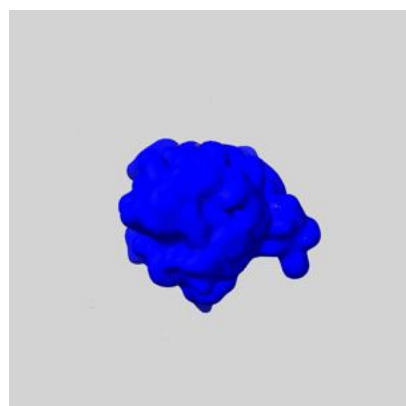
## 6.6 Mask visualisation [i](#)

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

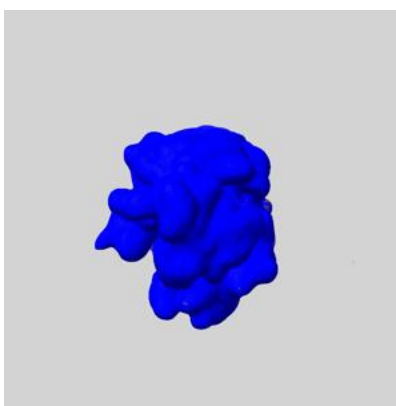
A mask typically either:

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

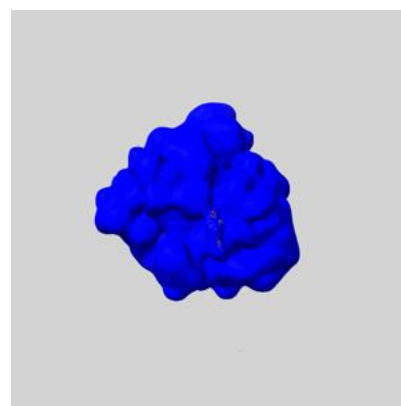
### 6.6.1 emd\_12930\_msk\_1.map [i](#)



X



Y



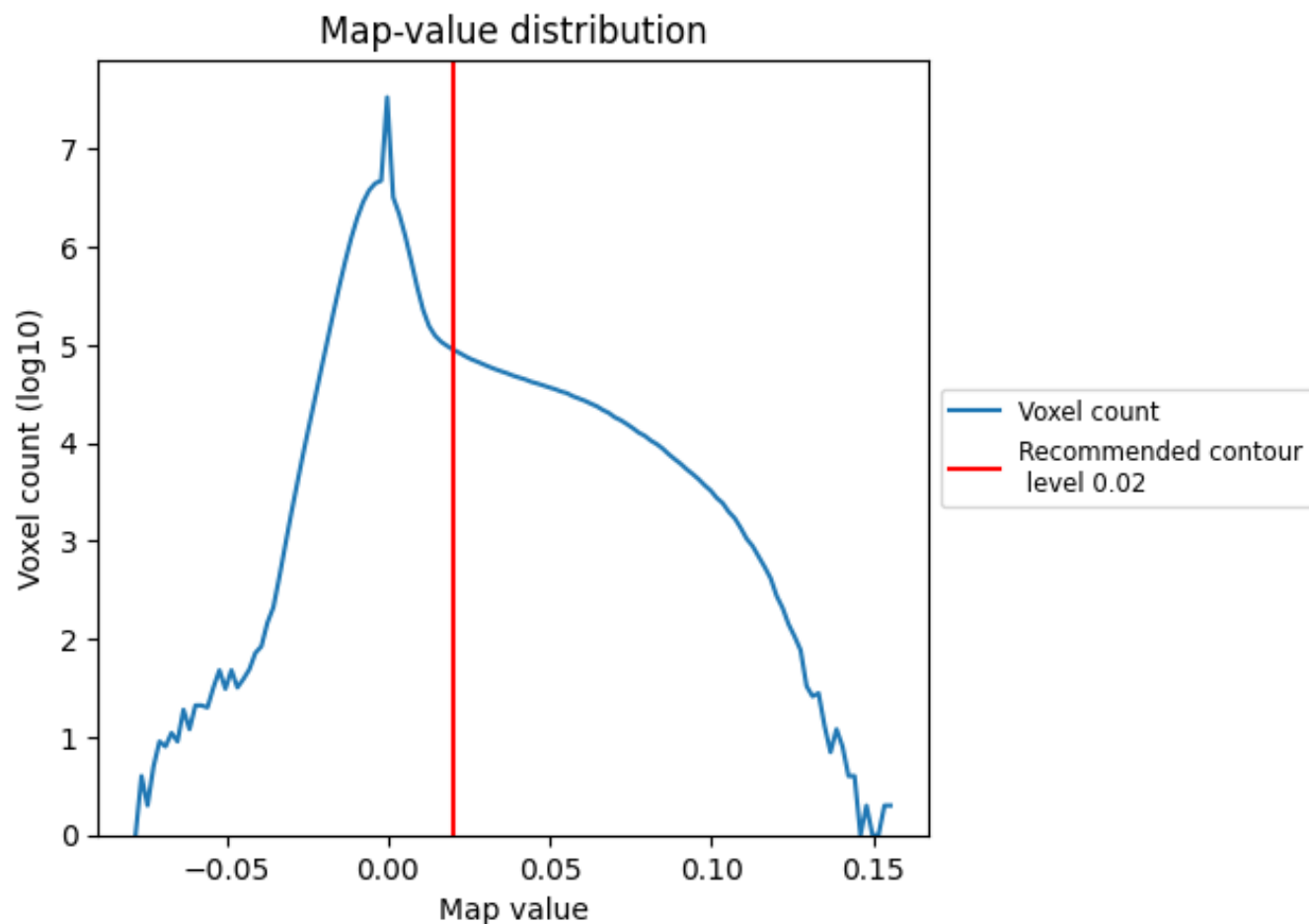
Z



## 7 Map analysis [i](#)

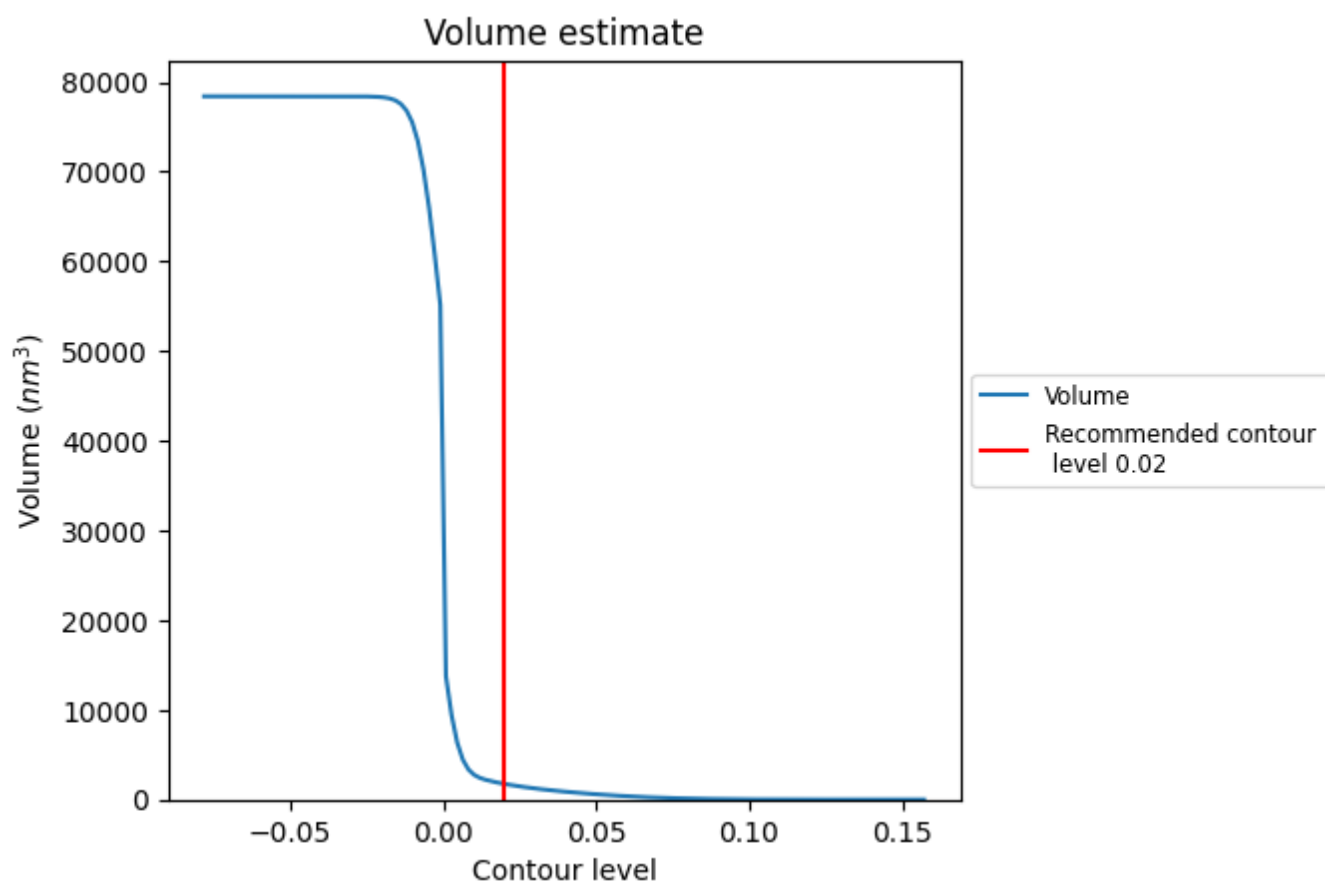
This section contains the results of statistical analysis of the map.

### 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.

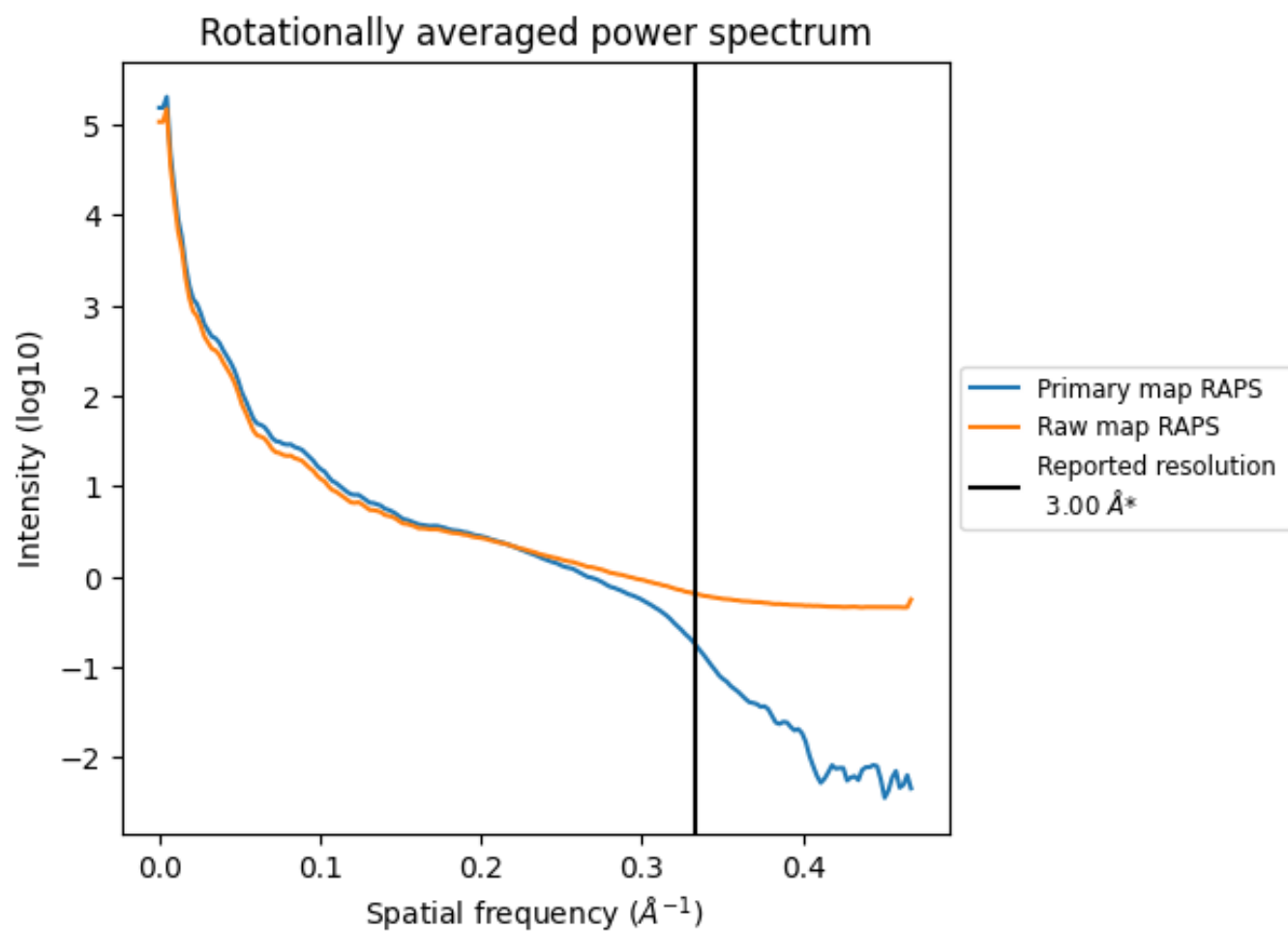
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1748 nm<sup>3</sup>; this corresponds to an approximate mass of 1579 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 ⓘ

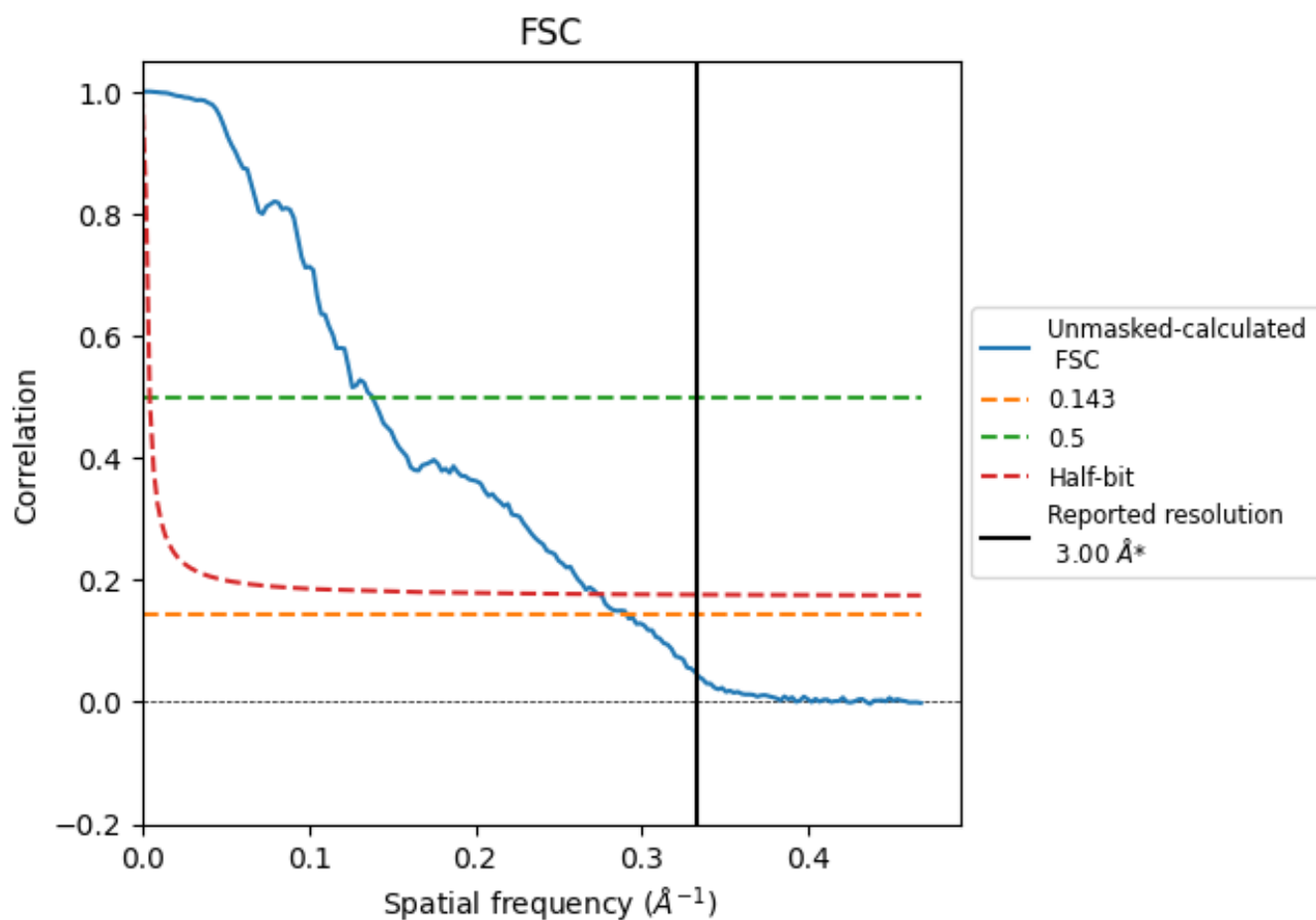


\*Reported resolution corresponds to spatial frequency of 0.333 Å<sup>-1</sup>

## 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 0.333  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

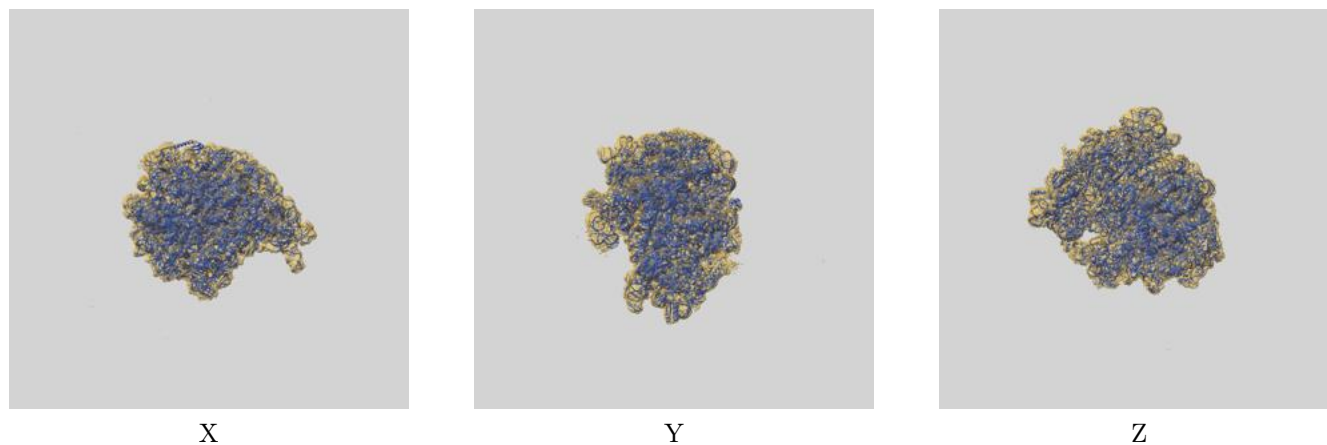
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 3.00                               | -    | -        |
| Author-provided FSC curve | -                                  | -    | -        |
| Unmasked-calculated*      | 3.44                               | 7.24 | 3.66     |

\*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 3.44 differs from the reported value 3.0 by more than 10 %

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

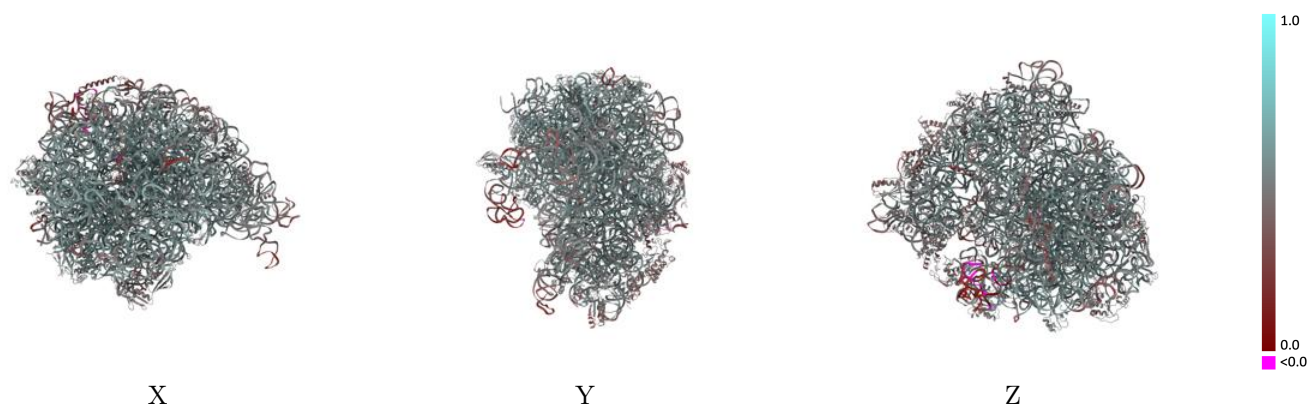
This section contains information regarding the fit between EMDB map EMD-12930 and PDB model 7OII. Per-residue inclusion information can be found in section 3 on page 15.

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



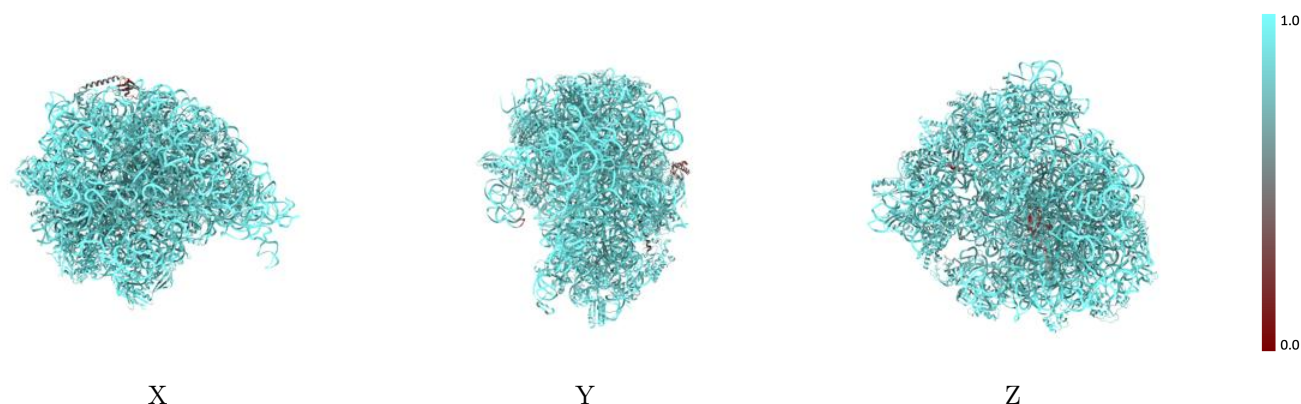
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



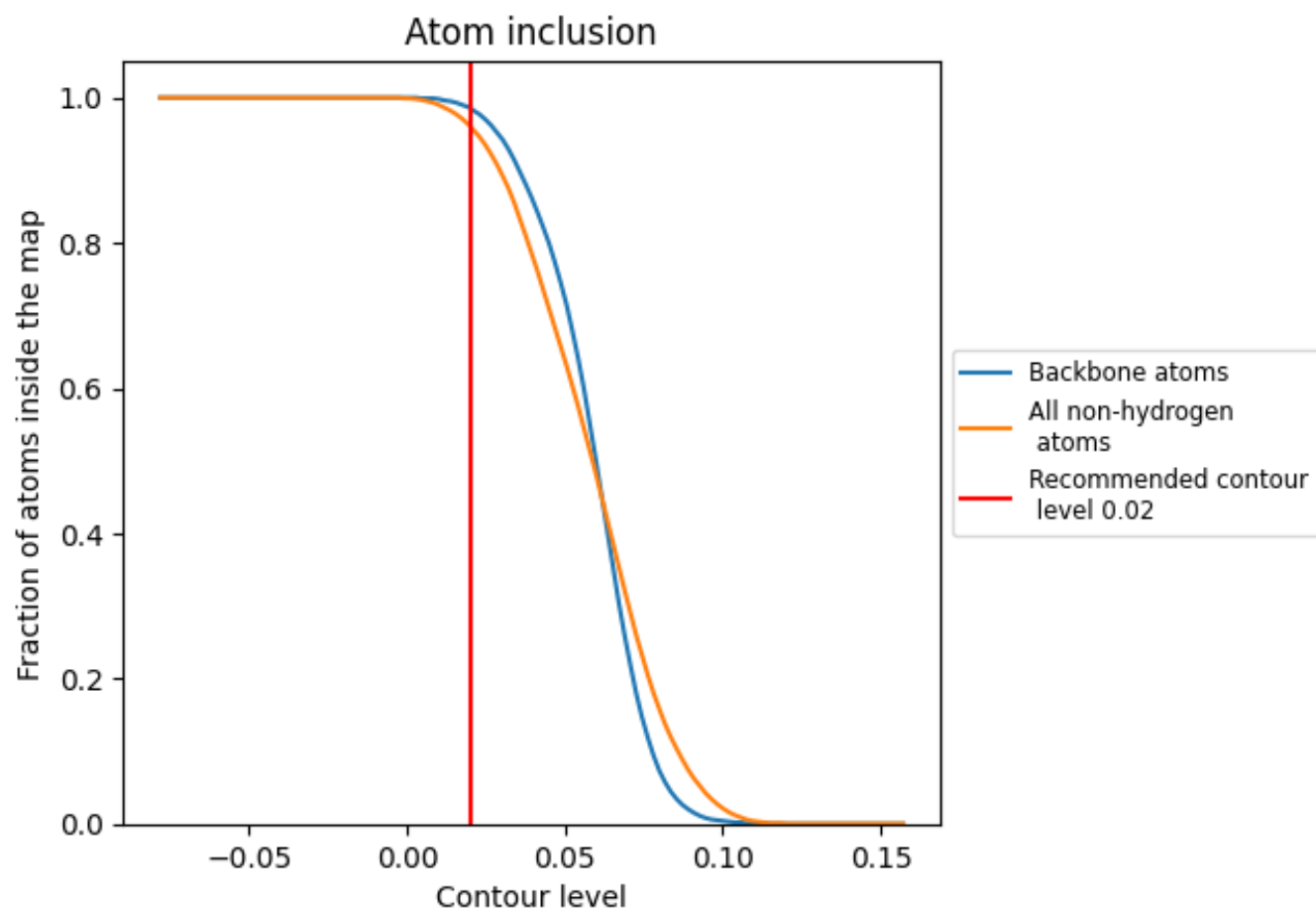
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 96% of all non-hydrogen atoms, are inside the map.



## 9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.9610   |  0.5180   |
| 1     |  0.9870   |  0.5310   |
| 2     |  0.9940   |  0.5240   |
| 3     |  0.9950   |  0.5230   |
| 4     |  0.9840   |  0.5110   |
| B     |  0.9160   |  0.2230   |
| C     |  0.9160   |  0.5640   |
| D     |  0.9320   |  0.5490   |
| E     |  0.9220   |  0.5170   |
| F     |  0.9020   |  0.4600   |
| G     |  0.9150   |  0.4660   |
| H     |  0.4990   |  0.3620   |
| I     |  0.9300   |  0.5430   |
| J     |  0.8830   |  0.5450   |
| K     |  0.9420  |  0.5390  |
| L     |  0.9150 |  0.5400 |
| M     |  0.9560 |  0.5530 |
| N     |  0.9370 |  0.4960 |
| O     |  0.9010 |  0.5410 |
| P     |  0.9440 |  0.5450 |
| Q     |  0.9310 |  0.5270 |
| R     |  0.8840 |  0.5280 |
| S     |  0.9000 |  0.5140 |
| T     |  0.9240 |  0.5050 |
| U     |  0.9050 |  0.5040 |
| V     |  0.8720 |  0.5510 |
| W     |  0.9150 |  0.5350 |
| X     |  0.8770 |  0.4450 |
| Y     |  0.9080 |  0.5260 |
| Z     |  0.8790 |  0.4050 |
| a     |  0.9070 |  0.5390 |
| b     |  0.8610 |  0.5080 |
| c     |  0.9040 |  0.5590 |
| d     |  0.9270 |  0.5700 |
| e     |  0.9040 |  0.5410 |



*Continued on next page...*

*Continued from previous page...*

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| f     |  0.8570   |  0.4310   |
| g     |  0.9040   |  0.4830   |
| h     |  0.9090   |  0.4790   |
| i     |  0.9120   |  0.5130   |
| j     |  0.9020   |  0.4670   |
| k     |  0.8720   |  0.4510   |
| l     |  0.9050   |  0.5130   |
| m     |  0.9130   |  0.4740   |
| n     |  0.8690   |  0.4370   |
| o     |  0.9120   |  0.4920   |
| p     |  0.8750   |  0.5200   |
| q     |  0.9150   |  0.4650   |
| r     |  0.9200   |  0.4970   |
| s     |  0.9220   |  0.4880   |
| t     |  0.9360   |  0.5040   |
| u     |  0.8880   |  0.4900   |
| v     |  0.8910   |  0.4900   |
| w     |  0.9300  |  0.4760  |
| x     |  0.9160 |  0.4820 |
| y     |  0.7460 |  0.3980 |
| z     |  0.9630 |  0.4710 |