



## Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 03:30 PM UTC

PDB ID : 7P7T / pdb\_00007p7t  
EMDB ID : EMD-13244  
Title : PoxA-EQ2 antibiotic resistance ABCF bound to E. faecalis 70S ribosome, state III  
Authors : Crowe-McAuliffe, C.; Wilson, D.N.  
Deposited on : 2021-07-20  
Resolution : 2.90 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

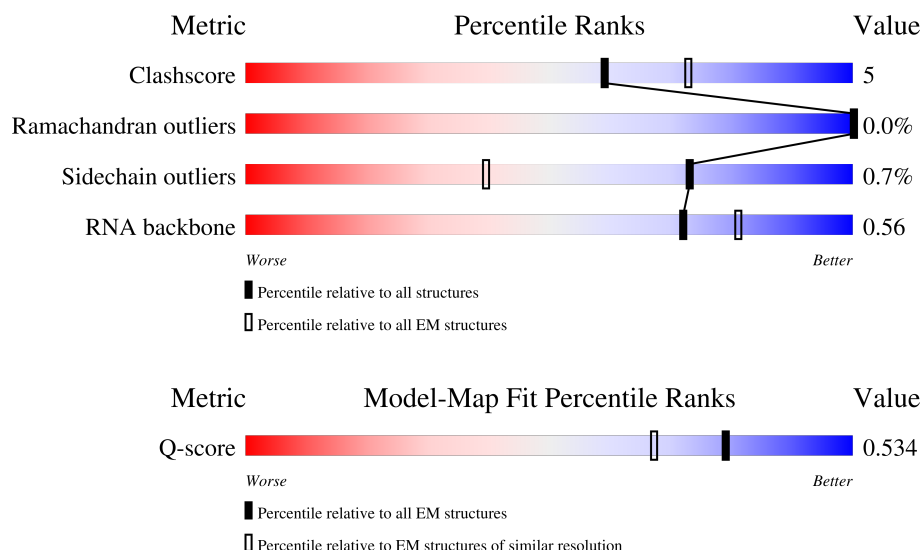
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

# 1 Overall quality at a glance

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

The reported resolution of this entry is 2.90 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                       | 13054 ( 2.40 - 3.40 )                                    |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | 0     | 586    |                  |
| 2   | 1     | 62     |                  |
| 3   | 2     | 59     |                  |

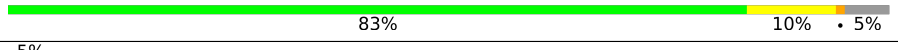
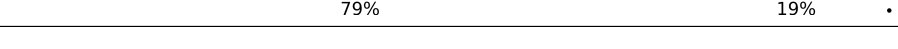
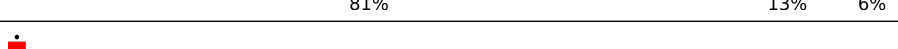
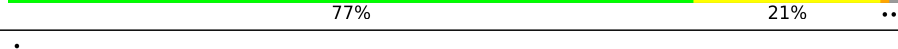
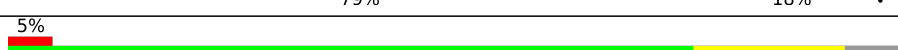
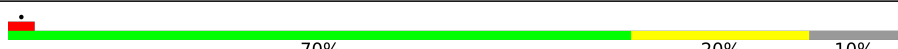
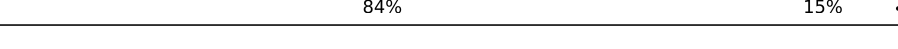
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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 4   | 3     | 89     |                  |
| 5   | 4     | 59     |                  |
| 6   | 5     | 49     |                  |
| 7   | 6     | 44     |                  |
| 8   | 7     | 66     |                  |
| 9   | 8     | 38     |                  |
| 10  | A     | 2912   |                  |
| 11  | B     | 116    |                  |
| 12  | C     | 76     |                  |
| 13  | D     | 77     |                  |
| 14  | F     | 229    |                  |
| 15  | G     | 276    |                  |
| 16  | H     | 209    |                  |
| 17  | I     | 207    |                  |
| 18  | J     | 179    |                  |
| 19  | K     | 178    |                  |
| 20  | M     | 147    |                  |
| 21  | N     | 122    |                  |
| 22  | O     | 146    |                  |
| 23  | P     | 144    |                  |
| 24  | Q     | 127    |                  |
| 25  | R     | 118    |                  |
| 26  | S     | 115    |                  |
| 27  | T     | 119    |                  |
| 28  | U     | 102    |                  |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 29  | V     | 115    |    |
| 30  | W     | 96     |    |
| 31  | X     | 103    |    |
| 32  | Y     | 95     |    |
| 33  | Z     | 62     |    |
| 34  | a     | 1558   |    |
| 35  | b     | 19     |    |
| 36  | c     | 261    |    |
| 37  | d     | 218    |    |
| 38  | e     | 203    |   |
| 39  | f     | 166    |  |
| 40  | g     | 100    |  |
| 41  | h     | 156    |  |
| 42  | i     | 132    |  |
| 43  | j     | 130    |  |
| 44  | k     | 102    |  |
| 45  | l     | 129    |  |
| 46  | m     | 137    |  |
| 47  | n     | 121    |  |
| 48  | o     | 61     |  |
| 49  | p     | 89     |  |
| 50  | q     | 91     |  |
| 51  | r     | 88     |  |
| 52  | s     | 79     |  |
| 53  | t     | 92     |  |

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| Mol | Chain | Length | Quality of chain                                |
|-----|-------|--------|-------------------------------------------------|
| 54  | u     | 83     | <div><div></div><div>94%</div><div></div></div> |

## 2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 149080 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called ARE-ABC-F family resistance factor PoxTA.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1   | 0     | 534      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4347  | 2789 | 720 | 823 | 15 |         |       |

- Molecule 2 is a protein called 50S ribosomal protein L29.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 2   | 1     | 59       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 491   | 307 | 91 | 92 | 1 |         |       |

- Molecule 3 is a protein called 50S ribosomal protein L30.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 3   | 2     | 57       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 428   | 266 | 80 | 81 | 1 |         |       |

- Molecule 4 is a protein called 50S ribosomal protein L31 type B.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 4   | 3     | 80       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 647   | 409 | 110 | 126 | 2 |         |       |

- Molecule 5 is a protein called 50S ribosomal protein L32.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 5   | 4     | 53       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 406   | 248 | 84 | 69 | 5 |         |       |

- Molecule 6 is a protein called 50S ribosomal protein L33.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 6   | 5     | 48       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 410   | 247 | 84 | 75 | 4 |         |       |

- Molecule 7 is a protein called 50S ribosomal protein L34.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 7   | 6     | 44       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 374   | 227 | 91 | 54 | 2 |         |       |

- Molecule 8 is a protein called 50S ribosomal protein L35.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 8   | 7     | 64       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 522   | 320 | 122 | 78 | 2 |         |       |

- Molecule 9 is a protein called 50S ribosomal protein L36.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 9   | 8     | 38       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 305   | 188 | 66 | 45 | 6 |         |       |

- Molecule 10 is a RNA chain called 23S rRNA.

| Mol | Chain | Residues | Atoms |       |       |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|-------|
| 10  | A     | 2901     | Total | C     | N     | O     | P    | 0       | 0     |
|     |       |          | 62268 | 27794 | 11451 | 20122 | 2901 |         |       |

- Molecule 11 is a RNA chain called 5S rRNA.

| Mol | Chain | Residues | Atoms |      |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|-------|
| 11  | B     | 114      | Total | C    | N   | O   | P   | 0       | 0     |
|     |       |          | 2439  | 1088 | 439 | 798 | 114 |         |       |

- Molecule 12 is a RNA chain called A-site tRNA.

| Mol | Chain | Residues | Atoms |     |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---|---------|-------|
| 12  | C     | 72       | Total | C   | N   | O   | P  | S | 0       | 0     |
|     |       |          | 1546  | 692 | 273 | 508 | 72 | 1 |         |       |

- Molecule 13 is a RNA chain called tRNA-fMet.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 13  | D     | 76       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 1624  | 724 | 295 | 529 | 76 |         |       |

- Molecule 14 is a protein called 50S ribosomal protein L1.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 14  | F     | 226      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1693  | 1073 | 287 | 327 | 6 |         |       |

- Molecule 15 is a protein called 50S ribosomal protein L2.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 15  | G     | 274      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2106  | 1305 | 414 | 380 | 7 |         |       |

- Molecule 16 is a protein called 50S ribosomal protein L3.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 16  | H     | 206      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1572  | 990 | 291 | 287 | 4 |         |       |

- Molecule 17 is a protein called 50S ribosomal protein L4.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 17  | I     | 205      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1572  | 984 | 289 | 297 | 2 |         |       |

- Molecule 18 is a protein called 50S ribosomal protein L5.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 18  | J     | 177      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1392  | 887 | 239 | 260 | 6 |         |       |

- Molecule 19 is a protein called 50S ribosomal protein L6.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 19  | K     | 174      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1335  | 838 | 242 | 251 | 4 |         |       |

- Molecule 20 is a protein called 50S ribosomal protein L13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 20  | M     | 147      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1146  | 726 | 207 | 209 | 4 |         |       |

- Molecule 21 is a protein called 50S ribosomal protein L14.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 21  | N     | 122      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 923   | 574 | 176 | 171 | 2 |         |       |

- Molecule 22 is a protein called 50S ribosomal protein L15.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 22  | O     | 146      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1096  | 677 | 212 | 206 | 1 |         |       |

- Molecule 23 is a protein called 50S ribosomal protein L16.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 23  | P     | 134      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1070  | 683 | 209 | 173 | 5 |         |       |

- Molecule 24 is a protein called 50S ribosomal protein L17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 24  | Q     | 125      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 997   | 615 | 192 | 187 | 3 |         |       |

- Molecule 25 is a protein called 50S ribosomal protein L18.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 25  | R     | 118      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 908   | 561 | 176 | 169 | 2 |         |       |

- Molecule 26 is a protein called 50S ribosomal protein L19.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 26  | S     | 114      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 925   | 582 | 185 | 158 |         |       |

- Molecule 27 is a protein called 50S ribosomal protein L20.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 27  | T     | 118      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 950   | 602 | 184 | 160 | 4 |         |       |

- Molecule 28 is a protein called 50S ribosomal protein L21.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 28  | U     | 101      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 779   | 497 | 138 | 142 | 2 |         |       |

- Molecule 29 is a protein called 50S ribosomal protein L22.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 29  | V     | 111      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 841   | 527 | 154 | 158 | 2 |         |       |

- Molecule 30 is a protein called 50S ribosomal protein L23.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 30  | W     | 91       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 736   | 469 | 129 | 134 | 4 |         |       |

- Molecule 31 is a protein called 50S ribosomal protein L24.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 31  | X     | 101      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 763   | 486 | 135 | 140 | 2 |         |       |

- Molecule 32 is a protein called 50S ribosomal protein L27.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 32  | Y     | 74       | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 559   | 344 | 107 | 108 |         |       |

- Molecule 33 is a protein called 50S ribosomal protein L28.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 33  | Z     | 61       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 480   | 299 | 97 | 82 | 2 |         |       |

- Molecule 34 is a RNA chain called 16S rRNA.

| Mol | Chain | Residues | Atoms |       |      |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|-------|
| 34  | a     | 1521     | Total | C     | N    | O     | P    | 0       | 0     |
|     |       |          | 32595 | 14542 | 5954 | 10578 | 1521 |         |       |

- Molecule 35 is a RNA chain called mRNA.

| Mol | Chain | Residues | Atoms |     |    |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|----|---------|-------|
| 35  | b     | 13       | Total | C   | N  | O  | P  | 0       | 0     |
|     |       |          | 287   | 128 | 59 | 87 | 13 |         |       |

- Molecule 36 is a protein called 30S ribosomal protein S2.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 36  | c     | 222      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1773  | 1126 | 312 | 326 | 9 |         |       |

- Molecule 37 is a protein called 30S ribosomal protein S3.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 37  | d     | 205      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1618  | 1018 | 304 | 293 | 3 |         |       |

- Molecule 38 is a protein called 30S ribosomal protein S4.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 38  | e     | 200      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1611  | 1010 | 301 | 296 | 4 |         |       |

- Molecule 39 is a protein called 30S ribosomal protein S5.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 39  | f     | 163      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1204  | 759 | 222 | 221 | 2 |         |       |

- Molecule 40 is a protein called 30S ribosomal protein S6.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 40  | g     | 96       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 786   | 496 | 135 | 152 | 3 |         |       |

- Molecule 41 is a protein called 30S ribosomal protein S7.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 41  | h     | 153      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1218  | 759 | 232 | 221 | 6 |         |       |

- Molecule 42 is a protein called 30S ribosomal protein S8.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 42  | i     | 131      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1041  | 662 | 184 | 193 | 2 |         |       |

- Molecule 43 is a protein called 30S ribosomal protein S9.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 43  | j     | 127      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 980   | 610 | 195 | 174 | 1 |         |       |

- Molecule 44 is a protein called 30S ribosomal protein S10.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 44  | k     | 96       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 773   | 487 | 142 | 142 | 2 |         |       |

- Molecule 45 is a protein called 30S ribosomal protein S11.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 45  | l     | 116      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 854   | 527 | 163 | 160 | 4 |         |       |

- Molecule 46 is a protein called 30S ribosomal protein S12.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 46  | m     | 134      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1051  | 652 | 211 | 186 | 2 |         |       |

- Molecule 47 is a protein called 30S ribosomal protein S13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 47  | n     | 114      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 902   | 552 | 183 | 166 | 1 |         |       |

- Molecule 48 is a protein called 30S ribosomal protein S14 type Z.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 48  | o     | 60       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 492   | 310 | 100 | 77 | 5 |         |       |

- Molecule 49 is a protein called 30S ribosomal protein S15.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 49  | p     | 85       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 716   | 440 | 146 | 129 | 1 |         |       |

- Molecule 50 is a protein called 30S ribosomal protein S16.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 50  | q     | 87       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 692   | 437 | 128 | 125 | 2 |         |       |

- Molecule 51 is a protein called 30S ribosomal protein S17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 51  | r     | 80       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 660   | 414 | 124 | 119 | 3 |         |       |

- Molecule 52 is a protein called 30S ribosomal protein S18.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 52  | s     | 63       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 511   | 328 | 95 | 87 | 1 |         |       |

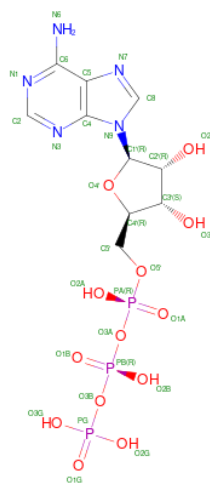
- Molecule 53 is a protein called 30S ribosomal protein S19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 53  | t     | 82       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 663   | 426 | 122 | 113 | 2 |         |       |

- Molecule 54 is a protein called 30S ribosomal protein S20.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 54  | u     | 81       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 608   | 371 | 118 | 117 | 2 |         |       |

- Molecule 55 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).



| Mol | Chain | Residues | Atoms       |         |        |         |        | AltConf |
|-----|-------|----------|-------------|---------|--------|---------|--------|---------|
| 55  | 0     | 1        | Total<br>31 | C<br>10 | N<br>5 | O<br>13 | P<br>3 | 0       |
| 55  | 0     | 1        | Total<br>31 | C<br>10 | N<br>5 | O<br>13 | P<br>3 | 0       |

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

| Mol | Chain | Residues | Atoms               | AltConf |
|-----|-------|----------|---------------------|---------|
| 56  | 0     | 2        | Total Mg<br>2 2     | 0       |
| 56  | A     | 117      | Total Mg<br>117 117 | 0       |
| 56  | B     | 1        | Total Mg<br>1 1     | 0       |
| 56  | G     | 1        | Total Mg<br>1 1     | 0       |
| 56  | a     | 39       | Total Mg<br>39 39   | 0       |
| 56  | n     | 1        | Total Mg<br>1 1     | 0       |

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

| Mol | Chain | Residues | Atoms           | AltConf |
|-----|-------|----------|-----------------|---------|
| 57  | 4     | 1        | Total Zn<br>1 1 | 0       |

*Continued on next page...*

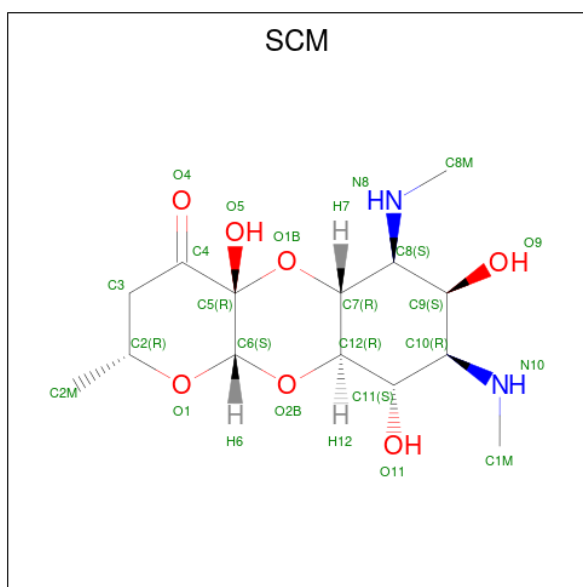
*Continued from previous page...*

| Mol | Chain | Residues | Atoms      |         | AltConf |
|-----|-------|----------|------------|---------|---------|
| 57  | 5     | 1        | Total<br>1 | Zn<br>1 | 0       |
| 57  | 8     | 1        | Total<br>1 | Zn<br>1 | 0       |
| 57  | o     | 1        | Total<br>1 | Zn<br>1 | 0       |

- Molecule 58 is POTASSIUM ION (CCD ID: K) (formula: K).

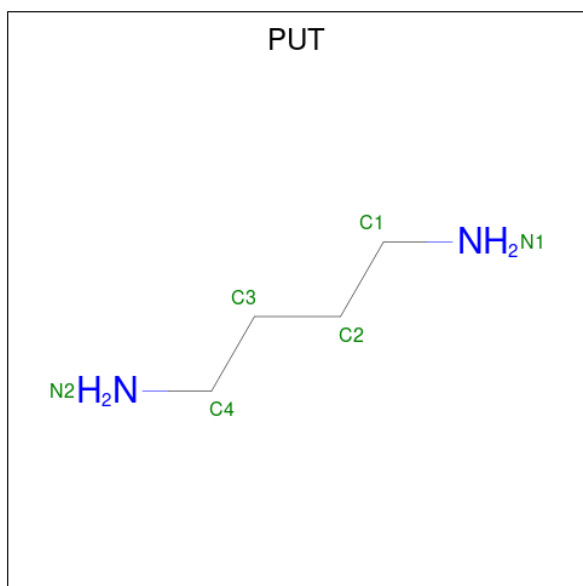
| Mol | Chain | Residues | Atoms       |         | AltConf |
|-----|-------|----------|-------------|---------|---------|
| 58  | 7     | 2        | Total<br>2  | K<br>2  | 0       |
| 58  | A     | 92       | Total<br>92 | K<br>92 | 0       |
| 58  | B     | 3        | Total<br>3  | K<br>3  | 0       |
| 58  | G     | 3        | Total<br>3  | K<br>3  | 0       |
| 58  | P     | 1        | Total<br>1  | K<br>1  | 0       |
| 58  | a     | 35       | Total<br>35 | K<br>35 | 0       |
| 58  | g     | 1        | Total<br>1  | K<br>1  | 0       |
| 58  | o     | 1        | Total<br>1  | K<br>1  | 0       |

- Molecule 59 is SPECTINOMYCIN (CCD ID: SCM) (formula: C<sub>14</sub>H<sub>24</sub>N<sub>2</sub>O<sub>7</sub>).



| Mol | Chain | Residues | Atoms |    |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---------|
| 59  | a     | 1        | Total | C  | N | O | 0       |
|     |       |          | 23    | 14 | 2 | 7 |         |

- Molecule 60 is 1,4-DIAMINOBUTANE (CCD ID: PUT) (formula:  $C_4H_{12}N_2$ ).



| Mol | Chain | Residues | Atoms |   |   | AltConf |
|-----|-------|----------|-------|---|---|---------|
| 60  | a     | 1        | Total | C | N | 0       |
|     |       |          | 6     | 4 | 2 |         |

- Molecule 61 is water.

| Mol | Chain | Residues | Atoms |   | AltConf |
|-----|-------|----------|-------|---|---------|
| 61  | D     | 1        | Total | O | 0       |
|     |       |          | 1     | 1 |         |

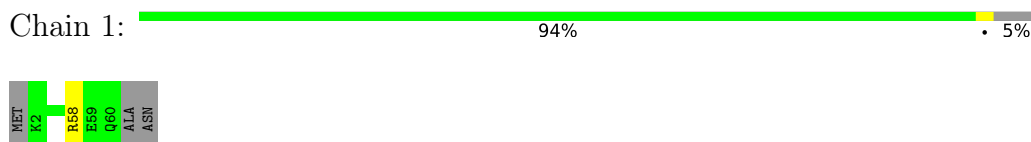
### 3 Residue-property plots

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.

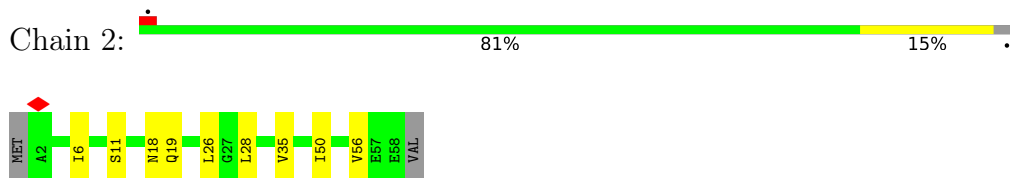
- Molecule 1: ARE-ABC-F family resistance factor PoxTA



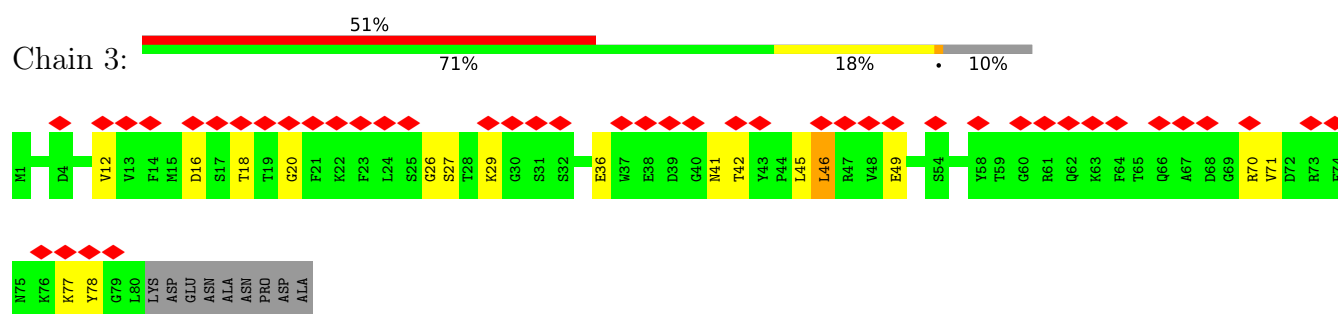
- Molecule 2: 50S ribosomal protein L29



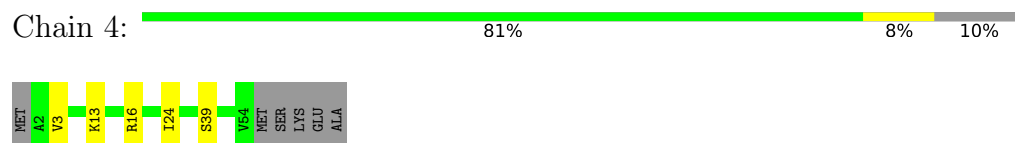
- Molecule 3: 50S ribosomal protein L30



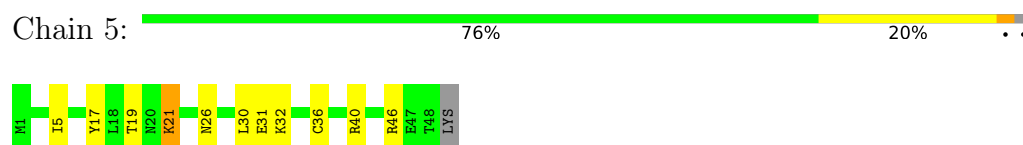
- Molecule 4: 50S ribosomal protein L31 type B



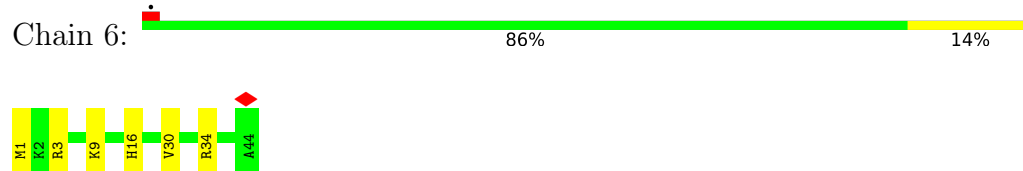
- Molecule 5: 50S ribosomal protein L32



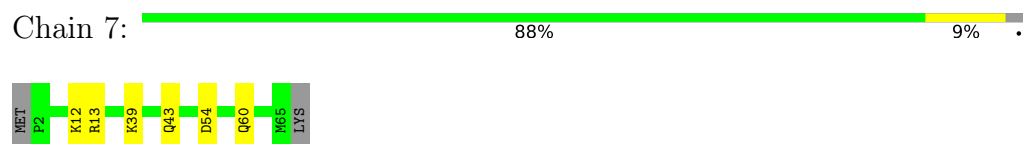
- Molecule 6: 50S ribosomal protein L33



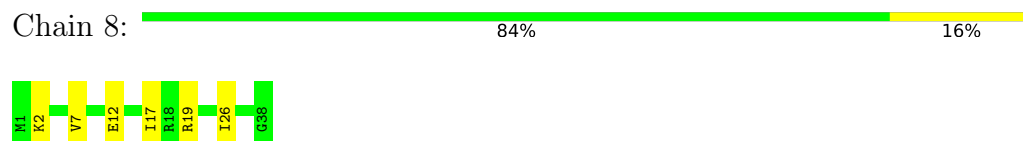
- Molecule 7: 50S ribosomal protein L34



- Molecule 8: 50S ribosomal protein L35

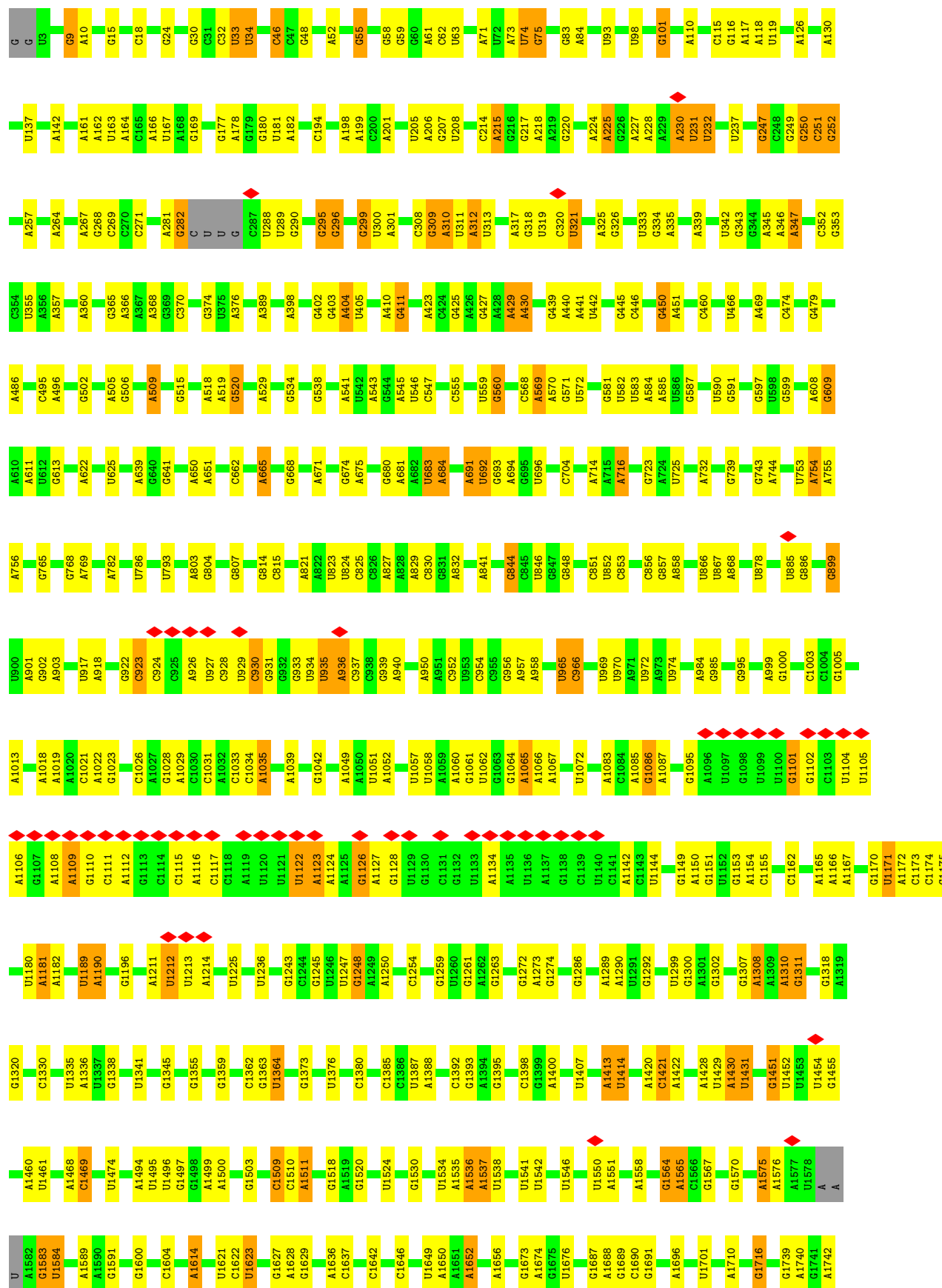


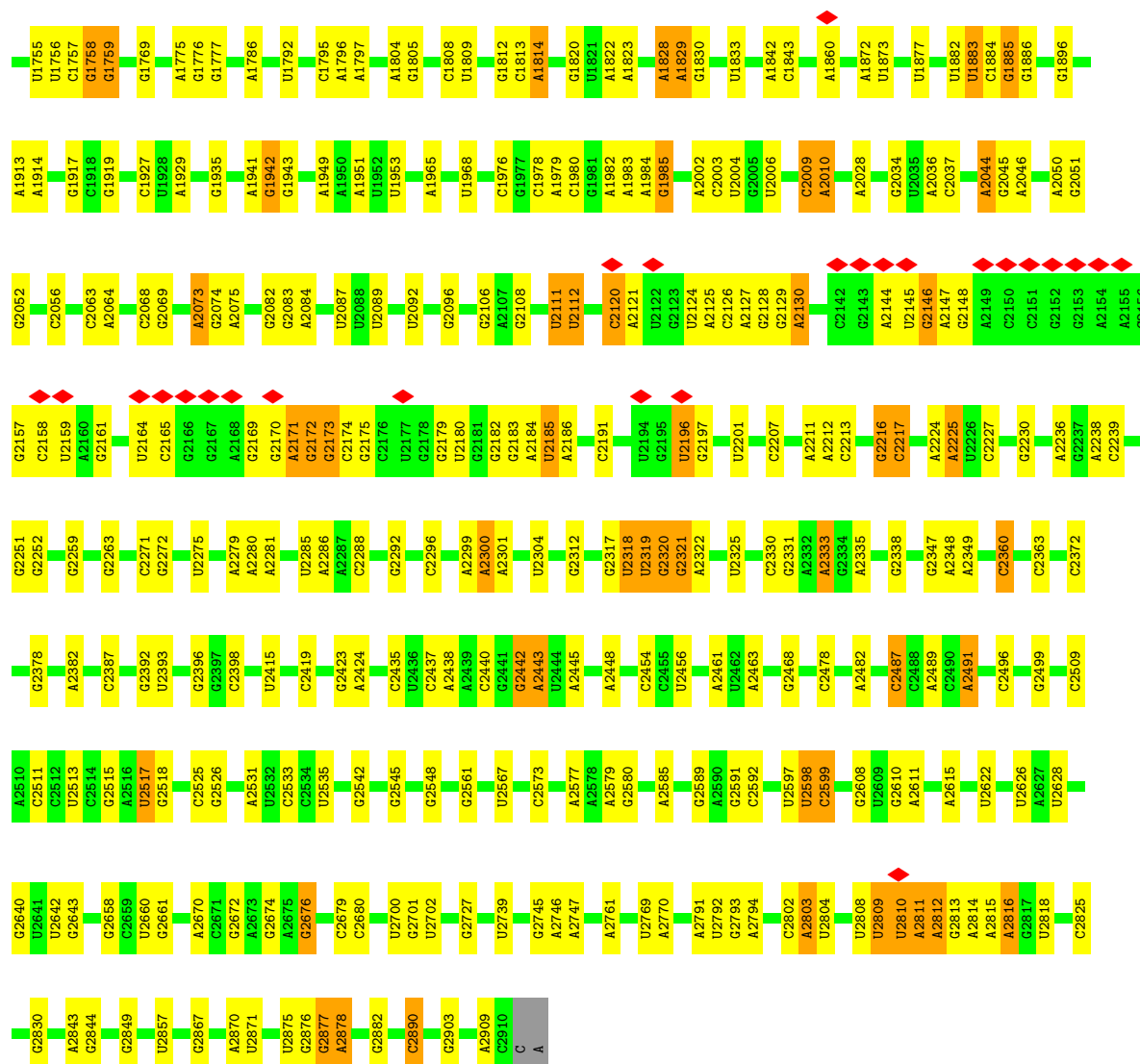
- Molecule 9: 50S ribosomal protein L36

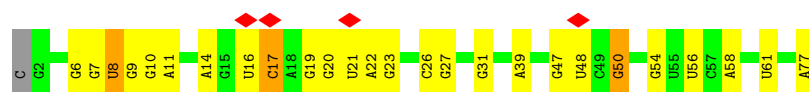


- Molecule 10: 23S rRNA

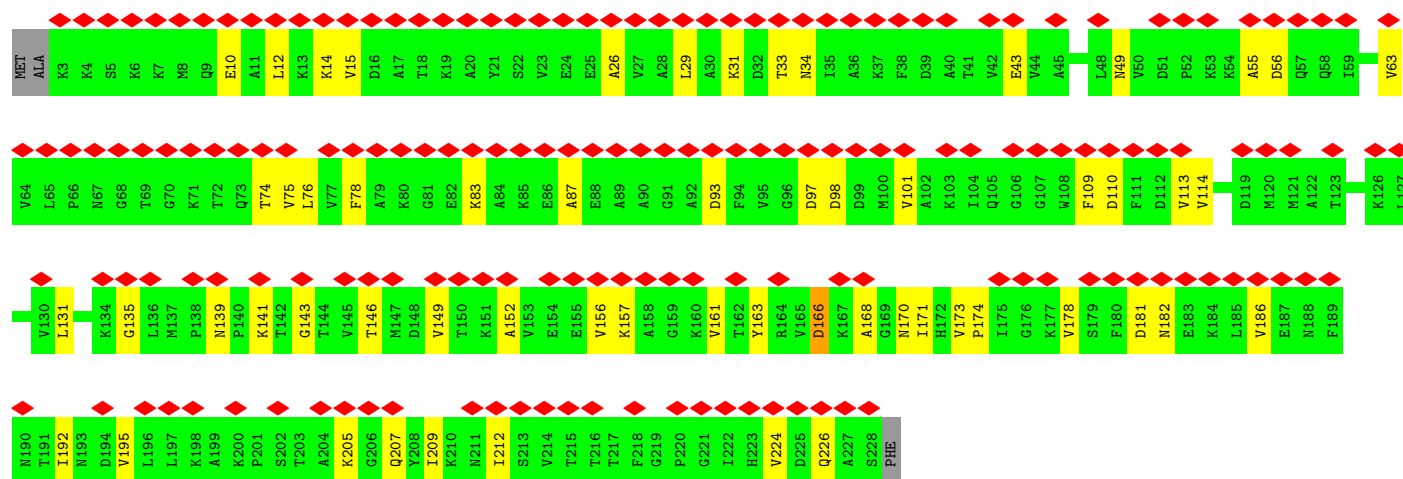
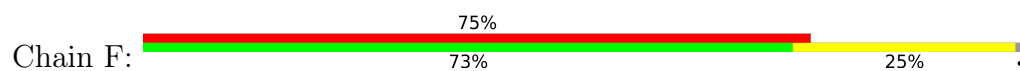




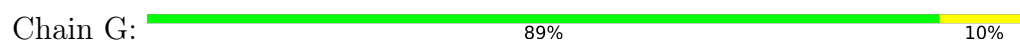




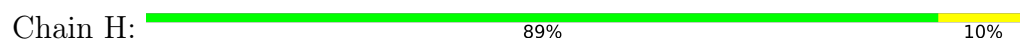
- Molecule 14: 50S ribosomal protein L1



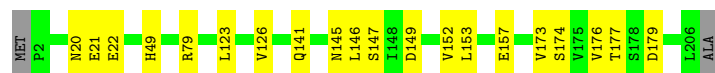
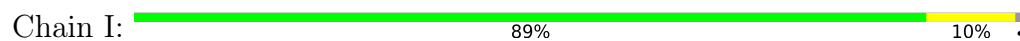
- Molecule 15: 50S ribosomal protein L2



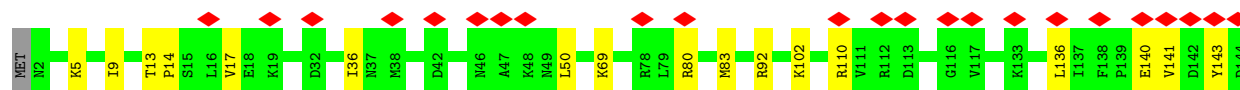
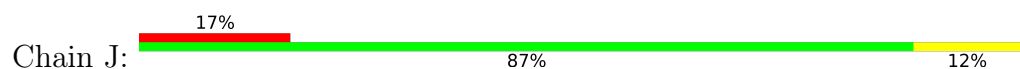
- Molecule 16: 50S ribosomal protein L3

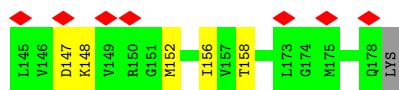


- Molecule 17: 50S ribosomal protein L4

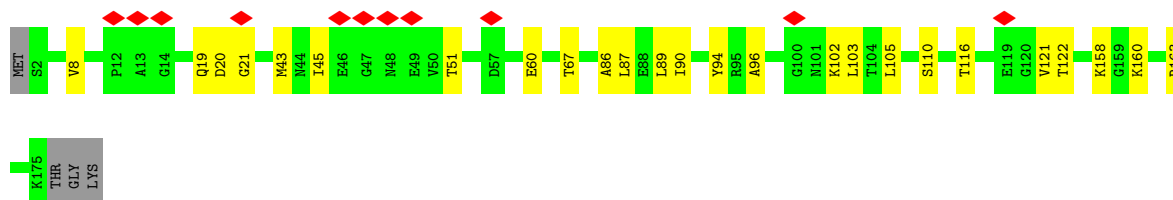
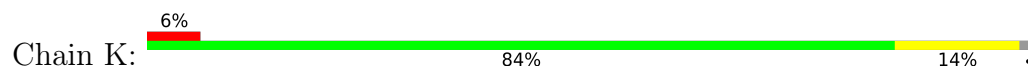


- Molecule 18: 50S ribosomal protein L5

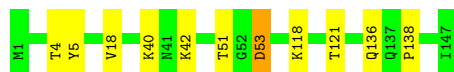




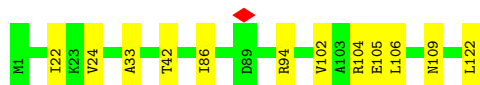
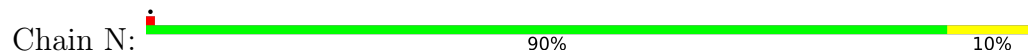
- Molecule 19: 50S ribosomal protein L6



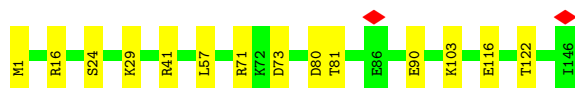
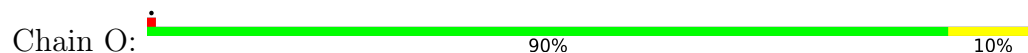
- Molecule 20: 50S ribosomal protein L13



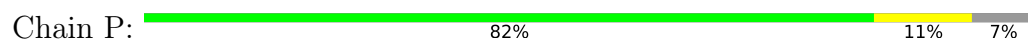
- Molecule 21: 50S ribosomal protein L14



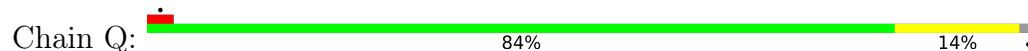
- Molecule 22: 50S ribosomal protein L15

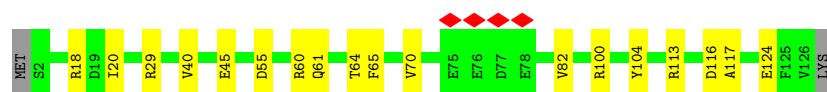


- Molecule 23: 50S ribosomal protein L16

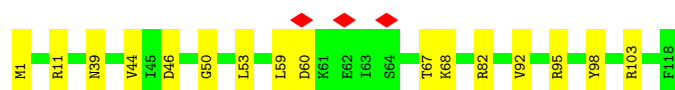
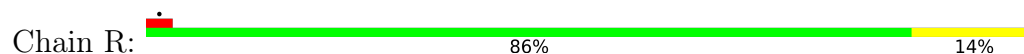


- Molecule 24: 50S ribosomal protein L17

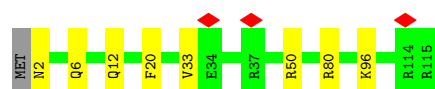




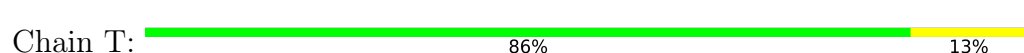
- Molecule 25: 50S ribosomal protein L18



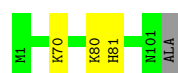
- Molecule 26: 50S ribosomal protein L19



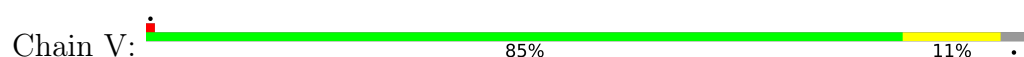
- Molecule 27: 50S ribosomal protein L20



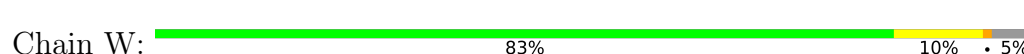
- Molecule 28: 50S ribosomal protein L21



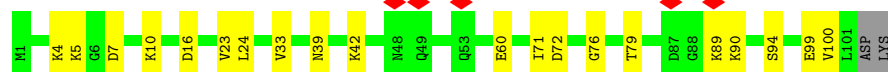
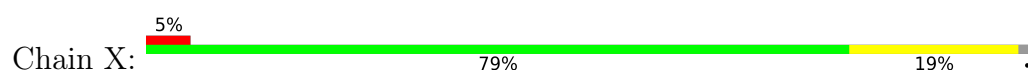
- Molecule 29: 50S ribosomal protein L22



- Molecule 30: 50S ribosomal protein L23



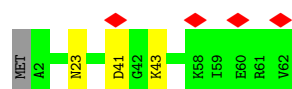
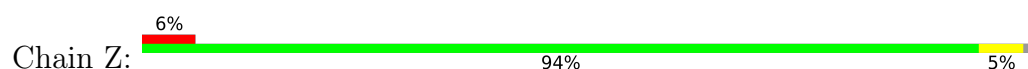
- Molecule 31: 50S ribosomal protein L24



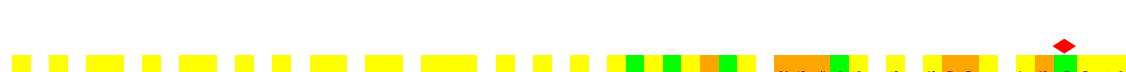
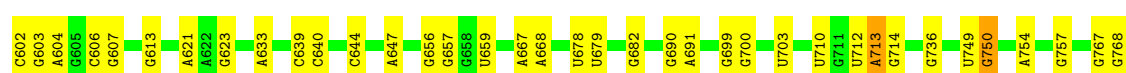
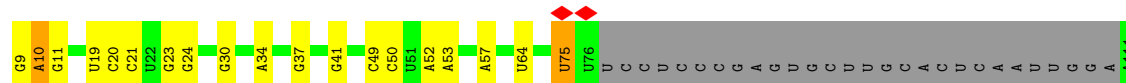
- Molecule 32: 50S ribosomal protein L27

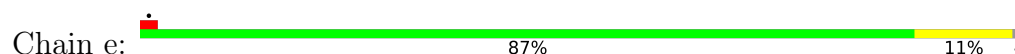


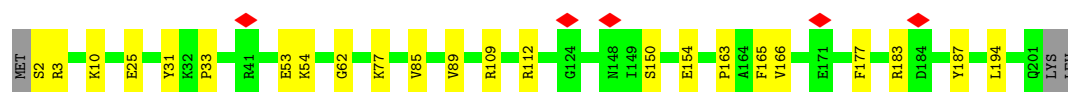
- Molecule 33: 50S ribosomal protein L28



- Molecule 34: 16S rRNA







- Molecule 39: 30S ribosomal protein S5

Chain f: 85% 13%



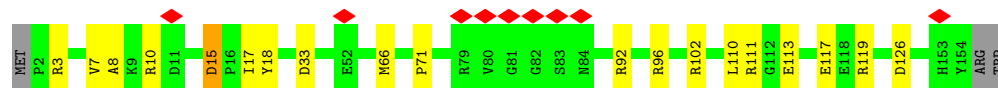
- Molecule 40: 30S ribosomal protein S6

Chain g: 13% 87% 9%



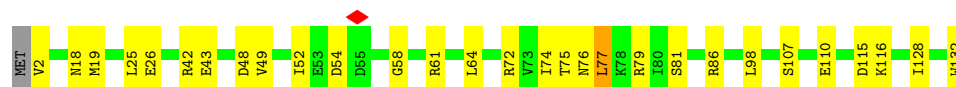
- Molecule 41: 30S ribosomal protein S7

Chain h: 6% 86% 12%



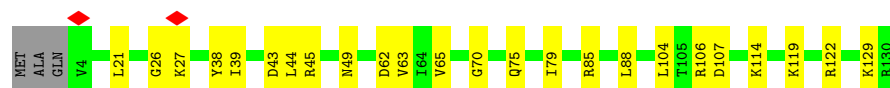
- Molecule 42: 30S ribosomal protein S8

Chain i: 77% 21%



- Molecule 43: 30S ribosomal protein S9

Chain j: 79% 18%

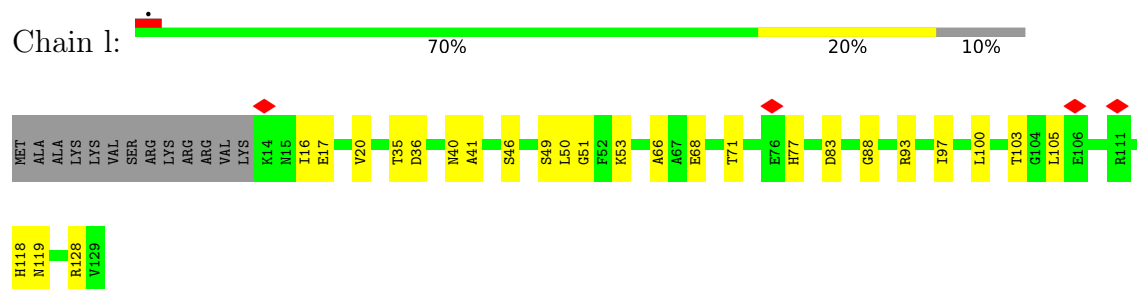


- Molecule 44: 30S ribosomal protein S10

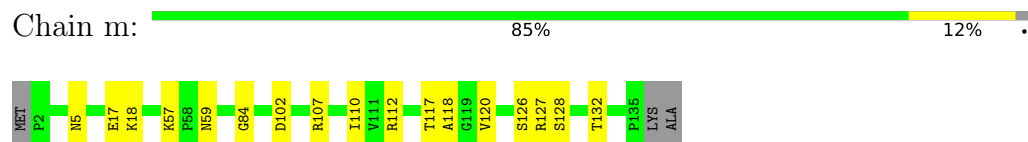
Chain k: 5% 77% 17% 6%



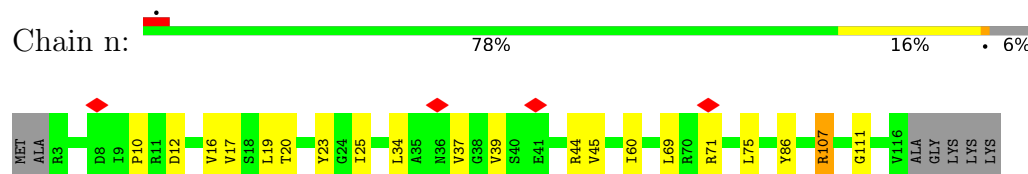
- Molecule 45: 30S ribosomal protein S11



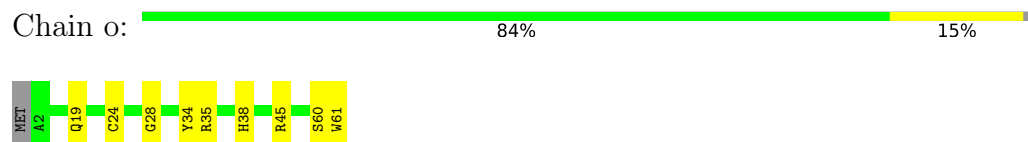
- Molecule 46: 30S ribosomal protein S12



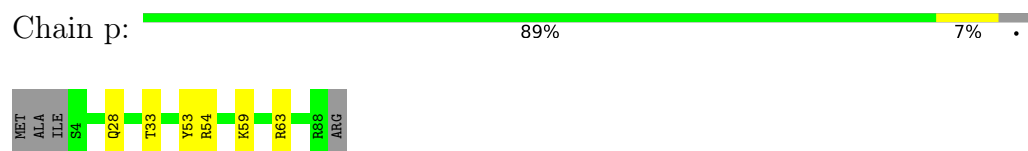
- Molecule 47: 30S ribosomal protein S13



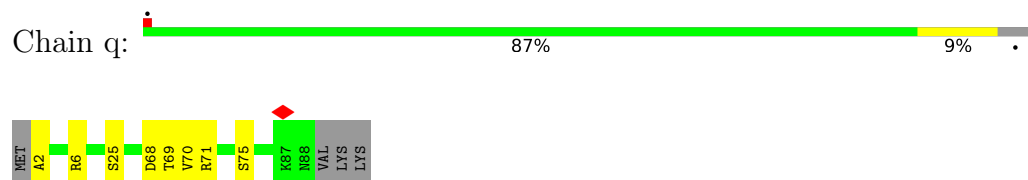
- Molecule 48: 30S ribosomal protein S14 type Z



- Molecule 49: 30S ribosomal protein S15



- Molecule 50: 30S ribosomal protein S16

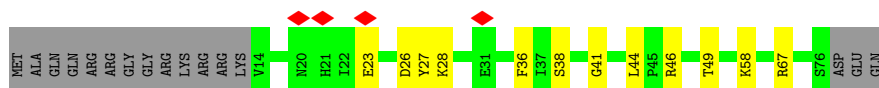


- Molecule 51: 30S ribosomal protein S17





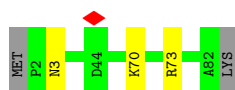
- Molecule 52: 30S ribosomal protein S18



- Molecule 53: 30S ribosomal protein S19



- Molecule 54: 30S ribosomal protein S20



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 23806                                   | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | FEI TITAN KRIOS                         | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 30.255                                  | Depositor |
| Minimum defocus (nm)                 | 500                                     | Depositor |
| Maximum defocus (nm)                 | 1500                                    | Depositor |
| Magnification                        | 165000                                  | Depositor |
| Image detector                       | GATAN K2 QUANTUM (4k x 4k)              | Depositor |
| Maximum map value                    | 0.059                                   | Depositor |
| Minimum map value                    | -0.010                                  | Depositor |
| Average map value                    | 0.002                                   | Depositor |
| Map value standard deviation         | 0.004                                   | Depositor |
| Recommended contour level            | 0.014                                   | Depositor |
| Map size ( $\text{\AA}$ )            | 344.4, 344.4, 344.4                     | wwPDB     |
| Map dimensions                       | 420, 420, 420                           | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 0.82, 0.82, 0.82                        | Depositor |

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PSU, PUT, K, 5MU, T6A, SCM, MG, U8U, ZN, ATP

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

| Mol | Chain | Bond lengths |             | Bond angles |             |
|-----|-------|--------------|-------------|-------------|-------------|
|     |       | RMSZ         | $\# Z  > 5$ | RMSZ        | $\# Z  > 5$ |
| 1   | 0     | 0.09         | 0/4421      | 0.23        | 0/5951      |
| 2   | 1     | 0.08         | 0/492       | 0.17        | 0/654       |
| 3   | 2     | 0.09         | 0/430       | 0.23        | 0/579       |
| 4   | 3     | 0.11         | 0/664       | 0.24        | 0/896       |
| 5   | 4     | 0.11         | 0/413       | 0.26        | 0/549       |
| 6   | 5     | 0.13         | 0/414       | 0.21        | 0/552       |
| 7   | 6     | 0.13         | 0/377       | 0.22        | 0/491       |
| 8   | 7     | 0.11         | 0/528       | 0.24        | 0/689       |
| 9   | 8     | 0.15         | 0/310       | 0.25        | 0/409       |
| 10  | A     | 0.12         | 0/69752     | 0.22        | 0/108803    |
| 11  | B     | 0.10         | 0/2728      | 0.19        | 0/4252      |
| 12  | C     | 0.16         | 0/1595      | 0.25        | 0/2477      |
| 13  | D     | 0.10         | 0/1815      | 0.20        | 0/2828      |
| 14  | F     | 0.08         | 0/1717      | 0.24        | 0/2318      |
| 15  | G     | 0.10         | 0/2141      | 0.23        | 0/2881      |
| 16  | H     | 0.11         | 0/1594      | 0.24        | 0/2140      |
| 17  | I     | 0.11         | 0/1595      | 0.21        | 0/2157      |
| 18  | J     | 0.09         | 0/1411      | 0.23        | 0/1897      |
| 19  | K     | 0.08         | 0/1355      | 0.21        | 0/1825      |
| 20  | M     | 0.12         | 0/1167      | 0.22        | 0/1576      |
| 21  | N     | 0.12         | 0/930       | 0.21        | 0/1247      |
| 22  | O     | 0.11         | 0/1106      | 0.22        | 0/1474      |
| 23  | P     | 0.11         | 0/1093      | 0.21        | 0/1457      |
| 24  | Q     | 0.10         | 0/1006      | 0.20        | 0/1349      |
| 25  | R     | 0.11         | 0/917       | 0.23        | 0/1226      |
| 26  | S     | 0.11         | 0/939       | 0.23        | 0/1262      |
| 27  | T     | 0.11         | 0/963       | 0.21        | 0/1280      |
| 28  | U     | 0.13         | 0/791       | 0.22        | 0/1061      |
| 29  | V     | 0.12         | 0/850       | 0.23        | 0/1145      |
| 30  | W     | 0.12         | 0/743       | 0.24        | 0/993       |
| 31  | X     | 0.11         | 0/772       | 0.24        | 0/1035      |
| 32  | Y     | 0.10         | 0/565       | 0.24        | 0/755       |

| Mol | Chain | Bond lengths |          | Bond angles |          |
|-----|-------|--------------|----------|-------------|----------|
|     |       | RMSZ         | # Z  >5  | RMSZ        | # Z  >5  |
| 33  | Z     | 0.09         | 0/486    | 0.19        | 0/648    |
| 34  | a     | 0.11         | 0/36487  | 0.21        | 0/56905  |
| 35  | b     | 0.11         | 0/322    | 0.29        | 0/499    |
| 36  | c     | 0.09         | 0/1803   | 0.24        | 0/2430   |
| 37  | d     | 0.10         | 0/1643   | 0.21        | 0/2208   |
| 38  | e     | 0.09         | 0/1641   | 0.22        | 0/2206   |
| 39  | f     | 0.10         | 0/1217   | 0.22        | 0/1641   |
| 40  | g     | 0.08         | 0/798    | 0.21        | 0/1075   |
| 41  | h     | 0.08         | 0/1238   | 0.21        | 0/1668   |
| 42  | i     | 0.09         | 0/1054   | 0.23        | 0/1417   |
| 43  | j     | 0.09         | 0/993    | 0.21        | 0/1331   |
| 44  | k     | 0.10         | 0/785    | 0.22        | 0/1059   |
| 45  | l     | 0.08         | 0/869    | 0.21        | 0/1174   |
| 46  | m     | 0.10         | 0/1068   | 0.26        | 0/1435   |
| 47  | n     | 0.08         | 0/908    | 0.21        | 0/1219   |
| 48  | o     | 0.10         | 0/504    | 0.21        | 0/669    |
| 49  | p     | 0.08         | 0/726    | 0.20        | 0/969    |
| 50  | q     | 0.09         | 0/704    | 0.26        | 0/945    |
| 51  | r     | 0.09         | 0/668    | 0.24        | 0/891    |
| 52  | s     | 0.08         | 0/518    | 0.20        | 0/694    |
| 53  | t     | 0.10         | 0/680    | 0.23        | 0/911    |
| 54  | u     | 0.09         | 0/611    | 0.21        | 0/818    |
| All | All   | 0.11         | 0/161317 | 0.22        | 0/241020 |

There are no bond length outliers.

There are no bond angle outliers.

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   | 0     | 4347  | 0        | 4448     | 40      | 0            |
| 2   | 1     | 491   | 0        | 527      | 0       | 0            |
| 3   | 2     | 428   | 0        | 463      | 6       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 4   | 3     | 647   | 0        | 616      | 17      | 0            |
| 5   | 4     | 406   | 0        | 417      | 5       | 0            |
| 6   | 5     | 410   | 0        | 422      | 8       | 0            |
| 7   | 6     | 374   | 0        | 424      | 6       | 0            |
| 8   | 7     | 522   | 0        | 575      | 7       | 0            |
| 9   | 8     | 305   | 0        | 337      | 5       | 0            |
| 10  | A     | 62268 | 0        | 31272    | 376     | 0            |
| 11  | B     | 2439  | 0        | 1228     | 12      | 0            |
| 12  | C     | 1546  | 0        | 790      | 9       | 0            |
| 13  | D     | 1624  | 0        | 824      | 11      | 0            |
| 14  | F     | 1693  | 0        | 1751     | 36      | 0            |
| 15  | G     | 2106  | 0        | 2189     | 21      | 0            |
| 16  | H     | 1572  | 0        | 1654     | 15      | 0            |
| 17  | I     | 1572  | 0        | 1614     | 14      | 0            |
| 18  | J     | 1392  | 0        | 1454     | 18      | 0            |
| 19  | K     | 1335  | 0        | 1369     | 18      | 0            |
| 20  | M     | 1146  | 0        | 1191     | 9       | 0            |
| 21  | N     | 923   | 0        | 985      | 9       | 0            |
| 22  | O     | 1096  | 0        | 1149     | 9       | 0            |
| 23  | P     | 1070  | 0        | 1136     | 9       | 0            |
| 24  | Q     | 997   | 0        | 1033     | 13      | 0            |
| 25  | R     | 908   | 0        | 944      | 9       | 0            |
| 26  | S     | 925   | 0        | 979      | 6       | 0            |
| 27  | T     | 950   | 0        | 1009     | 14      | 0            |
| 28  | U     | 779   | 0        | 821      | 2       | 0            |
| 29  | V     | 841   | 0        | 898      | 9       | 0            |
| 30  | W     | 736   | 0        | 795      | 9       | 0            |
| 31  | X     | 763   | 0        | 823      | 13      | 0            |
| 32  | Y     | 559   | 0        | 568      | 13      | 0            |
| 33  | Z     | 480   | 0        | 522      | 2       | 0            |
| 34  | a     | 32595 | 0        | 16412    | 234     | 0            |
| 35  | b     | 287   | 0        | 143      | 2       | 0            |
| 36  | c     | 1773  | 0        | 1810     | 21      | 0            |
| 37  | d     | 1618  | 0        | 1664     | 19      | 0            |
| 38  | e     | 1611  | 0        | 1628     | 16      | 0            |
| 39  | f     | 1204  | 0        | 1280     | 17      | 0            |
| 40  | g     | 786   | 0        | 781      | 7       | 0            |
| 41  | h     | 1218  | 0        | 1246     | 15      | 0            |
| 42  | i     | 1041  | 0        | 1092     | 20      | 0            |
| 43  | j     | 980   | 0        | 1027     | 15      | 0            |
| 44  | k     | 773   | 0        | 814      | 13      | 0            |
| 45  | l     | 854   | 0        | 869      | 17      | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 46  | m     | 1051   | 0        | 1115     | 13      | 0            |
| 47  | n     | 902    | 0        | 956      | 14      | 0            |
| 48  | o     | 492    | 0        | 508      | 7       | 0            |
| 49  | p     | 716    | 0        | 727      | 5       | 0            |
| 50  | q     | 692    | 0        | 724      | 6       | 0            |
| 51  | r     | 660    | 0        | 699      | 13      | 0            |
| 52  | s     | 511    | 0        | 549      | 9       | 0            |
| 53  | t     | 663    | 0        | 675      | 22      | 0            |
| 54  | u     | 608    | 0        | 635      | 2       | 0            |
| 55  | 0     | 62     | 0        | 23       | 4       | 0            |
| 56  | 0     | 2      | 0        | 0        | 0       | 0            |
| 56  | A     | 117    | 0        | 0        | 0       | 0            |
| 56  | B     | 1      | 0        | 0        | 0       | 0            |
| 56  | G     | 1      | 0        | 0        | 0       | 0            |
| 56  | a     | 39     | 0        | 0        | 0       | 0            |
| 56  | n     | 1      | 0        | 0        | 0       | 0            |
| 57  | 4     | 1      | 0        | 0        | 0       | 0            |
| 57  | 5     | 1      | 0        | 0        | 0       | 0            |
| 57  | 8     | 1      | 0        | 0        | 0       | 0            |
| 57  | o     | 1      | 0        | 0        | 0       | 0            |
| 58  | 7     | 2      | 0        | 0        | 0       | 0            |
| 58  | A     | 92     | 0        | 0        | 0       | 0            |
| 58  | B     | 3      | 0        | 0        | 0       | 0            |
| 58  | G     | 3      | 0        | 0        | 0       | 0            |
| 58  | P     | 1      | 0        | 0        | 0       | 0            |
| 58  | a     | 35     | 0        | 0        | 0       | 0            |
| 58  | g     | 1      | 0        | 0        | 0       | 0            |
| 58  | o     | 1      | 0        | 0        | 0       | 0            |
| 59  | a     | 23     | 0        | 23       | 4       | 0            |
| 60  | a     | 6      | 0        | 12       | 0       | 0            |
| 61  | D     | 1      | 0        | 0        | 1       | 0            |
| All | All   | 149080 | 0        | 100639   | 1068    | 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 5.

All (1068) 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) |
|----------------|----------------|--------------------------|-------------------|
| 12:C:54:5MU:C5 | 12:C:54:5MU:C4 | 1.80                     | 1.67              |
| 10:A:295:G:O2' | 10:A:296:G:O5' | 1.85                     | 0.95              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:A:1828:A:O2'   | 10:A:1829:A:O5'   | 1.86                     | 0.93              |
| 34:a:623:G:O2'    | 51:r:40:ARG:NH1   | 2.04                     | 0.91              |
| 10:A:1591:G:OP2   | 10:A:1591:G:N2    | 2.05                     | 0.90              |
| 34:a:9:G:O2'      | 34:a:10:A:OP1     | 1.90                     | 0.90              |
| 10:A:1413:A:O2'   | 10:A:1414:U:O5'   | 1.89                     | 0.89              |
| 10:A:1065:A:OP2   | 10:A:1173:C:O2'   | 1.89                     | 0.88              |
| 13:D:17:C:OP1     | 13:D:61:U:O2'     | 1.91                     | 0.87              |
| 12:C:69:G:O2'     | 12:C:70:C:OP1     | 1.93                     | 0.87              |
| 10:A:1792:U:OP2   | 10:A:1797:A:N6    | 2.08                     | 0.86              |
| 10:A:2125:A:N6    | 10:A:2182:G:O6    | 2.08                     | 0.86              |
| 10:A:319:U:O2'    | 10:A:321:U:OP2    | 1.95                     | 0.85              |
| 34:a:849:G:HO2'   | 42:i:2:VAL:N      | 1.75                     | 0.85              |
| 34:a:1386:A:OP2   | 48:o:35:ARG:NH2   | 2.11                     | 0.84              |
| 14:F:10:GLU:OE1   | 14:F:14:LYS:NZ    | 2.11                     | 0.84              |
| 10:A:2496:C:N3    | 23:P:124:LYS:NZ   | 2.25                     | 0.84              |
| 10:A:2849:G:O2'   | 24:Q:45:GLU:OE1   | 1.96                     | 0.84              |
| 34:a:227:A:O2'    | 34:a:228:A:O5'    | 1.95                     | 0.83              |
| 34:a:9:G:O6       | 39:f:97:LYS:NZ    | 2.11                     | 0.82              |
| 14:F:161:VAL:HG11 | 14:F:173:VAL:HG23 | 1.62                     | 0.81              |
| 10:A:1083:A:O2'   | 10:A:1150:A:N1    | 2.14                     | 0.80              |
| 10:A:1263:G:N7    | 27:T:16:LYS:NZ    | 2.28                     | 0.80              |
| 10:A:1691:G:O2'   | 24:Q:116:ASP:OD2  | 1.99                     | 0.80              |
| 1:O:180:LEU:HB3   | 1:O:208:VAL:HG23  | 1.64                     | 0.79              |
| 10:A:1882:U:O2    | 10:A:1885:G:N2    | 2.16                     | 0.79              |
| 9:8:2:LYS:NZ      | 10:A:2491:A:OP2   | 2.15                     | 0.79              |
| 41:h:113:GLU:N    | 41:h:113:GLU:OE1  | 2.16                     | 0.79              |
| 10:A:2144:A:O4'   | 10:A:2171:A:N6    | 2.15                     | 0.78              |
| 34:a:1341:U:O2'   | 34:a:1386:A:N3    | 2.16                     | 0.78              |
| 17:I:177:THR:OG1  | 17:I:179:ASP:OD1  | 2.01                     | 0.78              |
| 10:A:917:U:O2     | 10:A:940:A:N6     | 2.15                     | 0.78              |
| 10:A:1245:G:O2'   | 10:A:1273:A:N1    | 2.16                     | 0.78              |
| 10:A:137:U:O2     | 10:A:142:A:N6     | 2.17                     | 0.78              |
| 34:a:1402:U:O4    | 41:h:10:ARG:NH1   | 2.17                     | 0.77              |
| 34:a:446:U:O2'    | 34:a:449:G:O6     | 2.02                     | 0.77              |
| 11:B:29:C:O2      | 11:B:51:A:N6      | 2.17                     | 0.77              |
| 11:B:41:C:O2      | 18:J:92:ARG:NH1   | 2.17                     | 0.77              |
| 10:A:1104:U:O2    | 10:A:1112:A:N6    | 2.18                     | 0.77              |
| 10:A:1067:A:N3    | 10:A:2499:G:O2'   | 2.17                     | 0.77              |
| 16:H:90:GLU:O     | 16:H:95:LYS:NZ    | 2.15                     | 0.77              |
| 41:h:111:ARG:NH2  | 41:h:126:ASP:OD2  | 2.19                     | 0.76              |
| 10:A:2463:A:O2'   | 13:D:77:A:N1      | 2.18                     | 0.76              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:A:1189:U:O2'   | 10:A:1190:A:O5'   | 2.04                     | 0.76              |
| 34:a:573:A:OP2    | 38:e:2:SER:N      | 2.19                     | 0.76              |
| 10:A:2044:A:N3    | 10:A:2468:G:O2'   | 2.18                     | 0.75              |
| 37:d:25:GLU:OE2   | 44:k:11:LYS:NZ    | 2.14                     | 0.75              |
| 15:G:121:GLU:N    | 15:G:121:GLU:OE1  | 2.19                     | 0.75              |
| 53:t:12:ASP:OD2   | 53:t:35:SER:OG    | 2.04                     | 0.75              |
| 37:d:187:GLU:OE1  | 37:d:194:LYS:NZ   | 2.18                     | 0.75              |
| 15:G:274:ARG:O    | 15:G:275:THR:OG1  | 2.03                     | 0.75              |
| 10:A:1311:G:OP2   | 10:A:1687:G:O2'   | 2.02                     | 0.75              |
| 34:a:1020:G:O2'   | 34:a:1021:A:N7    | 2.20                     | 0.74              |
| 34:a:1079:U:O2'   | 34:a:1082:A:OP2   | 2.00                     | 0.74              |
| 14:F:75:VAL:HG22  | 14:F:156:VAL:HG11 | 1.69                     | 0.74              |
| 43:j:65:VAL:HG11  | 43:j:79:ILE:HG12  | 1.69                     | 0.74              |
| 42:i:26:GLU:OE2   | 42:i:61:ARG:NH1   | 2.19                     | 0.74              |
| 11:B:34:C:N4      | 11:B:47:C:O2      | 2.17                     | 0.74              |
| 34:a:868:U:O2'    | 34:a:871:C:N4     | 2.20                     | 0.74              |
| 10:A:295:G:HO2'   | 10:A:296:G:C5'    | 2.00                     | 0.74              |
| 34:a:529:A:OP2    | 46:m:126:SER:OG   | 2.04                     | 0.74              |
| 34:a:845:A:O2'    | 34:a:846:U:OP1    | 2.06                     | 0.74              |
| 42:i:79:ARG:NH1   | 42:i:81:SER:O     | 2.21                     | 0.73              |
| 34:a:1286:U:OP1   | 34:a:1310:C:O2'   | 2.03                     | 0.73              |
| 10:A:2535:U:O2'   | 10:A:2660:U:OP1   | 2.07                     | 0.73              |
| 34:a:1178:G:OP1   | 44:k:70:HIS:ND1   | 2.21                     | 0.73              |
| 9:8:12:GLU:N      | 9:8:12:GLU:OE1    | 2.21                     | 0.73              |
| 10:A:1420:A:O2'   | 10:A:1431:U:O2    | 2.06                     | 0.73              |
| 18:J:110:ARG:NH1  | 18:J:136:LEU:O    | 2.21                     | 0.73              |
| 53:t:35:SER:OG    | 53:t:38:SER:OG    | 2.06                     | 0.73              |
| 34:a:712:U:O2'    | 34:a:713:A:OP2    | 2.06                     | 0.73              |
| 10:A:2680:C:N3    | 19:K:110:SER:OG   | 2.19                     | 0.73              |
| 22:O:90:GLU:OE1   | 22:O:122:THR:OG1  | 2.01                     | 0.72              |
| 15:G:23:GLU:N     | 15:G:23:GLU:OE1   | 2.22                     | 0.72              |
| 18:J:136:LEU:HD23 | 18:J:141:VAL:HG11 | 1.72                     | 0.72              |
| 34:a:1342:G:N7    | 53:t:7:LYS:NZ     | 2.37                     | 0.72              |
| 10:A:429:A:O2'    | 10:A:430:A:O5'    | 2.06                     | 0.72              |
| 10:A:1034:C:O2    | 20:M:4:THR:OG1    | 2.07                     | 0.72              |
| 34:a:768:G:OP1    | 49:p:59:LYS:NZ    | 2.22                     | 0.72              |
| 4:3:36:GLU:N      | 4:3:36:GLU:OE1    | 2.23                     | 0.72              |
| 10:A:1828:A:HO2'  | 10:A:1829:A:P     | 2.12                     | 0.72              |
| 34:a:1107:A:OP1   | 39:f:52:LYS:NZ    | 2.22                     | 0.72              |
| 16:H:87:GLU:N     | 16:H:87:GLU:OE1   | 2.22                     | 0.72              |
| 37:d:90:LEU:O     | 37:d:94:THR:HG22  | 1.88                     | 0.72              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 10:A:2349:A:H61  | 32:Y:52:THR:HG21  | 1.54                     | 0.71              |
| 34:a:369:U:O2'   | 34:a:372:G:O6     | 2.06                     | 0.71              |
| 42:i:110:GLU:N   | 42:i:110:GLU:OE1  | 2.23                     | 0.71              |
| 36:c:75:GLN:OE1  | 36:c:75:GLN:N     | 2.24                     | 0.71              |
| 10:A:1355:G:OP2  | 10:A:1355:G:N2    | 2.19                     | 0.71              |
| 30:W:57:ASN:OD1  | 30:W:76:ARG:NH1   | 2.23                     | 0.71              |
| 34:a:1013:A:N3   | 53:t:52:TYR:OH    | 2.23                     | 0.71              |
| 34:a:1519:A:O2'  | 34:a:1520:A:O4'   | 2.08                     | 0.71              |
| 10:A:2815:A:O2'  | 10:A:2816:A:O5'   | 2.08                     | 0.70              |
| 43:j:26:GLY:N    | 43:j:62:ASP:OD1   | 2.24                     | 0.70              |
| 14:F:143:GLY:O   | 14:F:146:THR:HG23 | 1.91                     | 0.70              |
| 19:K:20:ASP:OD1  | 19:K:21:GLY:N     | 2.24                     | 0.70              |
| 33:Z:41:ASP:OD1  | 33:Z:43:LYS:NZ    | 2.20                     | 0.70              |
| 46:m:84:GLY:O    | 46:m:112:ARG:NH2  | 2.24                     | 0.70              |
| 8:7:39:LYS:NZ    | 10:A:2378:G:N7    | 2.38                     | 0.70              |
| 34:a:323:G:N2    | 34:a:326:A:OP2    | 2.20                     | 0.70              |
| 34:a:1035:C:O2'  | 34:a:1036:U:OP1   | 2.06                     | 0.70              |
| 52:s:23:GLU:N    | 52:s:23:GLU:OE1   | 2.25                     | 0.70              |
| 10:A:965:U:O2'   | 10:A:966:C:OP1    | 2.10                     | 0.70              |
| 10:A:2304:U:OP1  | 10:A:2393:U:O2'   | 2.09                     | 0.70              |
| 10:A:668:G:N2    | 10:A:671:A:OP2    | 2.24                     | 0.69              |
| 34:a:433:A:OP1   | 38:e:109:ARG:NH1  | 2.25                     | 0.69              |
| 31:X:10:LYS:HB2  | 31:X:71:ILE:HD11  | 1.73                     | 0.69              |
| 10:A:832:A:OP2   | 10:A:2084:A:O2'   | 2.11                     | 0.69              |
| 45:l:88:GLY:O    | 45:l:93:ARG:NH2   | 2.25                     | 0.69              |
| 10:A:2236:A:OP1  | 15:G:171:TYR:OH   | 2.10                     | 0.69              |
| 21:N:105:GLU:OE1 | 21:N:105:GLU:N    | 2.25                     | 0.69              |
| 14:F:76:LEU:HD12 | 14:F:114:VAL:HG13 | 1.74                     | 0.69              |
| 17:I:21:GLU:N    | 17:I:21:GLU:OE1   | 2.26                     | 0.69              |
| 10:A:846:U:OP2   | 22:O:41:ARG:NH2   | 2.26                     | 0.69              |
| 37:d:52:SER:OG   | 37:d:111:ASP:OD2  | 2.06                     | 0.69              |
| 34:a:1247:G:O3'  | 53:t:77:THR:HG21  | 1.93                     | 0.69              |
| 21:N:22:ILE:HD11 | 21:N:42:THR:OG1   | 1.93                     | 0.68              |
| 31:X:5:LYS:NZ    | 31:X:24:LEU:O     | 2.26                     | 0.68              |
| 46:m:112:ARG:NH1 | 46:m:118:ALA:O    | 2.26                     | 0.68              |
| 34:a:1343:C:O2   | 53:t:37:ARG:NH2   | 2.26                     | 0.68              |
| 10:A:199:A:N6    | 10:A:2443:A:O2'   | 2.26                     | 0.68              |
| 34:a:1230:A:O2'  | 37:d:194:LYS:NZ   | 2.27                     | 0.68              |
| 34:a:302:G:OP1   | 51:r:17:SER:OG    | 2.09                     | 0.68              |
| 22:O:71:ARG:NE   | 22:O:73:ASP:OD1   | 2.27                     | 0.68              |
| 34:a:401:U:OP1   | 50:q:69:THR:OG1   | 2.11                     | 0.68              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:A:2263:G:O2'   | 10:A:2509:C:OP1   | 2.12                     | 0.68              |
| 29:V:73:SER:OG    | 29:V:114:GLU:OE1  | 2.12                     | 0.68              |
| 10:A:1451:G:O2'   | 10:A:1452:U:O5'   | 2.11                     | 0.68              |
| 36:c:117:ILE:HD11 | 36:c:137:LEU:HB3  | 1.76                     | 0.68              |
| 10:A:1105:U:N3    | 10:A:1108:A:OP2   | 2.27                     | 0.68              |
| 25:R:95:ARG:NH1   | 25:R:98:TYR:O     | 2.27                     | 0.68              |
| 37:d:110:LEU:O    | 37:d:203:ARG:NH1  | 2.27                     | 0.67              |
| 13:D:54:G:OP2     | 61:D:101:HOH:O    | 2.11                     | 0.67              |
| 34:a:1372:A:OP1   | 43:j:122:ARG:NH1  | 2.26                     | 0.67              |
| 11:B:11:A:O2'     | 11:B:13:A:OP2     | 2.11                     | 0.67              |
| 4:3:71:VAL:HG23   | 53:t:67:VAL:HG21  | 1.76                     | 0.67              |
| 10:A:83:G:H1      | 10:A:101:G:HO2'   | 1.41                     | 0.67              |
| 10:A:2146:G:O2'   | 10:A:2147:A:OP2   | 2.11                     | 0.67              |
| 10:A:2318:U:O2'   | 10:A:2319:U:O5'   | 2.10                     | 0.67              |
| 10:A:1122:U:HO2'  | 10:A:1123:A:C2'   | 2.08                     | 0.66              |
| 18:J:140:GLU:OE1  | 18:J:140:GLU:N    | 2.27                     | 0.66              |
| 34:a:1292:G:N2    | 34:a:1295:A:OP2   | 2.22                     | 0.66              |
| 9:8:19:ARG:NE     | 10:A:2769:U:OP2   | 2.25                     | 0.66              |
| 47:n:107:ARG:NH1  | 47:n:111:GLY:O    | 2.29                     | 0.66              |
| 10:A:205:U:OP2    | 10:A:206:A:O2'    | 2.08                     | 0.66              |
| 18:J:36:ILE:HD11  | 18:J:152:MET:SD   | 2.36                     | 0.66              |
| 10:A:335:A:N3     | 10:A:355:U:O2'    | 2.29                     | 0.66              |
| 10:A:899:G:O2'    | 10:A:956:G:O6     | 2.10                     | 0.66              |
| 34:a:850:U:O4'    | 42:i:2:VAL:N      | 2.29                     | 0.66              |
| 10:A:572:U:O2'    | 27:T:49:ASP:OD2   | 2.09                     | 0.66              |
| 10:A:732:A:O2'    | 10:A:1388:A:N3    | 2.28                     | 0.66              |
| 34:a:431:U:O4     | 38:e:2:SER:OG     | 2.12                     | 0.66              |
| 10:A:1060:A:O2'   | 10:A:1162:C:OP1   | 2.14                     | 0.65              |
| 34:a:1192:G:N1    | 34:a:1195:A:OP2   | 2.29                     | 0.65              |
| 38:e:183:ARG:NH2  | 38:e:187:TYR:O    | 2.29                     | 0.65              |
| 10:A:502:G:N2     | 10:A:505:A:OP2    | 2.28                     | 0.65              |
| 25:R:46:ASP:O     | 25:R:50:GLY:N     | 2.29                     | 0.65              |
| 32:Y:81:LYS:N     | 32:Y:85:LYS:O     | 2.29                     | 0.65              |
| 10:A:1758:G:O2'   | 10:A:1759:G:OP2   | 2.12                     | 0.65              |
| 10:A:2349:A:H61   | 32:Y:52:THR:CG2   | 2.08                     | 0.65              |
| 45:l:71:THR:OG1   | 45:l:100:LEU:HD23 | 1.96                     | 0.65              |
| 47:n:12:ASP:O     | 47:n:44:ARG:NH1   | 2.28                     | 0.65              |
| 10:A:683:U:O2'    | 10:A:684:A:OP1    | 2.10                     | 0.65              |
| 10:A:1189:U:HO2'  | 10:A:1190:A:C5'   | 2.08                     | 0.65              |
| 10:A:509:A:OP1    | 17:I:79:ARG:NH2   | 2.28                     | 0.65              |
| 10:A:1236:U:H1'   | 27:T:4:VAL:HG22   | 1.78                     | 0.65              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 10:A:1376:U:OP2  | 10:A:1429:U:O2'   | 2.10                     | 0.65              |
| 34:a:621:A:N6    | 34:a:667:A:O2'    | 2.28                     | 0.65              |
| 10:A:84:A:N1     | 10:A:98:U:O2'     | 2.31                     | 0.64              |
| 36:c:188:ASP:OD1 | 36:c:189:THR:N    | 2.30                     | 0.64              |
| 34:a:925:G:N2    | 34:a:928:A:OP2    | 2.30                     | 0.64              |
| 30:W:88:GLU:N    | 30:W:88:GLU:OE1   | 2.30                     | 0.64              |
| 10:A:1029:A:O2'  | 10:A:1031:C:OP2   | 2.14                     | 0.64              |
| 34:a:228:A:HO2'  | 34:a:247:C:HO2'   | 1.41                     | 0.64              |
| 10:A:450:G:OP2   | 10:A:2419:C:O2'   | 2.10                     | 0.64              |
| 10:A:1302:G:O6   | 29:V:18:SER:OG    | 2.15                     | 0.64              |
| 23:P:51:ARG:HG3  | 23:P:66:ILE:HD11  | 1.80                     | 0.64              |
| 4:3:71:VAL:HG21  | 53:t:42:PRO:HG3   | 1.79                     | 0.64              |
| 10:A:625:U:OP1   | 22:O:16:ARG:NH2   | 2.31                     | 0.64              |
| 11:B:29:C:O2'    | 11:B:51:A:N1      | 2.29                     | 0.64              |
| 10:A:1537:A:N3   | 10:A:1622:C:O2'   | 2.31                     | 0.64              |
| 10:A:2672:G:OP2  | 19:K:158:LYS:NZ   | 2.28                     | 0.64              |
| 13:D:56:U:O2'    | 13:D:58:A:N7      | 2.27                     | 0.64              |
| 34:a:1516:G:O2'  | 34:a:1517:U:O5'   | 2.16                     | 0.64              |
| 11:B:39:G:OP1    | 11:B:41:C:N4      | 2.29                     | 0.63              |
| 14:F:98:ASP:O    | 14:F:101:VAL:HG22 | 1.98                     | 0.63              |
| 14:F:207:GLN:NE2 | 14:F:226:GLN:OE1  | 2.31                     | 0.63              |
| 37:d:69:THR:HG22 | 37:d:71:LYS:H     | 1.63                     | 0.63              |
| 46:m:5:ASN:OD1   | 51:r:39:LYS:NZ    | 2.30                     | 0.63              |
| 47:n:17:VAL:O    | 47:n:20:THR:OG1   | 2.16                     | 0.63              |
| 14:F:76:LEU:HD11 | 14:F:78:PHE:CZ    | 2.33                     | 0.63              |
| 42:i:48:ASP:OD1  | 42:i:49:VAL:N     | 2.31                     | 0.63              |
| 15:G:61:GLN:O    | 15:G:63:ARG:NH1   | 2.31                     | 0.63              |
| 45:l:36:ASP:OD1  | 45:l:40:ASN:N     | 2.32                     | 0.63              |
| 19:K:19:GLN:NE2  | 19:K:43:MET:SD    | 2.71                     | 0.63              |
| 45:l:71:THR:HG23 | 45:l:105:LEU:CD1  | 2.29                     | 0.63              |
| 10:A:680:G:N2    | 10:A:683:U:OP2    | 2.30                     | 0.63              |
| 10:A:2216:G:O2'  | 10:A:2217:C:OP2   | 2.13                     | 0.63              |
| 15:G:123:ASP:OD1 | 15:G:124:ILE:N    | 2.32                     | 0.63              |
| 10:A:1061:G:N2   | 10:A:1062:U:O4    | 2.26                     | 0.63              |
| 27:T:48:ARG:NH1  | 27:T:49:ASP:OD1   | 2.32                     | 0.63              |
| 34:a:491:U:O2'   | 34:a:493:A:N7     | 2.28                     | 0.63              |
| 34:a:1376:A:O2'  | 41:h:33:ASP:OD1   | 2.16                     | 0.63              |
| 6:5:17:TYR:HH    | 10:A:2360:C:HO2'  | 1.37                     | 0.62              |
| 10:A:24:G:O2'    | 29:V:83:GLU:O     | 2.16                     | 0.62              |
| 10:A:1123:A:O2'  | 10:A:1124:A:N7    | 2.32                     | 0.62              |
| 25:R:39:ASN:ND2  | 25:R:59:LEU:HD21  | 2.14                     | 0.62              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 34:a:350:G:N1    | 34:a:353:A:OP2    | 2.32                     | 0.62              |
| 10:A:1122:U:O2'  | 10:A:1123:A:O2'   | 2.03                     | 0.62              |
| 10:A:2092:U:O2'  | 33:Z:23:ASN:OD1   | 2.18                     | 0.62              |
| 24:Q:45:GLU:OE2  | 24:Q:104:TYR:N    | 2.32                     | 0.62              |
| 34:a:1209:U:O2'  | 34:a:1210:G:OP1   | 2.14                     | 0.62              |
| 37:d:87:ARG:NH1  | 37:d:98:VAL:O     | 2.32                     | 0.62              |
| 4:3:41:ASN:OD1   | 4:3:42:THR:N      | 2.31                     | 0.62              |
| 10:A:1003:C:O2'  | 10:A:2286:A:N3    | 2.30                     | 0.62              |
| 10:A:515:G:N1    | 10:A:518:A:OP2    | 2.31                     | 0.62              |
| 10:A:1026:C:O2'  | 10:A:1039:A:N3    | 2.31                     | 0.62              |
| 10:A:1033:C:O2'  | 10:A:1035:A:OP1   | 2.16                     | 0.62              |
| 10:A:918:A:N6    | 10:A:939:G:O2'    | 2.33                     | 0.62              |
| 12:C:17:U:O2'    | 12:C:57:G:N2      | 2.32                     | 0.61              |
| 34:a:1150:A:O2'  | 44:k:39:PRO:O     | 2.16                     | 0.61              |
| 3:2:18:ASN:OD1   | 3:2:19:GLN:N      | 2.32                     | 0.61              |
| 10:A:958:A:N3    | 11:B:78:U:O2'     | 2.32                     | 0.61              |
| 21:N:104:ARG:N   | 21:N:122:LEU:OXT  | 2.33                     | 0.61              |
| 4:3:18:THR:OG1   | 4:3:49:GLU:OE1    | 2.19                     | 0.61              |
| 10:A:2815:A:HO2' | 10:A:2816:A:C5'   | 2.13                     | 0.61              |
| 10:A:641:G:N7    | 22:O:103:LYS:NZ   | 2.48                     | 0.61              |
| 40:g:87:ASN:OD1  | 40:g:89:ASP:N     | 2.34                     | 0.61              |
| 10:A:559:U:O2'   | 10:A:560:G:N7     | 2.32                     | 0.61              |
| 34:a:710:U:O2'   | 45:l:41:ALA:O     | 2.17                     | 0.61              |
| 10:A:30:G:O2'    | 10:A:1250:A:N3    | 2.33                     | 0.61              |
| 10:A:538:G:N1    | 10:A:541:A:OP2    | 2.34                     | 0.61              |
| 15:G:97:GLU:OE2  | 15:G:115:ARG:NH1  | 2.34                     | 0.61              |
| 32:Y:42:GLY:N    | 32:Y:73:ASP:OD1   | 2.34                     | 0.61              |
| 34:a:1342:G:N1   | 34:a:1345:A:OP2   | 2.34                     | 0.61              |
| 44:k:34:ALA:HB2  | 44:k:83:THR:HG21  | 1.82                     | 0.61              |
| 6:5:17:TYR:OH    | 10:A:2360:C:O2'   | 2.11                     | 0.61              |
| 15:G:129:ALA:C   | 15:G:130:LEU:HD12 | 2.26                     | 0.61              |
| 49:p:33:THR:OG1  | 49:p:63:ARG:NH1   | 2.34                     | 0.60              |
| 4:3:71:VAL:HG11  | 53:t:42:PRO:HG3   | 1.83                     | 0.60              |
| 14:F:181:ASP:OD1 | 14:F:182:ASN:N    | 2.34                     | 0.60              |
| 18:J:158:THR:O   | 25:R:1:MET:N      | 2.25                     | 0.60              |
| 19:K:89:LEU:O    | 19:K:89:LEU:HD12  | 1.99                     | 0.60              |
| 34:a:795:G:H4'   | 34:a:1540:A:H4'   | 1.82                     | 0.60              |
| 10:A:681:A:N1    | 10:A:2382:A:O2'   | 2.33                     | 0.60              |
| 45:l:51:GLY:O    | 45:l:53:LYS:NZ    | 2.34                     | 0.60              |
| 1:0:107:VAL:O    | 1:0:112:GLN:NE2   | 2.35                     | 0.60              |
| 10:A:249:G:OP2   | 10:A:251:C:N4     | 2.27                     | 0.60              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 39:f:148:LYS:NZ  | 42:i:75:THR:OG1   | 2.34                     | 0.60              |
| 34:a:37:G:O2'    | 46:m:128:SER:O    | 2.15                     | 0.60              |
| 37:d:76:ILE:HA   | 37:d:83:VAL:HG13  | 1.84                     | 0.60              |
| 42:i:19:MET:O    | 42:i:72:ARG:NH2   | 2.34                     | 0.60              |
| 43:j:106:ARG:NH1 | 43:j:107:ASP:O    | 2.34                     | 0.60              |
| 29:V:15:VAL:HG11 | 29:V:51:ILE:HG21  | 1.83                     | 0.60              |
| 1:0:14:GLU:OE2   | 1:0:233:HIS:NE2   | 2.35                     | 0.60              |
| 1:0:444:ASN:OD1  | 1:0:445:VAL:HG13  | 2.01                     | 0.60              |
| 34:a:783:U:O2'   | 34:a:906:C:O2     | 2.19                     | 0.60              |
| 10:A:782:A:O2'   | 10:A:1701:U:OP1   | 2.18                     | 0.60              |
| 34:a:1003:G:OP2  | 34:a:1384:U:O2'   | 2.20                     | 0.60              |
| 10:A:1469:C:O2'  | 10:A:1614:A:OP2   | 2.16                     | 0.59              |
| 34:a:165:G:O2'   | 34:a:1472:A:N3    | 2.27                     | 0.59              |
| 34:a:422:A:O2'   | 34:a:424:C:OP1    | 2.20                     | 0.59              |
| 15:G:2:ALA:N     | 15:G:20:ASP:OD2   | 2.35                     | 0.59              |
| 34:a:993:G:O2'   | 43:j:129:LYS:O    | 2.20                     | 0.59              |
| 45:l:71:THR:HG23 | 45:l:105:LEU:HD12 | 1.82                     | 0.59              |
| 36:c:34:GLU:N    | 36:c:34:GLU:OE1   | 2.36                     | 0.59              |
| 44:k:80:THR:OG1  | 44:k:83:THR:HG23  | 2.02                     | 0.59              |
| 16:H:42:GLU:N    | 16:H:42:GLU:OE1   | 2.32                     | 0.59              |
| 17:I:149:ASP:OD1 | 17:I:149:ASP:N    | 2.35                     | 0.59              |
| 19:K:60:GLU:N    | 19:K:60:GLU:OE1   | 2.35                     | 0.59              |
| 1:0:327:ARG:NH1  | 41:h:110:LEU:O    | 2.36                     | 0.59              |
| 34:a:837:C:O2'   | 34:a:928:A:N1     | 2.32                     | 0.59              |
| 38:e:150:SER:OG  | 38:e:154:GLU:OE2  | 2.21                     | 0.59              |
| 10:A:1310:A:N1   | 10:A:1330:C:O2'   | 2.29                     | 0.58              |
| 30:W:52:ASN:OD1  | 30:W:53:VAL:N     | 2.35                     | 0.58              |
| 10:A:1451:G:O2'  | 10:A:1452:U:O4'   | 2.21                     | 0.58              |
| 16:H:39:LYS:NZ   | 16:H:82:GLU:OE2   | 2.35                     | 0.58              |
| 34:a:678:U:O4    | 34:a:778:G:O2'    | 2.15                     | 0.58              |
| 41:h:117:GLU:OE1 | 41:h:117:GLU:N    | 2.33                     | 0.58              |
| 10:A:33:U:O2'    | 10:A:34:U:O5'     | 2.15                     | 0.58              |
| 10:A:2157:G:N2   | 10:A:2159:U:O2    | 2.36                     | 0.58              |
| 34:a:1346:C:O2   | 53:t:36:ARG:NH2   | 2.36                     | 0.58              |
| 42:i:76:ASN:OD1  | 42:i:77:LEU:N     | 2.36                     | 0.58              |
| 10:A:1106:A:N1   | 10:A:1134:A:O2'   | 2.27                     | 0.58              |
| 16:H:58:GLU:N    | 16:H:58:GLU:OE1   | 2.37                     | 0.58              |
| 34:a:1104:G:N2   | 34:a:1107:A:OP2   | 2.36                     | 0.58              |
| 10:A:1126:G:O6   | 10:A:1128:G:N2    | 2.35                     | 0.58              |
| 31:X:16:ASP:OD2  | 31:X:39:ASN:N     | 2.34                     | 0.58              |
| 39:f:157:ARG:NH2 | 42:i:43:GLU:OE1   | 2.36                     | 0.58              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 14:F:29:LEU:O    | 14:F:33:THR:HG23  | 2.03                     | 0.58              |
| 30:W:56:LEU:HD12 | 30:W:56:LEU:N     | 2.19                     | 0.58              |
| 10:A:1812:G:OP1  | 15:G:260:ARG:NH1  | 2.32                     | 0.57              |
| 17:I:146:LEU:O   | 17:I:147:SER:OG   | 2.21                     | 0.57              |
| 37:d:182:ASP:OD1 | 37:d:183:TYR:N    | 2.37                     | 0.57              |
| 51:r:60:ASP:N    | 51:r:60:ASP:OD1   | 2.38                     | 0.57              |
| 10:A:281:A:O2'   | 10:A:282:G:O5'    | 2.21                     | 0.57              |
| 14:F:15:VAL:HA   | 14:F:29:LEU:HD21  | 1.87                     | 0.57              |
| 27:T:88:ILE:HG22 | 27:T:90:ILE:HG22  | 1.85                     | 0.57              |
| 34:a:822:C:OP1   | 45:l:128:ARG:N    | 2.36                     | 0.57              |
| 1:0:330:LEU:HD21 | 1:0:376:LEU:HD22  | 1.86                     | 0.57              |
| 1:0:450:GLU:OE2  | 55:0:602:ATP:O3'  | 2.22                     | 0.57              |
| 10:A:1318:G:O2'  | 10:A:1320:G:N7    | 2.37                     | 0.57              |
| 10:A:2128:G:O2'  | 10:A:2180:U:O2    | 2.22                     | 0.57              |
| 13:D:31:G:OP1    | 34:a:1255:A:O2'   | 2.21                     | 0.57              |
| 5:4:16:ARG:NH2   | 10:A:1300:G:OP1   | 2.36                     | 0.57              |
| 11:B:12:U:OP2    | 11:B:68:C:O2'     | 2.23                     | 0.57              |
| 34:a:613:G:OP1   | 42:i:86:ARG:NH2   | 2.37                     | 0.57              |
| 1:0:358:ARG:NH2  | 1:0:491:PHE:O     | 2.38                     | 0.57              |
| 10:A:807:G:N2    | 10:A:1414:U:O2'   | 2.37                     | 0.57              |
| 14:F:75:VAL:HG22 | 14:F:156:VAL:CG1  | 2.35                     | 0.57              |
| 32:Y:49:GLN:OE1  | 32:Y:53:LYS:N     | 2.38                     | 0.57              |
| 46:m:120:VAL:O   | 46:m:132:THR:HG21 | 2.05                     | 0.57              |
| 10:A:1302:G:O5'  | 29:V:20:ARG:NH2   | 2.38                     | 0.57              |
| 13:D:7:G:O2'     | 13:D:50:G:O4'     | 2.23                     | 0.57              |
| 16:H:180:ASP:OD2 | 16:H:183:ARG:NH1  | 2.36                     | 0.57              |
| 34:a:607:G:N1    | 34:a:785:A:OP2    | 2.36                     | 0.56              |
| 34:a:1248:G:OP2  | 34:a:1348:C:N4    | 2.29                     | 0.56              |
| 4:3:71:VAL:HG11  | 53:t:42:PRO:CG    | 2.35                     | 0.56              |
| 10:A:846:U:O2'   | 10:A:2073:A:N1    | 2.38                     | 0.56              |
| 10:A:1755:U:O2'  | 10:A:1758:G:O6    | 2.14                     | 0.56              |
| 14:F:97:ASP:O    | 14:F:101:VAL:HG13 | 2.05                     | 0.56              |
| 41:h:66:MET:HE2  | 41:h:66:MET:HA    | 1.85                     | 0.56              |
| 23:P:26:GLU:N    | 23:P:26:GLU:OE1   | 2.37                     | 0.56              |
| 34:a:9:G:HO2'    | 34:a:10:A:P       | 2.25                     | 0.56              |
| 34:a:1131:G:OP1  | 36:c:110:ARG:NE   | 2.37                     | 0.56              |
| 10:A:1872:A:N6   | 10:A:1896:G:O2'   | 2.37                     | 0.56              |
| 10:A:295:G:C2'   | 10:A:296:G:O5'    | 2.53                     | 0.56              |
| 20:M:118:LYS:O   | 20:M:121:THR:OG1  | 2.24                     | 0.56              |
| 31:X:79:THR:HG21 | 31:X:94:SER:OG    | 2.05                     | 0.56              |
| 10:A:2128:G:H2'  | 10:A:2130:A:H62   | 1.70                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 34:a:1209:U:O2'   | 34:a:1211:G:OP2   | 2.24                     | 0.56              |
| 42:i:54:ASP:OD1   | 42:i:58:GLY:N     | 2.31                     | 0.56              |
| 38:e:10:LYS:HG3   | 38:e:33:PRO:HB3   | 1.86                     | 0.56              |
| 34:a:1403:A:OP1   | 41:h:92:ARG:NH2   | 2.36                     | 0.56              |
| 34:a:1557:G:O2'   | 34:a:1558:A:OP2   | 2.16                     | 0.56              |
| 43:j:27:LYS:N     | 43:j:62:ASP:OD1   | 2.39                     | 0.56              |
| 7:6:9:LYS:NZ      | 10:A:1345:G:OP2   | 2.29                     | 0.56              |
| 10:A:2271:C:O2'   | 10:A:2440:C:OP2   | 2.24                     | 0.56              |
| 23:P:75:THR:HG22  | 23:P:90:PRO:HA    | 1.88                     | 0.56              |
| 34:a:1087:U:OP1   | 48:o:45:ARG:NH2   | 2.37                     | 0.55              |
| 34:a:1266:U:OP1   | 41:h:119:ARG:NH2  | 2.40                     | 0.55              |
| 51:r:84:GLU:N     | 51:r:84:GLU:OE1   | 2.39                     | 0.55              |
| 14:F:34:ASN:O     | 14:F:34:ASN:ND2   | 2.40                     | 0.55              |
| 22:O:116:GLU:N    | 22:O:116:GLU:OE1  | 2.39                     | 0.55              |
| 6:5:5:ILE:HD13    | 6:5:21:LYS:HG2    | 1.87                     | 0.55              |
| 10:A:1792:U:O2    | 10:A:1796:A:N6    | 2.39                     | 0.55              |
| 34:a:382:A:N3     | 34:a:394:U:O2'    | 2.34                     | 0.55              |
| 40:g:32:ILE:O     | 40:g:36:ASN:ND2   | 2.39                     | 0.55              |
| 42:i:115:ASP:OD1  | 42:i:116:LYS:N    | 2.40                     | 0.55              |
| 10:A:368:A:O2'    | 10:A:370:C:OP2    | 2.25                     | 0.55              |
| 10:A:1805:G:O2'   | 10:A:1843:C:OP1   | 2.23                     | 0.55              |
| 39:f:115:LEU:HD13 | 39:f:123:ILE:HG21 | 1.88                     | 0.55              |
| 6:5:31:GLU:OE2    | 6:5:46:ARG:NE     | 2.35                     | 0.55              |
| 37:d:94:THR:HG23  | 37:d:96:LYS:H     | 1.71                     | 0.55              |
| 41:h:71:PRO:O     | 41:h:96:ARG:NE    | 2.40                     | 0.55              |
| 36:c:80:ILE:HD11  | 36:c:93:ASN:HB3   | 1.88                     | 0.55              |
| 36:c:113:ARG:HH22 | 36:c:137:LEU:HD22 | 1.71                     | 0.55              |
| 53:t:64:GLU:O     | 53:t:67:VAL:HG22  | 2.06                     | 0.55              |
| 34:a:214:U:O2     | 51:r:68:ARG:NH1   | 2.40                     | 0.55              |
| 34:a:553:G:O2'    | 34:a:561:A:N1     | 2.24                     | 0.55              |
| 53:t:50:ALA:HB1   | 53:t:57:HIS:HB3   | 1.89                     | 0.55              |
| 34:a:633:A:OP1    | 34:a:657:G:N2     | 2.37                     | 0.54              |
| 10:A:429:A:O2'    | 10:A:430:A:O4'    | 2.25                     | 0.54              |
| 10:A:935:U:H3'    | 10:A:936:A:H4'    | 1.89                     | 0.54              |
| 17:I:153:LEU:HD11 | 17:I:176:VAL:HG22 | 1.89                     | 0.54              |
| 10:A:2589:G:O2'   | 10:A:2592:C:OP2   | 2.26                     | 0.54              |
| 53:t:26:GLU:OE1   | 53:t:26:GLU:N     | 2.38                     | 0.54              |
| 1:0:187:ASN:OD1   | 1:0:188:HIS:N     | 2.41                     | 0.54              |
| 4:3:16:ASP:O      | 4:3:20:GLY:N      | 2.34                     | 0.54              |
| 10:A:2317:G:H22   | 10:A:2325:U:H3    | 1.55                     | 0.54              |
| 24:Q:29:ARG:NH1   | 24:Q:124:GLU:OE1  | 2.40                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:F:161:VAL:CG1  | 14:F:173:VAL:HG23 | 2.36                     | 0.54              |
| 22:O:80:ASP:OD1   | 22:O:81:THR:N     | 2.38                     | 0.54              |
| 10:A:75:G:H22     | 10:A:110:A:H2     | 1.56                     | 0.54              |
| 37:d:69:THR:HG21  | 37:d:75:VAL:HG21  | 1.90                     | 0.54              |
| 42:i:18:ASN:ND2   | 42:i:74:ILE:O     | 2.41                     | 0.54              |
| 46:m:59:ASN:ND2   | 46:m:102:ASP:OD1  | 2.39                     | 0.54              |
| 36:c:187:VAL:HG21 | 36:c:199:VAL:HG23 | 1.90                     | 0.54              |
| 43:j:88:LEU:HD11  | 43:j:104:LEU:HD22 | 1.90                     | 0.54              |
| 10:A:247:G:O2'    | 10:A:423:A:N1     | 2.33                     | 0.54              |
| 10:A:2146:G:HO2'  | 10:A:2147:A:P     | 2.30                     | 0.54              |
| 34:a:1170:G:N2    | 34:a:1172:A:H62   | 2.06                     | 0.54              |
| 34:a:1281:G:O2'   | 34:a:1284:G:N3    | 2.38                     | 0.54              |
| 52:s:41:GLY:O     | 52:s:67:ARG:NH2   | 2.37                     | 0.54              |
| 10:A:1913:A:O2'   | 10:A:1914:A:OP1   | 2.24                     | 0.54              |
| 31:X:99:GLU:OE1   | 31:X:100:VAL:N    | 2.41                     | 0.54              |
| 8:7:13:ARG:NH2    | 10:A:252:G:OP1    | 2.40                     | 0.54              |
| 34:a:399:A:O2'    | 34:a:477:A:N7     | 2.41                     | 0.53              |
| 34:a:1331:G:O2'   | 34:a:1332:A:OP2   | 2.24                     | 0.53              |
| 39:f:39:VAL:HG12  | 39:f:67:ALA:HB1   | 1.90                     | 0.53              |
| 10:A:83:G:O2'     | 10:A:101:G:N2     | 2.41                     | 0.53              |
| 10:A:1583:G:O2'   | 10:A:1584:U:P     | 2.67                     | 0.53              |
| 10:A:2890:C:O3'   | 24:Q:100:ARG:NH2  | 2.42                     | 0.53              |
| 34:a:1209:U:HO2'  | 34:a:1210:G:P     | 2.30                     | 0.53              |
| 40:g:29:PHE:HA    | 40:g:32:ILE:HD12  | 1.90                     | 0.53              |
| 6:5:30:LEU:HD11   | 6:5:32:LYS:HE2    | 1.89                     | 0.53              |
| 37:d:34:GLU:OE2   | 37:d:58:ARG:NH1   | 2.40                     | 0.53              |
| 10:A:1373:G:O2'   | 10:A:1428:A:N1    | 2.40                     | 0.53              |
| 10:A:2146:G:N2    | 10:A:2170:G:O2'   | 2.42                     | 0.53              |
| 26:S:33:VAL:HG23  | 26:S:33:VAL:O     | 2.08                     | 0.53              |
| 34:a:1563:C:O2'   | 34:a:1564:U:P     | 2.66                     | 0.53              |
| 10:A:2598:U:H1'   | 10:A:2599:C:OP2   | 2.09                     | 0.53              |
| 32:Y:65:ASP:OD1   | 32:Y:67:THR:HG23  | 2.08                     | 0.53              |
| 39:f:159:LYS:NZ   | 42:i:42:ARG:O     | 2.41                     | 0.53              |
| 10:A:345:A:N3     | 10:A:365:G:O2'    | 2.40                     | 0.53              |
| 10:A:2670:A:O3'   | 19:K:160:LYS:NZ   | 2.41                     | 0.53              |
| 10:A:2148:G:O4'   | 10:A:2172:G:O2'   | 2.26                     | 0.53              |
| 31:X:72:ASP:O     | 31:X:76:GLY:N     | 2.35                     | 0.53              |
| 34:a:1444:A:N6    | 34:a:1509:G:O2'   | 2.41                     | 0.53              |
| 1:0:522:ASP:OD1   | 1:0:523:ASN:N     | 2.42                     | 0.53              |
| 14:F:152:ALA:O    | 14:F:156:VAL:HG23 | 2.09                     | 0.53              |
| 34:a:1212:G:N2    | 48:o:61:TRP:OXT   | 2.39                     | 0.53              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 5:4:13:LYS:NZ    | 10:A:1299:U:OP1   | 2.38                     | 0.52              |
| 10:A:281:A:HO2'  | 10:A:282:G:P      | 2.32                     | 0.52              |
| 19:K:96:ALA:HB2  | 19:K:105:LEU:HD23 | 1.91                     | 0.52              |
| 10:A:691:A:OP2   | 10:A:692:U:O2'    | 2.25                     | 0.52              |
| 34:a:1177:A:OP1  | 44:k:44:THR:HG22  | 2.09                     | 0.52              |
| 10:A:1398:C:O2'  | 10:A:1822:A:N3    | 2.37                     | 0.52              |
| 34:a:1425:C:O2   | 34:a:1529:A:N6    | 2.41                     | 0.52              |
| 10:A:613:G:O2'   | 10:A:1290:A:OP1   | 2.28                     | 0.52              |
| 10:A:1421:C:O2'  | 10:A:1511:A:N3    | 2.41                     | 0.52              |
| 34:a:177:A:H2'   | 34:a:178:A:O4'    | 2.09                     | 0.52              |
| 34:a:276:A:N6    | 34:a:301:G:O6     | 2.43                     | 0.52              |
| 1:0:352:GLN:O    | 1:0:512:ARG:NH2   | 2.38                     | 0.52              |
| 10:A:2770:A:N1   | 19:K:67:THR:OG1   | 2.35                     | 0.52              |
| 16:H:16:PHE:O    | 26:S:12:GLN:NE2   | 2.39                     | 0.52              |
| 34:a:527:C:OP1   | 46:m:127:ARG:NH2  | 2.39                     | 0.52              |
| 34:a:872:G:O2'   | 34:a:873:C:P      | 2.68                     | 0.52              |
| 37:d:169:GLU:OE1 | 37:d:170:GLY:N    | 2.41                     | 0.52              |
| 10:A:569:A:OP1   | 10:A:597:G:N1     | 2.43                     | 0.52              |
| 10:A:662:C:O2'   | 10:A:696:U:OP1    | 2.27                     | 0.52              |
| 10:A:965:U:HO2'  | 10:A:966:C:P      | 2.31                     | 0.52              |
| 31:X:89:LYS:NZ   | 31:X:90:LYS:O     | 2.41                     | 0.52              |
| 34:a:227:A:O2'   | 34:a:228:A:O4'    | 2.26                     | 0.52              |
| 6:5:21:LYS:NZ    | 6:5:26:ASN:O      | 2.26                     | 0.52              |
| 10:A:2318:U:O2'  | 10:A:2319:U:P     | 2.68                     | 0.52              |
| 43:j:45:ARG:O    | 43:j:49:ASN:ND2   | 2.42                     | 0.52              |
| 1:0:317:MET:SD   | 1:0:484:ILE:HD13  | 2.49                     | 0.52              |
| 10:A:1042:G:O2'  | 10:A:1049:A:N1    | 2.42                     | 0.52              |
| 14:F:166:ASP:OD1 | 14:F:168:ALA:N    | 2.40                     | 0.52              |
| 34:a:21:C:OP2    | 39:f:132:THR:OG1  | 2.26                     | 0.51              |
| 34:a:1097:U:O5'  | 39:f:30:ARG:NH2   | 2.43                     | 0.51              |
| 10:A:2148:G:N7   | 10:A:2169:G:N2    | 2.59                     | 0.51              |
| 24:Q:20:ILE:HG21 | 24:Q:40:VAL:HG21  | 1.93                     | 0.51              |
| 5:4:39:SER:OG    | 10:A:2825:C:O2'   | 2.28                     | 0.51              |
| 6:5:36:CYS:O     | 6:5:40:ARG:N      | 2.42                     | 0.51              |
| 13:D:39:A:O2'    | 34:a:816:A:OP1    | 2.24                     | 0.51              |
| 34:a:1204:G:N2   | 34:a:1207:G:OP2   | 2.43                     | 0.51              |
| 37:d:35:ASP:OD1  | 37:d:58:ARG:NH2   | 2.40                     | 0.51              |
| 48:o:34:TYR:O    | 48:o:38:HIS:N     | 2.44                     | 0.51              |
| 39:f:105:VAL:O   | 39:f:112:ARG:NH1  | 2.44                     | 0.51              |
| 10:A:1211:A:N3   | 10:A:1214:A:N6    | 2.57                     | 0.51              |
| 10:A:1646:C:O2'  | 10:A:1652:A:N1    | 2.39                     | 0.51              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 30:W:13:THR:H    | 30:W:16:SER:HG    | 1.58                     | 0.51              |
| 34:a:281:G:OP1   | 51:r:74:LYS:NZ    | 2.38                     | 0.51              |
| 4:3:29:LYS:HD3   | 4:3:46:LEU:HD11   | 1.92                     | 0.51              |
| 10:A:55:G:O2'    | 10:A:126:A:N1     | 2.41                     | 0.51              |
| 21:N:105:GLU:O   | 21:N:109:ASN:ND2  | 2.40                     | 0.51              |
| 34:a:556:G:O2'   | 34:a:557:U:OP1    | 2.28                     | 0.51              |
| 34:a:868:U:N3    | 34:a:870:C:OP1    | 2.44                     | 0.51              |
| 8:7:54:ASP:OD2   | 10:A:2372:C:O2'   | 2.19                     | 0.50              |
| 10:A:520:G:O2'   | 10:A:545:A:N6     | 2.44                     | 0.50              |
| 10:A:555:C:O2'   | 29:V:23:ARG:NH2   | 2.44                     | 0.50              |
| 10:A:1058:U:O2'  | 10:A:1060:A:N7    | 2.44                     | 0.50              |
| 34:a:52:A:O2'    | 34:a:386:G:N2     | 2.45                     | 0.50              |
| 34:a:584:G:OP2   | 34:a:585:A:O2'    | 2.26                     | 0.50              |
| 34:a:1035:C:HO2' | 34:a:1036:U:P     | 2.32                     | 0.50              |
| 34:a:1393:C:P    | 43:j:114:LYS:HZ1  | 2.34                     | 0.50              |
| 1:0:369:LYS:N    | 55:0:601:ATP:O1B  | 2.41                     | 0.50              |
| 4:3:71:VAL:HG23  | 53:t:67:VAL:CG2   | 2.41                     | 0.50              |
| 14:F:63:VAL:HG11 | 14:F:192:ILE:HD13 | 1.92                     | 0.50              |
| 34:a:604:A:O2'   | 34:a:754:A:N3     | 2.38                     | 0.50              |
| 34:a:1018:U:O2'  | 34:a:1019:U:OP2   | 2.26                     | 0.50              |
| 34:a:1457:C:H2'  | 34:a:1458:G:O4'   | 2.12                     | 0.50              |
| 34:a:1480:U:O2'  | 34:a:1481:G:P     | 2.69                     | 0.50              |
| 1:0:208:VAL:O    | 1:0:208:VAL:HG13  | 2.11                     | 0.50              |
| 10:A:2608:G:N2   | 10:A:2611:A:OP2   | 2.36                     | 0.50              |
| 34:a:179:A:H3'   | 34:a:180:C:O4'    | 2.11                     | 0.50              |
| 10:A:1101:G:H2'  | 10:A:1102:G:O4'   | 2.12                     | 0.50              |
| 48:o:24:CYS:O    | 48:o:28:GLY:N     | 2.38                     | 0.50              |
| 20:M:18:VAL:HG23 | 20:M:138:PRO:HB2  | 1.93                     | 0.50              |
| 34:a:1002:A:H4'  | 34:a:1003:G:H5''  | 1.92                     | 0.50              |
| 53:t:13:ASP:OD1  | 53:t:14:HIS:N     | 2.44                     | 0.50              |
| 3:2:26:LEU:HD12  | 3:2:50:ILE:HD11   | 1.94                     | 0.50              |
| 10:A:411:G:O2'   | 10:A:439:G:O6     | 2.26                     | 0.50              |
| 11:B:3:U:OP1     | 11:B:59:U:O2'     | 2.24                     | 0.50              |
| 17:I:20:ASN:OD1  | 17:I:22:GLU:N     | 2.43                     | 0.50              |
| 31:X:4:LYS:N     | 31:X:7:ASP:OD2    | 2.43                     | 0.50              |
| 44:k:78:ASN:O    | 44:k:78:ASN:ND2   | 2.44                     | 0.50              |
| 10:A:1259:G:N7   | 28:U:70:LYS:NZ    | 2.60                     | 0.50              |
| 10:A:2640:G:O2'  | 10:A:2794:A:N1    | 2.37                     | 0.50              |
| 16:H:103:GLN:N   | 16:H:106:ASP:OD2  | 2.40                     | 0.50              |
| 34:a:427:C:O2'   | 34:a:647:A:N3     | 2.35                     | 0.50              |
| 50:q:71:ARG:NH2  | 50:q:75:SER:OG    | 2.45                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 19:K:8:VAL:HG12   | 19:K:51:THR:HG22  | 1.92                     | 0.50              |
| 34:a:1356:U:OP1   | 47:n:25:ILE:N     | 2.44                     | 0.50              |
| 36:c:113:ARG:HH12 | 36:c:117:ILE:HD13 | 1.75                     | 0.50              |
| 8:7:12:LYS:NZ     | 10:A:251:C:O2     | 2.43                     | 0.50              |
| 10:A:1019:A:N3    | 10:A:2050:A:O2'   | 2.38                     | 0.50              |
| 10:A:2419:C:OP2   | 10:A:2424:A:N6    | 2.42                     | 0.50              |
| 12:C:69:G:HO2'    | 12:C:70:C:P       | 2.25                     | 0.50              |
| 13:D:7:G:H3'      | 13:D:8:U:C5'      | 2.42                     | 0.50              |
| 23:P:38:GLU:HB2   | 23:P:127:VAL:HG13 | 1.94                     | 0.50              |
| 34:a:289:A:OP1    | 54:u:73:ARG:NE    | 2.38                     | 0.50              |
| 34:a:1217:A:N6    | 59:a:1615:SCM:H11 | 2.26                     | 0.50              |
| 10:A:754:A:N1     | 49:p:53:TYR:OH    | 2.37                     | 0.49              |
| 34:a:64:U:O2'     | 34:a:405:C:O2     | 2.30                     | 0.49              |
| 43:j:21:LEU:CD2   | 43:j:63:VAL:HG22  | 2.42                     | 0.49              |
| 3:2:28:LEU:HD21   | 3:2:35:VAL:HG12   | 1.92                     | 0.49              |
| 10:A:194:C:O2'    | 10:A:841:A:N3     | 2.45                     | 0.49              |
| 10:A:1812:G:N7    | 15:G:178:SER:OG   | 2.41                     | 0.49              |
| 10:A:2111:U:O2'   | 10:A:2112:U:P     | 2.70                     | 0.49              |
| 34:a:399:A:N1     | 34:a:417:C:O2'    | 2.35                     | 0.49              |
| 38:e:166:VAL:HG12 | 38:e:177:PHE:CD1  | 2.47                     | 0.49              |
| 10:A:1180:U:H4'   | 10:A:1181:A:O4'   | 2.12                     | 0.49              |
| 10:A:1536:A:O2'   | 10:A:1537:A:P     | 2.70                     | 0.49              |
| 10:A:2808:U:O2'   | 10:A:2809:U:OP1   | 2.22                     | 0.49              |
| 34:a:771:U:OP1    | 34:a:878:C:O2'    | 2.30                     | 0.49              |
| 34:a:966:G:O3'    | 41:h:102:ARG:NH1  | 2.45                     | 0.49              |
| 10:A:1570:G:N1    | 10:A:1589:A:OP2   | 2.40                     | 0.49              |
| 14:F:43:GLU:OE1   | 14:F:43:GLU:N     | 2.46                     | 0.49              |
| 1:0:173:LEU:HD13  | 1:0:200:TYR:OH    | 2.12                     | 0.49              |
| 10:A:1814:A:OP2   | 15:G:150:LYS:NZ   | 2.38                     | 0.49              |
| 34:a:865:G:O2'    | 34:a:866:G:P      | 2.71                     | 0.49              |
| 10:A:2877:G:O2'   | 10:A:2878:A:P     | 2.70                     | 0.49              |
| 34:a:682:G:O2'    | 49:p:28:GLN:OE1   | 2.23                     | 0.49              |
| 34:a:845:A:H4'    | 34:a:846:U:OP2    | 2.12                     | 0.49              |
| 34:a:1101:G:O2'   | 34:a:1128:A:N1    | 2.42                     | 0.49              |
| 41:h:15:ASP:OD1   | 41:h:17:ILE:N     | 2.43                     | 0.49              |
| 42:i:98:LEU:HD11  | 42:i:132:TRP:CD1  | 2.48                     | 0.49              |
| 10:A:1583:G:O2'   | 10:A:1584:U:O5'   | 2.31                     | 0.49              |
| 15:G:274:ARG:C    | 15:G:275:THR:HG1  | 2.14                     | 0.49              |
| 20:M:42:LYS:NZ    | 20:M:51:THR:O     | 2.24                     | 0.49              |
| 36:c:205:ASP:OD1  | 36:c:205:ASP:O    | 2.31                     | 0.49              |
| 10:A:250:G:O2'    | 10:A:2445:A:OP1   | 2.29                     | 0.49              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 29:V:85:PRO:O      | 29:V:105:THR:OG1  | 2.24                     | 0.49              |
| 34:a:794:A:N3      | 34:a:1539:U:O2'   | 2.46                     | 0.49              |
| 10:A:901:A:N3      | 11:B:77:G:O2'     | 2.45                     | 0.49              |
| 19:K:87:LEU:N      | 19:K:87:LEU:HD12  | 2.27                     | 0.49              |
| 34:a:907:C:OP1     | 46:m:5:ASN:ND2    | 2.39                     | 0.49              |
| 59:a:1615:SCM:H2M1 | 39:f:27:GLY:HA2   | 1.95                     | 0.49              |
| 47:n:19:LEU:HD11   | 47:n:34:LEU:HD21  | 1.95                     | 0.49              |
| 10:A:1965:A:OP1    | 21:N:42:THR:HG21  | 2.12                     | 0.48              |
| 34:a:1035:C:O2'    | 34:a:1036:U:P     | 2.70                     | 0.48              |
| 10:A:2217:C:OP2    | 15:G:150:LYS:NZ   | 2.36                     | 0.48              |
| 30:W:56:LEU:HD11   | 30:W:79:ILE:CD1   | 2.44                     | 0.48              |
| 34:a:865:G:HO2'    | 34:a:866:G:P      | 2.36                     | 0.48              |
| 34:a:1004:A:O2'    | 34:a:1006:C:OP2   | 2.26                     | 0.48              |
| 10:A:1833:U:OP1    | 15:G:177:ASN:ND2  | 2.43                     | 0.48              |
| 14:F:139:ASN:OD1   | 14:F:141:LYS:N    | 2.47                     | 0.48              |
| 26:S:2:ASN:OD1     | 26:S:6:GLN:NE2    | 2.46                     | 0.48              |
| 34:a:75:U:O4       | 34:a:112:A:N6     | 2.46                     | 0.48              |
| 34:a:606:C:H2'     | 34:a:607:G:O4'    | 2.13                     | 0.48              |
| 10:A:1917:G:O2'    | 10:A:1941:A:N1    | 2.44                     | 0.48              |
| 34:a:1006:C:O2     | 48:o:19:GLN:NE2   | 2.47                     | 0.48              |
| 34:a:1028:U:H3     | 34:a:1065:A:H61   | 1.61                     | 0.48              |
| 34:a:1313:A:N3     | 34:a:1379:G:O2'   | 2.32                     | 0.48              |
| 36:c:86:ARG:NH1    | 36:c:219:ASP:OD1  | 2.40                     | 0.48              |
| 39:f:74:VAL:HG11   | 39:f:144:LEU:HD13 | 1.95                     | 0.48              |
| 10:A:9:G:O2'       | 10:A:2812:A:N6    | 2.46                     | 0.48              |
| 34:a:750:G:OP2     | 34:a:858:G:N2     | 2.46                     | 0.48              |
| 10:A:18:C:OP1      | 27:T:26:GLY:N     | 2.43                     | 0.48              |
| 10:A:923:C:H2'     | 10:A:924:C:C6     | 2.49                     | 0.48              |
| 39:f:25:VAL:HG22   | 39:f:26:LYS:N     | 2.29                     | 0.48              |
| 1:0:104:LEU:HD11   | 1:0:119:MET:HE2   | 1.95                     | 0.48              |
| 9:8:17:ILE:HD11    | 9:8:26:ILE:HD12   | 1.96                     | 0.48              |
| 34:a:960:G:N7      | 41:h:3:ARG:NH1    | 2.60                     | 0.48              |
| 10:A:52:A:OP2      | 10:A:116:G:N1     | 2.37                     | 0.48              |
| 25:R:60:ASP:OD2    | 25:R:82:ARG:NH1   | 2.46                     | 0.48              |
| 34:a:159:G:O2'     | 34:a:228:A:N1     | 2.42                     | 0.48              |
| 38:e:166:VAL:HG12  | 38:e:177:PHE:CE1  | 2.48                     | 0.48              |
| 40:g:38:ALA:HB1    | 40:g:68:VAL:CG2   | 2.43                     | 0.48              |
| 40:g:38:ALA:HB1    | 40:g:68:VAL:HG21  | 1.96                     | 0.48              |
| 10:A:342:U:H2'     | 10:A:343:G:O4'    | 2.13                     | 0.48              |
| 10:A:2443:A:N3     | 10:A:2443:A:H2'   | 2.29                     | 0.48              |
| 32:Y:48:ARG:HH11   | 32:Y:67:THR:HG21  | 1.79                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 38:e:163:PRO:O    | 38:e:166:VAL:HG22 | 2.14                     | 0.48              |
| 20:M:5:TYR:O      | 27:T:64:ARG:NH2   | 2.45                     | 0.48              |
| 34:a:1563:C:O2'   | 34:a:1564:U:OP1   | 2.30                     | 0.48              |
| 10:A:180:G:H2'    | 10:A:181:U:O4'    | 2.14                     | 0.47              |
| 10:A:2304:U:O2'   | 10:A:2387:C:O2    | 2.31                     | 0.47              |
| 34:a:402:G:H5''   | 50:q:6:ARG:HB2    | 1.96                     | 0.47              |
| 34:a:690:G:H22    | 34:a:767:G:H1     | 1.60                     | 0.47              |
| 37:d:69:THR:HG21  | 37:d:75:VAL:CG2   | 2.44                     | 0.47              |
| 10:A:1877:U:OP1   | 10:A:2423:G:O2'   | 2.31                     | 0.47              |
| 31:X:60:GLU:OE1   | 31:X:60:GLU:N     | 2.43                     | 0.47              |
| 42:i:107:SER:HB2  | 42:i:128:ILE:HD11 | 1.96                     | 0.47              |
| 43:j:43:ASP:OD1   | 43:j:44:LEU:N     | 2.47                     | 0.47              |
| 44:k:26:VAL:HG13  | 44:k:36:VAL:HG21  | 1.96                     | 0.47              |
| 44:k:73:LEU:O     | 44:k:74:ILE:HD13  | 2.13                     | 0.47              |
| 10:A:59:G:O2'     | 10:A:74:U:OP2     | 2.27                     | 0.47              |
| 10:A:1509:C:O2'   | 10:A:1510:C:OP2   | 2.27                     | 0.47              |
| 10:A:2658:G:H4'   | 10:A:2745:G:O2'   | 2.14                     | 0.47              |
| 34:a:783:U:H2'    | 34:a:784:G:O4'    | 2.14                     | 0.47              |
| 37:d:39:ARG:NH1   | 37:d:54:ILE:O     | 2.47                     | 0.47              |
| 45:l:71:THR:HG21  | 45:l:103:THR:OG1  | 2.14                     | 0.47              |
| 10:A:693:G:N3     | 10:A:693:G:H2'    | 2.30                     | 0.47              |
| 10:A:2184:A:H1'   | 10:A:2185:U:C2    | 2.48                     | 0.47              |
| 10:A:2279:A:H4'   | 10:A:2280:A:O5'   | 2.15                     | 0.47              |
| 10:A:2525:C:H2'   | 10:A:2526:G:O4'   | 2.15                     | 0.47              |
| 14:F:192:ILE:O    | 14:F:195:VAL:HG12 | 2.14                     | 0.47              |
| 19:K:89:LEU:HD13  | 19:K:94:TYR:HB3   | 1.96                     | 0.47              |
| 34:a:1213:G:N3    | 48:o:60:SER:OG    | 2.48                     | 0.47              |
| 50:q:68:ASP:OD1   | 50:q:69:THR:N     | 2.45                     | 0.47              |
| 52:s:49:THR:O     | 52:s:49:THR:HG22  | 2.14                     | 0.47              |
| 1:0:241:ASP:OD1   | 1:0:241:ASP:N     | 2.47                     | 0.47              |
| 10:A:856:C:O2'    | 10:A:878:U:OP1    | 2.33                     | 0.47              |
| 10:A:1005:G:O4'   | 10:A:2280:A:N6    | 2.48                     | 0.47              |
| 10:A:1170:G:N2    | 10:A:1171:U:O4    | 2.40                     | 0.47              |
| 10:A:1758:G:O2'   | 10:A:1759:G:P     | 2.73                     | 0.47              |
| 18:J:156:ILE:N    | 18:J:156:ILE:HD12 | 2.30                     | 0.47              |
| 23:P:127:VAL:HG12 | 23:P:128:LYS:O    | 2.15                     | 0.47              |
| 34:a:30:G:O2'     | 34:a:322:U:OP1    | 2.31                     | 0.47              |
| 34:a:1275:C:O2'   | 43:j:75:GLN:OE1   | 2.29                     | 0.47              |
| 45:l:46:SER:N     | 45:l:49:SER:OG    | 2.42                     | 0.47              |
| 47:n:10:PRO:O     | 47:n:45:VAL:HG21  | 2.15                     | 0.47              |
| 10:A:441:A:H2'    | 10:A:442:U:O4'    | 2.15                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:A:1086:G:N2    | 10:A:1149:G:O2'   | 2.48                     | 0.47              |
| 32:Y:57:GLY:N     | 32:Y:88:VAL:O     | 2.45                     | 0.47              |
| 34:a:1171:C:H4'   | 34:a:1172:A:O5'   | 2.15                     | 0.47              |
| 34:a:1347:U:OP2   | 34:a:1348:C:O2'   | 2.33                     | 0.47              |
| 11:B:10:G:O4'     | 32:Y:80:ARG:NH2   | 2.48                     | 0.47              |
| 36:c:33:THR:HG22  | 36:c:34:GLU:N     | 2.29                     | 0.47              |
| 45:l:35:THR:HG22  | 45:l:41:ALA:HA    | 1.97                     | 0.47              |
| 4:3:12:VAL:HG11   | 4:3:27:SER:HB3    | 1.96                     | 0.47              |
| 10:A:519:A:O2'    | 31:X:42:LYS:O     | 2.33                     | 0.47              |
| 10:A:927:U:O2'    | 10:A:930:C:O2'    | 2.32                     | 0.47              |
| 10:A:1095:G:C2'   | 10:A:1142:A:H61   | 2.28                     | 0.47              |
| 10:A:1254:C:OP2   | 27:T:15:LYS:NZ    | 2.32                     | 0.47              |
| 20:M:136:GLN:OE1  | 20:M:136:GLN:N    | 2.48                     | 0.47              |
| 34:a:1183:A:N7    | 34:a:1206:A:N6    | 2.63                     | 0.47              |
| 45:l:20:VAL:HG22  | 45:l:83:ASP:OD1   | 2.14                     | 0.47              |
| 10:A:325:A:H2'    | 10:A:326:G:O4'    | 2.15                     | 0.46              |
| 10:A:1564:G:OP2   | 10:A:1565:A:O2'   | 2.11                     | 0.46              |
| 10:A:2875:U:OP2   | 10:A:2876:G:O2'   | 2.20                     | 0.46              |
| 34:a:699:G:H2'    | 34:a:700:G:C8     | 2.51                     | 0.46              |
| 34:a:1563:C:H42   | 35:b:3:A:H62      | 1.62                     | 0.46              |
| 10:A:793:U:O2'    | 10:A:1308:A:N1    | 2.45                     | 0.46              |
| 45:l:68:GLU:HA    | 45:l:103:THR:HG21 | 1.97                     | 0.46              |
| 47:n:86:TYR:N     | 53:t:73:GLU:OE1   | 2.43                     | 0.46              |
| 23:P:42:ILE:HD12  | 23:P:97:VAL:HG21  | 1.97                     | 0.46              |
| 34:a:1043:A:O2'   | 34:a:1243:C:O2'   | 2.33                     | 0.46              |
| 51:r:30:THR:HG22  | 51:r:31:LYS:N     | 2.29                     | 0.46              |
| 10:A:827:A:OP1    | 10:A:830:C:N4     | 2.41                     | 0.46              |
| 10:A:2857:U:OP1   | 26:S:96:LYS:NZ    | 2.42                     | 0.46              |
| 34:a:1275:C:O2'   | 43:j:70:GLY:O     | 2.34                     | 0.46              |
| 36:c:75:GLN:NE2   | 36:c:205:ASP:OD1  | 2.47                     | 0.46              |
| 10:A:1739:G:OP2   | 10:A:1740:A:O2'   | 2.32                     | 0.46              |
| 10:A:1820:G:N2    | 10:A:1823:A:OP2   | 2.42                     | 0.46              |
| 51:r:30:THR:HG22  | 51:r:31:LYS:H     | 1.81                     | 0.46              |
| 1:0:456:LEU:HD13  | 1:0:484:ILE:HD11  | 1.98                     | 0.46              |
| 10:A:333:U:H2'    | 10:A:334:G:O4'    | 2.16                     | 0.46              |
| 10:A:1407:U:O2'   | 10:A:2225:A:N3    | 2.41                     | 0.46              |
| 10:A:2877:G:C2'   | 10:A:2878:A:OP2   | 2.64                     | 0.46              |
| 14:F:113:VAL:HG11 | 14:F:156:VAL:HG21 | 1.98                     | 0.46              |
| 14:F:209:ILE:HG21 | 14:F:212:ILE:HG12 | 1.97                     | 0.46              |
| 25:R:44:VAL:O     | 25:R:53:LEU:N     | 2.49                     | 0.46              |
| 20:M:5:TYR:O      | 27:T:64:ARG:NH1   | 2.47                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 34:a:668:A:N3     | 42:i:107:SER:OG   | 2.46                     | 0.46              |
| 34:a:1052:U:O2'   | 34:a:1053:C:O5'   | 2.27                     | 0.46              |
| 4:3:27:SER:OG     | 18:J:140:GLU:OE2  | 2.32                     | 0.46              |
| 10:A:622:A:N1     | 10:A:848:G:O2'    | 2.46                     | 0.46              |
| 15:G:130:LEU:HD13 | 15:G:192:ILE:CD1  | 2.46                     | 0.46              |
| 21:N:86:ILE:HG22  | 21:N:94:ARG:HG3   | 1.97                     | 0.46              |
| 37:d:122:GLN:NE2  | 37:d:135:GLN:OE1  | 2.48                     | 0.46              |
| 10:A:228:A:O2'    | 10:A:231:U:O4     | 2.31                     | 0.46              |
| 12:C:37:T6A:N11   | 12:C:37:T6A:N1    | 2.62                     | 0.46              |
| 16:H:19:SER:O     | 26:S:80:ARG:NE    | 2.44                     | 0.46              |
| 34:a:1480:U:O2'   | 34:a:1481:G:O5'   | 2.30                     | 0.46              |
| 10:A:743:G:O2'    | 10:A:744:A:OP2    | 2.30                     | 0.46              |
| 10:A:2127:A:H2'   | 10:A:2128:G:O4'   | 2.16                     | 0.46              |
| 10:A:2213:C:O2    | 10:A:2239:C:N4    | 2.45                     | 0.45              |
| 10:A:2545:G:O2'   | 10:A:2670:A:N1    | 2.45                     | 0.45              |
| 14:F:131:LEU:O    | 14:F:135:GLY:N    | 2.49                     | 0.45              |
| 23:P:20:GLU:OE2   | 23:P:99:ARG:NE    | 2.47                     | 0.45              |
| 36:c:14:VAL:HG22  | 36:c:209:ALA:HB1  | 1.97                     | 0.45              |
| 51:r:52:GLU:OE1   | 51:r:52:GLU:N     | 2.43                     | 0.45              |
| 1:0:362:VAL:HG12  | 1:0:363:GLY:N     | 2.31                     | 0.45              |
| 14:F:31:LYS:NZ    | 14:F:178:VAL:O    | 2.49                     | 0.45              |
| 17:I:153:LEU:HD11 | 17:I:176:VAL:CG2  | 2.46                     | 0.45              |
| 20:M:53:ASP:OD1   | 20:M:53:ASP:N     | 2.49                     | 0.45              |
| 23:P:44:ASN:OD1   | 23:P:45:ARG:N     | 2.49                     | 0.45              |
| 34:a:1027:U:H3'   | 34:a:1028:U:C5'   | 2.46                     | 0.45              |
| 5:4:24:ILE:HG23   | 5:4:24:ILE:O      | 2.16                     | 0.45              |
| 10:A:220:G:H22    | 10:A:237:U:H4'    | 1.81                     | 0.45              |
| 10:A:739:G:O2'    | 10:A:1674:A:N3    | 2.39                     | 0.45              |
| 10:A:753:U:O2'    | 10:A:755:A:N7     | 2.24                     | 0.45              |
| 10:A:902:G:H2'    | 10:A:903:A:O4'    | 2.15                     | 0.45              |
| 17:I:141:GLN:OE1  | 17:I:145:ASN:ND2  | 2.43                     | 0.45              |
| 34:a:358:G:OP2    | 54:u:3:ASN:N      | 2.41                     | 0.45              |
| 34:a:754:A:OP1    | 49:p:54:ARG:NH1   | 2.49                     | 0.45              |
| 39:f:25:VAL:HG22  | 39:f:26:LYS:H     | 1.80                     | 0.45              |
| 34:a:1340:C:OP1   | 53:t:6:LYS:NZ     | 2.50                     | 0.45              |
| 34:a:1516:G:O2'   | 34:a:1517:U:P     | 2.73                     | 0.45              |
| 46:m:110:ILE:CG2  | 46:m:117:THR:HG21 | 2.47                     | 0.45              |
| 52:s:26:ASP:OD1   | 52:s:28:LYS:N     | 2.45                     | 0.45              |
| 1:0:474:ASN:O     | 1:0:475:HIS:HB2   | 2.16                     | 0.45              |
| 4:3:27:SER:HG     | 18:J:140:GLU:CD   | 2.25                     | 0.45              |
| 10:A:299:G:O2'    | 10:A:460:C:OP2    | 2.15                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:A:2545:G:N2    | 10:A:2676:G:O2'   | 2.49                     | 0.45              |
| 19:K:45:ILE:HD12  | 19:K:45:ILE:N     | 2.32                     | 0.45              |
| 34:a:703:U:O2     | 34:a:803:A:O2'    | 2.34                     | 0.45              |
| 34:a:1097:U:OP1   | 39:f:30:ARG:NH1   | 2.50                     | 0.45              |
| 34:a:1335:G:H2'   | 34:a:1336:C:O4'   | 2.17                     | 0.45              |
| 10:A:1086:G:O2'   | 10:A:1087:A:OP2   | 2.33                     | 0.45              |
| 17:I:153:LEU:HD12 | 17:I:174:SER:O    | 2.17                     | 0.45              |
| 30:W:14:GLU:OE1   | 30:W:14:GLU:N     | 2.43                     | 0.45              |
| 38:e:165:PHE:CD1  | 38:e:166:VAL:HG13 | 2.52                     | 0.45              |
| 1:0:29:VAL:HB     | 1:0:209:LEU:HD22  | 1.98                     | 0.45              |
| 1:0:351:PHE:HB3   | 1:0:521:ILE:HD11  | 1.98                     | 0.45              |
| 6:5:19:THR:OG1    | 10:A:2299:A:N6    | 2.50                     | 0.45              |
| 10:A:309:G:O2'    | 10:A:310:A:OP2    | 2.30                     | 0.45              |
| 10:A:857:G:N1     | 10:A:1225:U:OP2   | 2.37                     | 0.45              |
| 10:A:1355:G:C2    | 10:A:1364:U:H5'   | 2.52                     | 0.45              |
| 10:A:2679:C:O2    | 10:A:2679:C:O4'   | 2.35                     | 0.45              |
| 15:G:132:LEU:O    | 15:G:167:LYS:NZ   | 2.49                     | 0.45              |
| 34:a:1032:C:O2'   | 34:a:1065:A:H2'   | 2.17                     | 0.45              |
| 1:0:373:LEU:HD11  | 1:0:498:VAL:HG23  | 1.98                     | 0.45              |
| 7:6:1:MET:HE2     | 7:6:3:ARG:HH21    | 1.82                     | 0.45              |
| 10:A:33:U:HO2'    | 10:A:34:U:P       | 2.35                     | 0.45              |
| 10:A:1189:U:O2'   | 10:A:1190:A:P     | 2.75                     | 0.45              |
| 10:A:2487:C:O4'   | 10:A:2487:C:O2    | 2.34                     | 0.45              |
| 12:C:37:T6A:H2'   | 12:C:38:A:O4'     | 2.16                     | 0.45              |
| 14:F:163:TYR:HB2  | 14:F:171:ILE:HD11 | 1.99                     | 0.45              |
| 21:N:24:VAL:HG13  | 21:N:33:ALA:HB2   | 1.99                     | 0.45              |
| 34:a:791:G:N1     | 34:a:838:G:O2'    | 2.38                     | 0.45              |
| 34:a:1476:U:H2'   | 34:a:1477:U:C6    | 2.51                     | 0.45              |
| 42:i:52:ILE:N     | 42:i:52:ILE:HD12  | 2.32                     | 0.45              |
| 4:3:70:ARG:HB2    | 53:t:67:VAL:HG23  | 1.98                     | 0.45              |
| 42:i:25:LEU:HD23  | 42:i:64:LEU:HD21  | 1.99                     | 0.45              |
| 17:I:157:GLU:OE1  | 17:I:157:GLU:N    | 2.38                     | 0.45              |
| 34:a:430:G:O2'    | 34:a:524:A:N1     | 2.47                     | 0.45              |
| 38:e:53:GLU:HG3   | 38:e:194:LEU:HD12 | 1.97                     | 0.45              |
| 50:q:2:ALA:N      | 50:q:25:SER:HG    | 2.15                     | 0.45              |
| 1:0:101:TYR:HA    | 1:0:104:LEU:HD12  | 1.99                     | 0.44              |
| 10:A:225:A:N1     | 10:A:446:C:O2'    | 2.38                     | 0.44              |
| 10:A:2330:C:H2'   | 10:A:2331:G:O4'   | 2.17                     | 0.44              |
| 12:C:47:U:O3'     | 12:C:48:C:O4'     | 2.35                     | 0.44              |
| 19:K:102:LYS:HZ3  | 19:K:116:THR:HG23 | 1.81                     | 0.44              |
| 34:a:199:A:H1'    | 34:a:201:A:N7     | 2.32                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 34:a:406:G:N2     | 34:a:409:A:OP2    | 2.38                     | 0.44              |
| 1:0:121:TRP:HZ3   | 14:F:55:ALA:HB1   | 1.82                     | 0.44              |
| 10:A:429:A:HO2'   | 10:A:430:A:P      | 2.39                     | 0.44              |
| 10:A:2700:U:H2'   | 10:A:2701:G:O4'   | 2.17                     | 0.44              |
| 15:G:130:LEU:HD13 | 15:G:192:ILE:HD13 | 1.99                     | 0.44              |
| 17:I:152:VAL:CG1  | 17:I:173:VAL:HG22 | 2.48                     | 0.44              |
| 34:a:639:C:OP1    | 38:e:77:LYS:NZ    | 2.50                     | 0.44              |
| 10:A:83:G:N1      | 10:A:101:G:O2'    | 2.41                     | 0.44              |
| 10:A:115:C:H2'    | 10:A:116:G:O4'    | 2.17                     | 0.44              |
| 10:A:2867:G:N2    | 10:A:2870:A:OP2   | 2.50                     | 0.44              |
| 14:F:12:LEU:HD13  | 14:F:12:LEU:O     | 2.17                     | 0.44              |
| 34:a:388:G:N1     | 34:a:391:U:OP2    | 2.50                     | 0.44              |
| 52:s:38:SER:HB3   | 52:s:44:LEU:HD21  | 1.98                     | 0.44              |
| 1:0:30:GLY:N      | 1:0:222:ILE:HD12  | 2.33                     | 0.44              |
| 10:A:743:G:O2'    | 10:A:765:G:N2     | 2.39                     | 0.44              |
| 10:A:852:U:O5'    | 22:O:24:SER:OG    | 2.36                     | 0.44              |
| 13:D:7:G:H3'      | 13:D:8:U:H5'      | 1.99                     | 0.44              |
| 34:a:194:G:OP2    | 34:a:194:G:N2     | 2.42                     | 0.44              |
| 34:a:221:A:H2'    | 34:a:222:G:O4'    | 2.17                     | 0.44              |
| 34:a:1563:C:H42   | 35:b:3:A:N6       | 2.15                     | 0.44              |
| 10:A:2089:U:O2    | 10:A:2089:U:O4'   | 2.36                     | 0.44              |
| 24:Q:70:VAL:HG13  | 24:Q:82:VAL:HG13  | 2.00                     | 0.44              |
| 27:T:24:TYR:O     | 27:T:29:HIS:ND1   | 2.46                     | 0.44              |
| 1:0:460:LEU:C     | 1:0:460:LEU:HD23  | 2.42                     | 0.44              |
| 10:A:264:A:N3     | 10:A:469:A:O2'    | 2.45                     | 0.44              |
| 10:A:1413:A:O2'   | 10:A:1414:U:P     | 2.75                     | 0.44              |
| 10:A:2010:A:OP2   | 16:H:130:ARG:NH1  | 2.50                     | 0.44              |
| 14:F:26:ALA:CB    | 14:F:224:VAL:HG12 | 2.48                     | 0.44              |
| 14:F:87:ALA:HB2   | 14:F:149:VAL:HG21 | 1.99                     | 0.44              |
| 34:a:865:G:O2'    | 34:a:866:G:O5'    | 2.35                     | 0.44              |
| 38:e:62:GLY:O     | 38:e:112:ARG:NH1  | 2.50                     | 0.44              |
| 1:0:28:LYS:NZ     | 1:0:202:LYS:O     | 2.51                     | 0.44              |
| 10:A:32:C:N4      | 10:A:486:A:OP2    | 2.50                     | 0.44              |
| 10:A:1018:A:H2'   | 10:A:1021:C:H41   | 1.82                     | 0.44              |
| 34:a:227:A:HO2'   | 34:a:228:A:C5'    | 2.26                     | 0.44              |
| 37:d:93:LEU:C     | 37:d:93:LEU:HD13  | 2.42                     | 0.44              |
| 44:k:92:LEU:N     | 44:k:92:LEU:HD12  | 2.32                     | 0.44              |
| 10:A:162:A:OP2    | 10:A:163:U:O2'    | 2.23                     | 0.44              |
| 10:A:1518:G:O2'   | 10:A:1558:A:N6    | 2.47                     | 0.44              |
| 10:A:1978:C:OP1   | 10:A:1979:A:O2'   | 2.35                     | 0.44              |
| 19:K:86:ALA:C     | 19:K:87:LEU:HD12  | 2.43                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:Q:20:ILE:CG2   | 24:Q:40:VAL:HG21  | 2.47                     | 0.44              |
| 31:X:23:VAL:HG13  | 31:X:33:VAL:CG2   | 2.48                     | 0.44              |
| 34:a:272:A:C2     | 34:a:308:A:C5     | 3.06                     | 0.44              |
| 34:a:1104:G:N1    | 34:a:1107:A:OP2   | 2.50                     | 0.44              |
| 10:A:267:A:N1     | 10:A:466:U:O2'    | 2.47                     | 0.44              |
| 30:W:12:ILE:HD12  | 30:W:12:ILE:N     | 2.33                     | 0.44              |
| 34:a:346:G:H2'    | 34:a:347:A:O4'    | 2.17                     | 0.44              |
| 34:a:767:G:H2'    | 34:a:768:G:O4'    | 2.18                     | 0.44              |
| 34:a:1476:U:H2'   | 34:a:1477:U:O4'   | 2.18                     | 0.44              |
| 47:n:25:ILE:CD1   | 47:n:60:ILE:HD12  | 2.48                     | 0.44              |
| 51:r:61:ILE:O     | 51:r:82:VAL:N     | 2.51                     | 0.44              |
| 34:a:1392:C:OP1   | 43:j:119:LYS:NZ   | 2.51                     | 0.43              |
| 1:0:69:GLN:NE2    | 55:0:602:ATP:O2G  | 2.47                     | 0.43              |
| 8:7:43:GLN:NE2    | 10:A:2378:G:O6    | 2.50                     | 0.43              |
| 34:a:1207:G:O2'   | 34:a:1208:G:N7    | 2.47                     | 0.43              |
| 10:A:1123:A:O4'   | 10:A:1144:U:O2'   | 2.36                     | 0.43              |
| 10:A:1421:C:OP2   | 10:A:1431:U:N3    | 2.46                     | 0.43              |
| 10:A:2577:A:OP1   | 10:A:2661:G:O2'   | 2.20                     | 0.43              |
| 3:2:6:ILE:HG12    | 3:2:56:VAL:HG12   | 2.00                     | 0.43              |
| 10:A:231:U:H1'    | 10:A:232:U:O4'    | 2.19                     | 0.43              |
| 10:A:1108:A:H4'   | 10:A:1109:A:H2'   | 1.99                     | 0.43              |
| 44:k:29:ALA:O     | 44:k:32:THR:OG1   | 2.27                     | 0.43              |
| 7:6:16:HIS:ND1    | 10:A:723:G:OP1    | 2.52                     | 0.43              |
| 10:A:853:C:H1'    | 10:A:1261:G:H21   | 1.83                     | 0.43              |
| 10:A:1116:A:H2'   | 10:A:1117:C:O4'   | 2.19                     | 0.43              |
| 10:A:1883:U:P     | 10:A:1883:U:O2    | 2.76                     | 0.43              |
| 18:J:147:ASP:OD1  | 18:J:148:LYS:N    | 2.52                     | 0.43              |
| 41:h:7:VAL:HG22   | 41:h:8:ALA:N      | 2.33                     | 0.43              |
| 47:n:37:VAL:HG12  | 47:n:39:VAL:HG23  | 2.01                     | 0.43              |
| 9:8:7:VAL:HG23    | 9:8:7:VAL:O       | 2.18                     | 0.43              |
| 10:A:1310:A:H4'   | 10:A:1311:G:OP1   | 2.19                     | 0.43              |
| 10:A:2174:C:H2'   | 10:A:2175:G:O4'   | 2.18                     | 0.43              |
| 19:K:90:ILE:HD12  | 19:K:163:ARG:HD2  | 2.00                     | 0.43              |
| 34:a:494:C:O2     | 34:a:494:C:O4'    | 2.36                     | 0.43              |
| 34:a:1500:G:H2'   | 34:a:1501:G:C8    | 2.54                     | 0.43              |
| 36:c:187:VAL:CG2  | 36:c:199:VAL:HG23 | 2.48                     | 0.43              |
| 1:0:39:LYS:NZ     | 55:0:602:ATP:O1G  | 2.51                     | 0.43              |
| 10:A:1575:A:OP2   | 10:A:1583:G:N2    | 2.45                     | 0.43              |
| 10:A:1965:A:C2    | 21:N:22:ILE:HG23  | 2.53                     | 0.43              |
| 21:N:102:VAL:HG11 | 21:N:106:LEU:HD12 | 2.01                     | 0.43              |
| 34:a:391:U:H5'    | 34:a:392:C:OP1    | 2.19                     | 0.43              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 43:j:38:TYR:HB3   | 43:j:39:ILE:HD12 | 2.00                     | 0.43              |
| 44:k:10:LEU:N     | 44:k:10:LEU:HD12 | 2.34                     | 0.43              |
| 47:n:16:VAL:CG1   | 47:n:34:LEU:HD12 | 2.48                     | 0.43              |
| 1:0:79:THR:HG22   | 1:0:80:VAL:N     | 2.33                     | 0.43              |
| 4:3:45:LEU:HD13   | 4:3:45:LEU:C     | 2.44                     | 0.43              |
| 10:A:590:U:H2'    | 10:A:591:G:O4'   | 2.19                     | 0.43              |
| 10:A:2299:A:H4'   | 10:A:2300:A:O4'  | 2.19                     | 0.43              |
| 13:D:26:C:H2'     | 13:D:27:G:O4'    | 2.19                     | 0.43              |
| 14:F:56:ASP:N     | 14:F:56:ASP:OD1  | 2.50                     | 0.43              |
| 18:J:50:LEU:HD13  | 18:J:50:LEU:C    | 2.43                     | 0.43              |
| 34:a:432:G:O3'    | 38:e:3:ARG:NH2   | 2.47                     | 0.43              |
| 34:a:591:U:OP2    | 34:a:592:G:O2'   | 2.24                     | 0.43              |
| 34:a:865:G:C2'    | 34:a:866:G:O5'   | 2.67                     | 0.43              |
| 53:t:38:SER:HB2   | 53:t:71:LEU:HD12 | 2.01                     | 0.43              |
| 10:A:162:A:N1     | 10:A:2230:G:O2'  | 2.49                     | 0.43              |
| 10:A:333:U:OP1    | 31:X:90:LYS:NZ   | 2.52                     | 0.43              |
| 10:A:824:U:H2'    | 10:A:825:C:C6    | 2.54                     | 0.43              |
| 10:A:1362:C:H2'   | 10:A:1363:G:O4'  | 2.18                     | 0.43              |
| 10:A:1494:A:C8    | 10:A:1499:A:N6   | 2.87                     | 0.43              |
| 10:A:1941:A:H2'   | 10:A:1942:G:O4'  | 2.18                     | 0.43              |
| 10:A:2063:C:H2'   | 10:A:2064:A:O4'  | 2.19                     | 0.43              |
| 14:F:31:LYS:HA    | 14:F:34:ASN:OD1  | 2.19                     | 0.43              |
| 18:J:136:LEU:HD22 | 18:J:143:TYR:HA  | 2.01                     | 0.43              |
| 34:a:131:G:H1'    | 34:a:132:A:N7    | 2.34                     | 0.43              |
| 34:a:213:A:H2'    | 34:a:214:U:O4'   | 2.18                     | 0.43              |
| 34:a:543:G:N2     | 34:a:559:A:OP2   | 2.45                     | 0.43              |
| 34:a:1149:U:H2'   | 34:a:1150:A:O4'  | 2.18                     | 0.43              |
| 36:c:86:ARG:NH2   | 36:c:219:ASP:OD1 | 2.49                     | 0.43              |
| 10:A:1882:U:HO2'  | 10:A:1885:G:N2   | 2.17                     | 0.43              |
| 10:A:1982:A:O2'   | 10:A:1985:G:N3   | 2.42                     | 0.43              |
| 10:A:2164:U:H2'   | 10:A:2165:C:C6   | 2.54                     | 0.43              |
| 10:A:2172:G:H2'   | 10:A:2173:G:O4'  | 2.19                     | 0.43              |
| 14:F:49:ASN:ND2   | 14:F:205:LYS:O   | 2.52                     | 0.43              |
| 34:a:1176:U:O4    | 34:a:1177:A:N6   | 2.52                     | 0.43              |
| 15:G:144:ILE:O    | 15:G:153:GLN:N   | 2.40                     | 0.42              |
| 34:a:656:G:H2'    | 34:a:657:G:O4'   | 2.18                     | 0.42              |
| 34:a:843:C:C4     | 34:a:845:A:H1'   | 2.53                     | 0.42              |
| 46:m:17:GLU:OE1   | 46:m:18:LYS:N    | 2.50                     | 0.42              |
| 4:3:26:GLY:O      | 18:J:102:LYS:NZ  | 2.51                     | 0.42              |
| 10:A:1421:C:H2'   | 10:A:1422:A:C8   | 2.54                     | 0.42              |
| 10:A:1710:A:O2'   | 10:A:1716:G:N7   | 2.25                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:A:2120:C:O2    | 10:A:2120:C:H2'   | 2.19                     | 0.42              |
| 10:A:2263:G:OP1   | 10:A:2288:C:O2'   | 2.33                     | 0.42              |
| 17:I:123:LEU:C    | 17:I:123:LEU:HD13 | 2.45                     | 0.42              |
| 10:A:2513:U:O2'   | 10:A:2517:U:O2    | 2.36                     | 0.42              |
| 14:F:76:LEU:HD13  | 14:F:76:LEU:C     | 2.45                     | 0.42              |
| 19:K:121:VAL:HG12 | 19:K:122:THR:N    | 2.34                     | 0.42              |
| 24:Q:60:ARG:O     | 24:Q:64:THR:HG23  | 2.19                     | 0.42              |
| 34:a:938:U:OP2    | 46:m:107:ARG:NH2  | 2.52                     | 0.42              |
| 10:A:271:C:O2     | 10:A:271:C:H2'    | 2.20                     | 0.42              |
| 34:a:1003:G:P     | 34:a:1384:U:O2'   | 2.77                     | 0.42              |
| 34:a:1069:U:H2'   | 34:a:1070:G:C8    | 2.55                     | 0.42              |
| 50:q:6:ARG:HA     | 50:q:70:VAL:HG21  | 2.01                     | 0.42              |
| 3:2:11:SER:OG     | 10:A:1028:G:OP2   | 2.34                     | 0.42              |
| 10:A:2333:A:N3    | 10:A:2333:A:H2'   | 2.33                     | 0.42              |
| 10:A:2585:A:N7    | 16:H:149:VAL:HG11 | 2.34                     | 0.42              |
| 10:A:2809:U:H2'   | 10:A:2810:U:O4'   | 2.19                     | 0.42              |
| 15:G:130:LEU:HD12 | 15:G:130:LEU:N    | 2.33                     | 0.42              |
| 18:J:80:ARG:HG3   | 18:J:83:MET:HE3   | 2.00                     | 0.42              |
| 24:Q:113:ARG:O    | 24:Q:117:ALA:N    | 2.50                     | 0.42              |
| 51:r:26:VAL:O     | 51:r:46:LYS:HA    | 2.19                     | 0.42              |
| 10:A:360:A:N6     | 10:A:374:G:O2'    | 2.45                     | 0.42              |
| 10:A:716:A:O2'    | 10:A:2083:G:O2'   | 2.20                     | 0.42              |
| 10:A:2182:G:H2'   | 10:A:2183:G:O4'   | 2.19                     | 0.42              |
| 10:A:2285:U:OP2   | 32:Y:27:SER:OG    | 2.28                     | 0.42              |
| 24:Q:61:GLN:O     | 24:Q:64:THR:OG1   | 2.19                     | 0.42              |
| 45:l:97:ILE:HA    | 45:l:100:LEU:HD12 | 2.02                     | 0.42              |
| 47:n:23:TYR:CE1   | 47:n:69:LEU:HD23  | 2.55                     | 0.42              |
| 10:A:714:A:N3     | 10:A:2456:U:O2'   | 2.48                     | 0.42              |
| 10:A:1086:G:HO2'  | 10:A:1087:A:P     | 2.43                     | 0.42              |
| 10:A:1965:A:N3    | 10:A:2573:C:O2'   | 2.46                     | 0.42              |
| 10:A:2009:C:H4'   | 10:A:2010:A:OP1   | 2.20                     | 0.42              |
| 18:J:5:LYS:O      | 18:J:9:ILE:HG22   | 2.20                     | 0.42              |
| 25:R:11:ARG:HD2   | 25:R:98:TYR:CZ    | 2.54                     | 0.42              |
| 34:a:148:C:O2'    | 34:a:288:A:N3     | 2.43                     | 0.42              |
| 34:a:1183:A:C2    | 34:a:1207:G:C4    | 3.08                     | 0.42              |
| 34:a:1467:G:O2'   | 34:a:1487:A:N6    | 2.50                     | 0.42              |
| 53:t:55:ARG:O     | 53:t:56:LYS:HG3   | 2.19                     | 0.42              |
| 10:A:1108:A:O2'   | 10:A:1112:A:N7    | 2.46                     | 0.42              |
| 27:T:35:ALA:O     | 27:T:39:VAL:HG23  | 2.19                     | 0.42              |
| 34:a:397:G:H2'    | 34:a:398:C:O4'    | 2.20                     | 0.42              |
| 34:a:1519:A:H5''  | 46:m:57:LYS:HA    | 2.02                     | 0.42              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 44:k:32:THR:OG1  | 44:k:83:THR:HG22  | 2.19                     | 0.42              |
| 52:s:23:GLU:O    | 52:s:58:LYS:NZ    | 2.51                     | 0.42              |
| 1:0:173:LEU:HD13 | 1:0:200:TYR:CZ    | 2.55                     | 0.42              |
| 1:0:332:VAL:HG21 | 1:0:351:PHE:CZ    | 2.54                     | 0.42              |
| 10:A:1536:A:O2'  | 10:A:1537:A:OP1   | 2.37                     | 0.42              |
| 10:A:2517:U:O2   | 10:A:2517:U:O4'   | 2.38                     | 0.42              |
| 12:C:47:U:H2'    | 12:C:48:C:C6      | 2.55                     | 0.42              |
| 20:M:5:TYR:CG    | 27:T:100:VAL:HG11 | 2.55                     | 0.42              |
| 34:a:178:A:H2'   | 34:a:179:A:O4'    | 2.19                     | 0.42              |
| 34:a:1306:A:O2'  | 34:a:1307:U:H5''  | 2.20                     | 0.42              |
| 8:7:54:ASP:HB3   | 22:O:57:LEU:HD22  | 2.02                     | 0.42              |
| 10:A:844:G:N2    | 10:A:868:A:OP1    | 2.52                     | 0.42              |
| 10:A:969:U:H2'   | 10:A:970:U:O4'    | 2.20                     | 0.42              |
| 10:A:2802:C:O2'  | 10:A:2803:A:OP2   | 2.26                     | 0.42              |
| 10:A:2814:A:O2'  | 10:A:2815:A:H5'   | 2.20                     | 0.42              |
| 11:B:39:G:O6     | 18:J:69:LYS:NZ    | 2.43                     | 0.42              |
| 24:Q:18:ARG:NE   | 24:Q:65:PHE:O     | 2.44                     | 0.42              |
| 34:a:866:G:H2'   | 34:a:867:U:O4'    | 2.20                     | 0.42              |
| 34:a:1461:G:H2'  | 34:a:1462:U:C6    | 2.55                     | 0.42              |
| 45:l:16:ILE:HG22 | 45:l:17:GLU:N     | 2.35                     | 0.42              |
| 1:0:415:VAL:O    | 1:0:415:VAL:HG12  | 2.20                     | 0.41              |
| 10:A:214:C:H2'   | 10:A:215:A:O4'    | 2.19                     | 0.41              |
| 10:A:427:G:N3    | 10:A:429:A:N6     | 2.68                     | 0.41              |
| 10:A:518:A:H4'   | 10:A:519:A:OP1    | 2.19                     | 0.41              |
| 10:A:572:U:HO2'  | 27:T:49:ASP:CG    | 2.19                     | 0.41              |
| 10:A:1673:G:N2   | 10:A:1676:U:OP2   | 2.42                     | 0.41              |
| 10:A:2320:G:H4'  | 10:A:2321:G:O4'   | 2.20                     | 0.41              |
| 10:A:2810:U:O2'  | 10:A:2811:A:OP2   | 2.27                     | 0.41              |
| 14:F:43:GLU:HA   | 14:F:174:PRO:HA   | 2.02                     | 0.41              |
| 34:a:1543:G:N1   | 34:a:1546:A:OP2   | 2.53                     | 0.41              |
| 39:f:16:VAL:HG21 | 39:f:38:VAL:HG23  | 2.02                     | 0.41              |
| 10:A:48:G:N1     | 10:A:178:A:OP2    | 2.47                     | 0.41              |
| 10:A:346:A:O2'   | 10:A:347:A:OP2    | 2.29                     | 0.41              |
| 10:A:852:U:H2'   | 10:A:853:C:C6     | 2.55                     | 0.41              |
| 10:A:1165:A:H4'  | 10:A:1166:A:C5'   | 2.50                     | 0.41              |
| 10:A:1413:A:O2'  | 10:A:1414:U:C6    | 2.71                     | 0.41              |
| 10:A:1792:U:H5   | 10:A:1797:A:N7    | 2.18                     | 0.41              |
| 18:J:13:THR:O    | 18:J:17:VAL:HG23  | 2.20                     | 0.41              |
| 34:a:846:U:H4'   | 34:a:847:G:OP2    | 2.19                     | 0.41              |
| 34:a:1006:C:O2   | 34:a:1006:C:H2'   | 2.20                     | 0.41              |
| 10:A:995:G:N2    | 10:A:999:A:OP2    | 2.47                     | 0.41              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 10:A:1211:A:H2'  | 10:A:1214:A:H61    | 1.85                     | 0.41              |
| 10:A:1541:U:H2'  | 10:A:1542:U:O4'    | 2.20                     | 0.41              |
| 34:a:268:C:O2'   | 34:a:271:U:OP1     | 2.25                     | 0.41              |
| 34:a:1540:A:H2'  | 34:a:1541:U:C6     | 2.55                     | 0.41              |
| 36:c:210:VAL:O   | 36:c:214:THR:HG23  | 2.20                     | 0.41              |
| 1:0:29:VAL:HA    | 1:0:224:LYS:O      | 2.19                     | 0.41              |
| 1:0:456:LEU:HD13 | 1:0:484:ILE:CD1    | 2.50                     | 0.41              |
| 10:A:1758:G:H2'  | 10:A:1758:G:N3     | 2.35                     | 0.41              |
| 10:A:2087:U:O2'  | 10:A:2610:G:H1'    | 2.21                     | 0.41              |
| 10:A:2196:U:H2'  | 10:A:2197:G:O4'    | 2.20                     | 0.41              |
| 19:K:96:ALA:HB1  | 19:K:103:LEU:HD11  | 2.03                     | 0.41              |
| 34:a:1443:G:O2'  | 34:a:1510:A:N6     | 2.50                     | 0.41              |
| 34:a:1516:G:H2'  | 34:a:1517:U:O4'    | 2.20                     | 0.41              |
| 51:r:34:HIS:HA   | 51:r:41:MET:HE2    | 2.03                     | 0.41              |
| 1:0:26:PHE:N     | 1:0:207:SER:OG     | 2.46                     | 0.41              |
| 10:A:404:A:H2'   | 10:A:405:U:O4'     | 2.21                     | 0.41              |
| 10:A:1108:A:H5'' | 10:A:1109:A:H2'    | 2.03                     | 0.41              |
| 10:A:2815:A:O2'  | 10:A:2816:A:P      | 2.78                     | 0.41              |
| 15:G:39:ASN:ND2  | 15:G:56:GLY:O      | 2.54                     | 0.41              |
| 28:U:80:LYS:O    | 28:U:81:HIS:C      | 2.63                     | 0.41              |
| 29:V:7:SER:HB3   | 29:V:113:THR:HG22  | 2.03                     | 0.41              |
| 34:a:19:U:H2'    | 34:a:20:C:C6       | 2.55                     | 0.41              |
| 34:a:1062:G:O2'  | 34:a:1063:A:O5'    | 2.36                     | 0.41              |
| 47:n:71:ARG:O    | 47:n:75:LEU:HD13   | 2.19                     | 0.41              |
| 10:A:74:U:H5''   | 10:A:75:G:O4'      | 2.20                     | 0.41              |
| 10:A:230:A:H3'   | 10:A:231:U:O4'     | 2.21                     | 0.41              |
| 10:A:569:A:OP1   | 10:A:597:G:N2      | 2.53                     | 0.41              |
| 10:A:1536:A:H2'  | 10:A:1537:A:C8     | 2.56                     | 0.41              |
| 10:A:1642:C:OP1  | 30:W:76:ARG:NH1    | 2.53                     | 0.41              |
| 10:A:1656:A:N6   | 29:V:97:SER:O      | 2.38                     | 0.41              |
| 10:A:1696:A:O2'  | 16:H:119:PHE:O     | 2.36                     | 0.41              |
| 10:A:2051:G:H2'  | 10:A:2052:G:O4'    | 2.20                     | 0.41              |
| 12:C:44:G:C2'    | 12:C:45:G:O5'      | 2.69                     | 0.41              |
| 16:H:56:LYS:N    | 16:H:76:PRO:O      | 2.51                     | 0.41              |
| 32:Y:24:ASP:OD1  | 32:Y:25:SER:N      | 2.51                     | 0.41              |
| 34:a:1322:C:H4'  | 34:a:1328:U:O4     | 2.20                     | 0.41              |
| 10:A:2126:C:H2'  | 10:A:2127:A:O4'    | 2.20                     | 0.41              |
| 34:a:272:A:N1    | 34:a:304:C:O2'     | 2.51                     | 0.41              |
| 34:a:1091:G:OP1  | 59:a:1615:SCM:H1M1 | 2.20                     | 0.41              |
| 34:a:1340:C:OP2  | 53:t:4:SER:OG      | 2.35                     | 0.41              |
| 40:g:32:ILE:HD13 | 40:g:83:LEU:HD13   | 2.01                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:7:60:GLN:OE1    | 10:A:704:C:O2'    | 2.30                     | 0.41              |
| 10:A:665:A:N1     | 10:A:674:G:O2'    | 2.49                     | 0.41              |
| 16:H:31:THR:O     | 16:H:32:PRO:C     | 2.62                     | 0.41              |
| 26:S:20:PHE:O     | 26:S:50:ARG:NH1   | 2.53                     | 0.41              |
| 34:a:522:G:H21    | 34:a:523:A:H5''   | 1.84                     | 0.41              |
| 34:a:783:U:OP1    | 34:a:848:A:O2'    | 2.39                     | 0.41              |
| 34:a:1299:C:H2'   | 34:a:1300:A:O4'   | 2.21                     | 0.41              |
| 40:g:77:ILE:N     | 40:g:77:ILE:HD12  | 2.35                     | 0.41              |
| 1:0:69:GLN:NE2    | 1:0:184:GLN:OE1   | 2.54                     | 0.41              |
| 3:2:18:ASN:OD1    | 3:2:19:GLN:HG3    | 2.21                     | 0.41              |
| 5:4:3:VAL:HG12    | 10:A:2028:A:C2    | 2.56                     | 0.41              |
| 7:6:1:MET:HE2     | 7:6:3:ARG:NH2     | 2.36                     | 0.41              |
| 10:A:207:G:O2'    | 10:A:208:U:OP2    | 2.39                     | 0.41              |
| 10:A:608:A:H5''   | 10:A:609:G:OP2    | 2.21                     | 0.41              |
| 10:A:856:C:H2'    | 10:A:857:G:O4'    | 2.21                     | 0.41              |
| 10:A:1153:G:O2'   | 10:A:1154:A:H5'   | 2.20                     | 0.41              |
| 10:A:2442:G:OP2   | 10:A:2443:A:OP2   | 2.38                     | 0.41              |
| 10:A:2769:U:H4'   | 10:A:2770:A:OP1   | 2.21                     | 0.41              |
| 14:F:93:ASP:OD1   | 14:F:157:LYS:NZ   | 2.49                     | 0.41              |
| 17:I:126:VAL:HG11 | 17:I:146:LEU:HD11 | 2.03                     | 0.41              |
| 18:J:13:THR:HB    | 18:J:14:PRO:HD3   | 2.01                     | 0.41              |
| 27:T:66:ASN:O     | 27:T:70:ARG:HG2   | 2.20                     | 0.41              |
| 34:a:23:G:H2'     | 34:a:24:G:C8      | 2.56                     | 0.41              |
| 34:a:991:A:N3     | 34:a:996:A:O2'    | 2.47                     | 0.41              |
| 34:a:1217:A:H61   | 59:a:1615:SCM:H11 | 1.86                     | 0.41              |
| 34:a:1376:A:H2'   | 34:a:1377:U:O4'   | 2.21                     | 0.41              |
| 41:h:15:ASP:OD1   | 41:h:18:TYR:N     | 2.44                     | 0.41              |
| 45:l:50:LEU:HD11  | 45:l:66:ALA:HA    | 2.03                     | 0.41              |
| 10:A:309:G:O2'    | 10:A:310:A:P      | 2.78                     | 0.41              |
| 10:A:312:A:H2'    | 10:A:313:U:O4'    | 2.21                     | 0.41              |
| 10:A:357:A:O2'    | 10:A:376:A:N3     | 2.54                     | 0.41              |
| 10:A:1086:G:O2'   | 10:A:1087:A:P     | 2.79                     | 0.41              |
| 10:A:1429:U:H2'   | 10:A:1430:A:O4'   | 2.21                     | 0.41              |
| 24:Q:55:ASP:OD1   | 24:Q:55:ASP:N     | 2.47                     | 0.41              |
| 34:a:131:G:O2'    | 34:a:132:A:C8     | 2.74                     | 0.41              |
| 34:a:571:C:OP1    | 38:e:54:LYS:NZ    | 2.54                     | 0.41              |
| 34:a:860:U:OP1    | 52:s:46:ARG:NH2   | 2.53                     | 0.41              |
| 34:a:1048:G:H2'   | 34:a:1049:C:O4'   | 2.20                     | 0.41              |
| 34:a:1209:U:H3'   | 34:a:1210:G:C5'   | 2.52                     | 0.41              |
| 36:c:33:THR:O     | 36:c:40:ILE:N     | 2.50                     | 0.41              |
| 36:c:176:ALA:HB3  | 36:c:183:ILE:HD11 | 2.03                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 52:s:26:ASP:OD1  | 52:s:27:TYR:N     | 2.54                     | 0.41              |
| 10:A:1359:G:C4   | 10:A:1363:G:O6    | 2.74                     | 0.40              |
| 10:A:1392:C:H2'  | 10:A:1393:G:O4'   | 2.20                     | 0.40              |
| 10:A:2128:G:O2'  | 10:A:2179:G:N2    | 2.54                     | 0.40              |
| 13:D:9:G:O2'     | 13:D:10:G:N7      | 2.54                     | 0.40              |
| 34:a:1401:A:H2'  | 34:a:1402:U:O4'   | 2.21                     | 0.40              |
| 38:e:85:VAL:O    | 38:e:89:VAL:HG23  | 2.21                     | 0.40              |
| 39:f:152:GLU:O   | 39:f:156:LEU:HD13 | 2.21                     | 0.40              |
| 1:0:361:VAL:HB   | 1:0:498:VAL:HG22  | 2.03                     | 0.40              |
| 10:A:58:G:O2'    | 10:A:73:A:N1      | 2.52                     | 0.40              |
| 10:A:1636:A:H2'  | 10:A:1637:C:O4'   | 2.21                     | 0.40              |
| 10:A:1808:C:H2'  | 10:A:1809:U:O4'   | 2.21                     | 0.40              |
| 34:a:1165:G:H1'  | 34:a:1166:U:OP2   | 2.22                     | 0.40              |
| 47:n:25:ILE:HD11 | 47:n:60:ILE:HD12  | 2.03                     | 0.40              |
| 1:0:90:ILE:HD11  | 1:0:129:PHE:HB3   | 2.02                     | 0.40              |
| 10:A:83:G:OP1    | 31:X:90:LYS:NZ    | 2.44                     | 0.40              |
| 10:A:1622:C:H2'  | 10:A:1623:U:C1'   | 2.52                     | 0.40              |
| 10:A:2272:G:C8   | 10:A:2440:C:C4    | 3.10                     | 0.40              |
| 25:R:68:LYS:HB3  | 25:R:103:ARG:HD3  | 2.04                     | 0.40              |
| 32:Y:59:ASN:ND2  | 32:Y:90:VAL:O     | 2.44                     | 0.40              |
| 34:a:945:A:H2'   | 34:a:946:A:O4'    | 2.22                     | 0.40              |
| 52:s:36:PHE:CD1  | 52:s:49:THR:HG21  | 2.57                     | 0.40              |
| 4:3:77:LYS:HB3   | 4:3:78:TYR:CD1    | 2.56                     | 0.40              |
| 10:A:166:A:H2'   | 10:A:167:U:O4'    | 2.22                     | 0.40              |
| 10:A:1247:U:H3'  | 10:A:1248:G:H5'   | 2.04                     | 0.40              |
| 10:A:2002:A:H2'  | 10:A:2003:C:O4'   | 2.22                     | 0.40              |
| 25:R:92:VAL:HG13 | 25:R:92:VAL:O     | 2.22                     | 0.40              |
| 34:a:431:U:O2'   | 34:a:524:A:H3'    | 2.21                     | 0.40              |
| 34:a:1128:A:H5'' | 36:c:171:ILE:HD11 | 2.03                     | 0.40              |
| 36:c:114:LEU:O   | 36:c:117:ILE:HG22 | 2.21                     | 0.40              |
| 45:l:118:HIS:O   | 45:l:119:ASN:HB2  | 2.21                     | 0.40              |
| 7:6:30:VAL:O     | 7:6:34:ARG:HG2    | 2.22                     | 0.40              |
| 7:6:34:ARG:HD3   | 10:A:506:G:OP2    | 2.22                     | 0.40              |
| 10:A:46:C:OP2    | 10:A:217:G:OP2    | 2.39                     | 0.40              |
| 10:A:1023:G:H2'  | 10:A:1023:G:N3    | 2.36                     | 0.40              |
| 10:A:1211:A:H3'  | 10:A:1212:U:H5''  | 2.04                     | 0.40              |
| 10:A:2037:C:O3'  | 16:H:153:ARG:NE   | 2.55                     | 0.40              |
| 10:A:2275:U:OP2  | 32:Y:25:SER:OG    | 2.30                     | 0.40              |
| 10:A:2808:U:H3   | 10:A:2811:A:H62   | 1.69                     | 0.40              |
| 34:a:125:A:C6    | 34:a:352:G:C6     | 3.10                     | 0.40              |
| 34:a:1328:U:C5   | 47:n:17:VAL:HG21  | 2.57                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed      | Favoured   | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|------------|---------|----------|-------------|-----|
| 1   | 0     | 532/586 (91%) | 521 (98%)  | 11 (2%) | 0        | 100         | 100 |
| 2   | 1     | 57/62 (92%)   | 57 (100%)  | 0       | 0        | 100         | 100 |
| 3   | 2     | 55/59 (93%)   | 53 (96%)   | 2 (4%)  | 0        | 100         | 100 |
| 4   | 3     | 78/89 (88%)   | 77 (99%)   | 1 (1%)  | 0        | 100         | 100 |
| 5   | 4     | 51/59 (86%)   | 49 (96%)   | 2 (4%)  | 0        | 100         | 100 |
| 6   | 5     | 46/49 (94%)   | 43 (94%)   | 3 (6%)  | 0        | 100         | 100 |
| 7   | 6     | 42/44 (96%)   | 42 (100%)  | 0       | 0        | 100         | 100 |
| 8   | 7     | 62/66 (94%)   | 62 (100%)  | 0       | 0        | 100         | 100 |
| 9   | 8     | 36/38 (95%)   | 36 (100%)  | 0       | 0        | 100         | 100 |
| 14  | F     | 224/229 (98%) | 216 (96%)  | 8 (4%)  | 0        | 100         | 100 |
| 15  | G     | 272/276 (99%) | 265 (97%)  | 6 (2%)  | 1 (0%)   | 30          | 59  |
| 16  | H     | 204/209 (98%) | 194 (95%)  | 10 (5%) | 0        | 100         | 100 |
| 17  | I     | 203/207 (98%) | 200 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 18  | J     | 175/179 (98%) | 167 (95%)  | 8 (5%)  | 0        | 100         | 100 |
| 19  | K     | 172/178 (97%) | 165 (96%)  | 7 (4%)  | 0        | 100         | 100 |
| 20  | M     | 145/147 (99%) | 144 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 21  | N     | 120/122 (98%) | 117 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 22  | O     | 144/146 (99%) | 138 (96%)  | 5 (4%)  | 1 (1%)   | 18          | 48  |
| 23  | P     | 132/144 (92%) | 132 (100%) | 0       | 0        | 100         | 100 |
| 24  | Q     | 123/127 (97%) | 120 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 25  | R     | 116/118 (98%) | 113 (97%)  | 3 (3%)  | 0        | 100         | 100 |
| 26  | S     | 112/115 (97%) | 109 (97%)  | 3 (3%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 27  | T     | 116/119 (98%)   | 114 (98%)  | 2 (2%)   | 0        | 100         | 100 |
| 28  | U     | 99/102 (97%)    | 96 (97%)   | 3 (3%)   | 0        | 100         | 100 |
| 29  | V     | 109/115 (95%)   | 108 (99%)  | 1 (1%)   | 0        | 100         | 100 |
| 30  | W     | 89/96 (93%)     | 88 (99%)   | 1 (1%)   | 0        | 100         | 100 |
| 31  | X     | 99/103 (96%)    | 94 (95%)   | 5 (5%)   | 0        | 100         | 100 |
| 32  | Y     | 72/95 (76%)     | 70 (97%)   | 2 (3%)   | 0        | 100         | 100 |
| 33  | Z     | 59/62 (95%)     | 57 (97%)   | 2 (3%)   | 0        | 100         | 100 |
| 36  | c     | 220/261 (84%)   | 214 (97%)  | 6 (3%)   | 0        | 100         | 100 |
| 37  | d     | 203/218 (93%)   | 200 (98%)  | 3 (2%)   | 0        | 100         | 100 |
| 38  | e     | 198/203 (98%)   | 195 (98%)  | 3 (2%)   | 0        | 100         | 100 |
| 39  | f     | 161/166 (97%)   | 158 (98%)  | 3 (2%)   | 0        | 100         | 100 |
| 40  | g     | 94/100 (94%)    | 92 (98%)   | 2 (2%)   | 0        | 100         | 100 |
| 41  | h     | 151/156 (97%)   | 149 (99%)  | 2 (1%)   | 0        | 100         | 100 |
| 42  | i     | 129/132 (98%)   | 125 (97%)  | 4 (3%)   | 0        | 100         | 100 |
| 43  | j     | 125/130 (96%)   | 120 (96%)  | 5 (4%)   | 0        | 100         | 100 |
| 44  | k     | 94/102 (92%)    | 92 (98%)   | 2 (2%)   | 0        | 100         | 100 |
| 45  | l     | 114/129 (88%)   | 111 (97%)  | 3 (3%)   | 0        | 100         | 100 |
| 46  | m     | 132/137 (96%)   | 126 (96%)  | 6 (4%)   | 0        | 100         | 100 |
| 47  | n     | 112/121 (93%)   | 108 (96%)  | 4 (4%)   | 0        | 100         | 100 |
| 48  | o     | 58/61 (95%)     | 55 (95%)   | 3 (5%)   | 0        | 100         | 100 |
| 49  | p     | 83/89 (93%)     | 82 (99%)   | 1 (1%)   | 0        | 100         | 100 |
| 50  | q     | 85/91 (93%)     | 81 (95%)   | 4 (5%)   | 0        | 100         | 100 |
| 51  | r     | 78/88 (89%)     | 75 (96%)   | 3 (4%)   | 0        | 100         | 100 |
| 52  | s     | 61/79 (77%)     | 59 (97%)   | 2 (3%)   | 0        | 100         | 100 |
| 53  | t     | 80/92 (87%)     | 78 (98%)   | 2 (2%)   | 0        | 100         | 100 |
| 54  | u     | 79/83 (95%)     | 78 (99%)   | 1 (1%)   | 0        | 100         | 100 |
| All | All   | 6001/6379 (94%) | 5845 (97%) | 154 (3%) | 2 (0%)   | 100         | 100 |

All (2) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 22  | O     | 29  | LYS  |
| 15  | G     | 155 | ILE  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 1   | 0     | 489/533 (92%)  | 484 (99%)  | 5 (1%)   | 68          | 89  |
| 2   | 1     | 54/56 (96%)    | 53 (98%)   | 1 (2%)   | 50          | 79  |
| 3   | 2     | 48/50 (96%)    | 48 (100%)  | 0        | 100         | 100 |
| 4   | 3     | 72/79 (91%)    | 71 (99%)   | 1 (1%)   | 59          | 85  |
| 5   | 4     | 43/48 (90%)    | 43 (100%)  | 0        | 100         | 100 |
| 6   | 5     | 48/49 (98%)    | 47 (98%)   | 1 (2%)   | 47          | 77  |
| 7   | 6     | 39/39 (100%)   | 39 (100%)  | 0        | 100         | 100 |
| 8   | 7     | 51/53 (96%)    | 51 (100%)  | 0        | 100         | 100 |
| 9   | 8     | 35/35 (100%)   | 35 (100%)  | 0        | 100         | 100 |
| 14  | F     | 181/183 (99%)  | 174 (96%)  | 7 (4%)   | 28          | 63  |
| 15  | G     | 224/226 (99%)  | 224 (100%) | 0        | 100         | 100 |
| 16  | H     | 169/172 (98%)  | 169 (100%) | 0        | 100         | 100 |
| 17  | I     | 172/173 (99%)  | 171 (99%)  | 1 (1%)   | 78          | 93  |
| 18  | J     | 154/156 (99%)  | 154 (100%) | 0        | 100         | 100 |
| 19  | K     | 145/148 (98%)  | 145 (100%) | 0        | 100         | 100 |
| 20  | M     | 124/124 (100%) | 122 (98%)  | 2 (2%)   | 55          | 83  |
| 21  | N     | 98/98 (100%)   | 98 (100%)  | 0        | 100         | 100 |
| 22  | O     | 112/112 (100%) | 111 (99%)  | 1 (1%)   | 70          | 90  |
| 23  | P     | 107/114 (94%)  | 106 (99%)  | 1 (1%)   | 70          | 90  |
| 24  | Q     | 107/109 (98%)  | 107 (100%) | 0        | 100         | 100 |
| 25  | R     | 92/92 (100%)   | 91 (99%)   | 1 (1%)   | 65          | 88  |
| 26  | S     | 97/98 (99%)    | 97 (100%)  | 0        | 100         | 100 |
| 27  | T     | 94/95 (99%)    | 94 (100%)  | 0        | 100         | 100 |
| 28  | U     | 83/83 (100%)   | 83 (100%)  | 0        | 100         | 100 |
| 29  | V     | 94/98 (96%)    | 94 (100%)  | 0        | 100         | 100 |
| 30  | W     | 82/85 (96%)    | 81 (99%)   | 1 (1%)   | 63          | 86  |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 31  | X     | 85/87 (98%)     | 85 (100%)  | 0        | 100         | 100 |
| 32  | Y     | 59/75 (79%)     | 59 (100%)  | 0        | 100         | 100 |
| 33  | Z     | 54/55 (98%)     | 54 (100%)  | 0        | 100         | 100 |
| 36  | c     | 187/220 (85%)   | 187 (100%) | 0        | 100         | 100 |
| 37  | d     | 163/174 (94%)   | 162 (99%)  | 1 (1%)   | 78          | 93  |
| 38  | e     | 174/177 (98%)   | 172 (99%)  | 2 (1%)   | 65          | 88  |
| 39  | f     | 126/128 (98%)   | 126 (100%) | 0        | 100         | 100 |
| 40  | g     | 85/88 (97%)     | 85 (100%)  | 0        | 100         | 100 |
| 41  | h     | 130/133 (98%)   | 129 (99%)  | 1 (1%)   | 73          | 90  |
| 42  | i     | 112/113 (99%)   | 111 (99%)  | 1 (1%)   | 70          | 90  |
| 43  | j     | 100/102 (98%)   | 99 (99%)   | 1 (1%)   | 68          | 89  |
| 44  | k     | 87/92 (95%)     | 86 (99%)   | 1 (1%)   | 65          | 88  |
| 45  | l     | 90/101 (89%)    | 89 (99%)   | 1 (1%)   | 65          | 88  |
| 46  | m     | 117/119 (98%)   | 117 (100%) | 0        | 100         | 100 |
| 47  | n     | 98/102 (96%)    | 97 (99%)   | 1 (1%)   | 68          | 89  |
| 48  | o     | 51/52 (98%)     | 51 (100%)  | 0        | 100         | 100 |
| 49  | p     | 76/79 (96%)     | 76 (100%)  | 0        | 100         | 100 |
| 50  | q     | 77/81 (95%)     | 77 (100%)  | 0        | 100         | 100 |
| 51  | r     | 74/81 (91%)     | 72 (97%)   | 2 (3%)   | 39          | 73  |
| 52  | s     | 54/67 (81%)     | 54 (100%)  | 0        | 100         | 100 |
| 53  | t     | 70/79 (89%)     | 70 (100%)  | 0        | 100         | 100 |
| 54  | u     | 62/64 (97%)     | 61 (98%)   | 1 (2%)   | 55          | 83  |
| All | All   | 5145/5377 (96%) | 5111 (99%) | 34 (1%)  | 73          | 92  |

All (34) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 0     | 88  | ARG  |
| 1   | 0     | 152 | PHE  |
| 1   | 0     | 245 | TYR  |
| 1   | 0     | 289 | ARG  |
| 1   | 0     | 346 | TYR  |
| 2   | 1     | 58  | ARG  |
| 4   | 3     | 46  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | 5     | 21  | LYS  |
| 14  | F     | 74  | THR  |
| 14  | F     | 83  | LYS  |
| 14  | F     | 109 | PHE  |
| 14  | F     | 110 | ASP  |
| 14  | F     | 166 | ASP  |
| 14  | F     | 170 | ASN  |
| 14  | F     | 186 | VAL  |
| 17  | I     | 49  | HIS  |
| 20  | M     | 40  | LYS  |
| 20  | M     | 53  | ASP  |
| 22  | O     | 1   | MET  |
| 23  | P     | 54  | MET  |
| 25  | R     | 67  | THR  |
| 30  | W     | 56  | LEU  |
| 37  | d     | 87  | ARG  |
| 38  | e     | 25  | GLU  |
| 38  | e     | 31  | TYR  |
| 41  | h     | 15  | ASP  |
| 42  | i     | 77  | LEU  |
| 43  | j     | 85  | ARG  |
| 44  | k     | 71  | LYS  |
| 45  | l     | 77  | HIS  |
| 47  | n     | 107 | ARG  |
| 51  | r     | 42  | LYS  |
| 51  | r     | 60  | ASP  |
| 54  | u     | 70  | LYS  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 0     | 22  | HIS  |
| 1   | 0     | 275 | GLN  |
| 1   | 0     | 279 | GLN  |
| 1   | 0     | 285 | HIS  |
| 1   | 0     | 475 | HIS  |
| 3   | 2     | 40  | ASN  |
| 6   | 5     | 33  | GLN  |
| 8   | 7     | 61  | GLN  |
| 9   | 8     | 13  | HIS  |
| 14  | F     | 170 | ASN  |
| 14  | F     | 211 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 14  | F     | 223 | HIS  |
| 16  | H     | 128 | GLN  |
| 17  | I     | 121 | ASN  |
| 17  | I     | 160 | ASN  |
| 17  | I     | 169 | ASN  |
| 20  | M     | 137 | GLN  |
| 21  | N     | 34  | ASN  |
| 22  | O     | 17  | ASN  |
| 24  | Q     | 27  | ASN  |
| 24  | Q     | 61  | GLN  |
| 24  | Q     | 87  | GLN  |
| 27  | T     | 72  | ASN  |
| 29  | V     | 65  | ASN  |
| 36  | c     | 59  | ASN  |
| 37  | d     | 85  | ASN  |
| 38  | e     | 59  | HIS  |
| 40  | g     | 67  | ASN  |
| 42  | i     | 99  | ASN  |
| 45  | l     | 119 | ASN  |
| 46  | m     | 125 | GLN  |
| 50  | q     | 72  | ASN  |
| 53  | t     | 23  | GLN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 10  | A     | 2898/2912 (99%) | 433 (14%)         | 21 (0%)         |
| 11  | B     | 113/116 (97%)   | 20 (17%)          | 0               |
| 12  | C     | 69/76 (90%)     | 20 (28%)          | 1 (1%)          |
| 13  | D     | 75/77 (97%)     | 13 (17%)          | 1 (1%)          |
| 34  | a     | 1518/1558 (97%) | 218 (14%)         | 0               |
| 35  | b     | 11/19 (57%)     | 0                 | 0               |
| All | All   | 4684/4758 (98%) | 704 (15%)         | 23 (0%)         |

All (704) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10  | A     | 10  | A    |
| 10  | A     | 15  | G    |
| 10  | A     | 34  | U    |
| 10  | A     | 46  | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10  | A     | 55  | G    |
| 10  | A     | 61  | A    |
| 10  | A     | 62  | C    |
| 10  | A     | 63  | U    |
| 10  | A     | 71  | A    |
| 10  | A     | 74  | U    |
| 10  | A     | 75  | G    |
| 10  | A     | 93  | U    |
| 10  | A     | 101 | G    |
| 10  | A     | 117 | A    |
| 10  | A     | 118 | A    |
| 10  | A     | 119 | U    |
| 10  | A     | 130 | A    |
| 10  | A     | 161 | A    |
| 10  | A     | 164 | A    |
| 10  | A     | 169 | G    |
| 10  | A     | 177 | G    |
| 10  | A     | 182 | A    |
| 10  | A     | 198 | A    |
| 10  | A     | 201 | A    |
| 10  | A     | 215 | A    |
| 10  | A     | 218 | A    |
| 10  | A     | 224 | A    |
| 10  | A     | 225 | A    |
| 10  | A     | 230 | A    |
| 10  | A     | 231 | U    |
| 10  | A     | 232 | U    |
| 10  | A     | 247 | G    |
| 10  | A     | 250 | G    |
| 10  | A     | 251 | C    |
| 10  | A     | 252 | G    |
| 10  | A     | 257 | A    |
| 10  | A     | 268 | G    |
| 10  | A     | 269 | C    |
| 10  | A     | 282 | G    |
| 10  | A     | 289 | U    |
| 10  | A     | 290 | G    |
| 10  | A     | 295 | G    |
| 10  | A     | 296 | G    |
| 10  | A     | 299 | G    |
| 10  | A     | 300 | U    |
| 10  | A     | 301 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10  | A     | 308 | C    |
| 10  | A     | 309 | G    |
| 10  | A     | 310 | A    |
| 10  | A     | 311 | U    |
| 10  | A     | 312 | A    |
| 10  | A     | 317 | A    |
| 10  | A     | 318 | G    |
| 10  | A     | 320 | C    |
| 10  | A     | 321 | U    |
| 10  | A     | 339 | A    |
| 10  | A     | 347 | A    |
| 10  | A     | 352 | C    |
| 10  | A     | 353 | G    |
| 10  | A     | 366 | A    |
| 10  | A     | 389 | A    |
| 10  | A     | 398 | A    |
| 10  | A     | 402 | G    |
| 10  | A     | 403 | G    |
| 10  | A     | 404 | A    |
| 10  | A     | 410 | A    |
| 10  | A     | 411 | G    |
| 10  | A     | 425 | G    |
| 10  | A     | 430 | A    |
| 10  | A     | 440 | A    |
| 10  | A     | 445 | G    |
| 10  | A     | 450 | G    |
| 10  | A     | 451 | A    |
| 10  | A     | 474 | C    |
| 10  | A     | 479 | G    |
| 10  | A     | 495 | C    |
| 10  | A     | 496 | A    |
| 10  | A     | 509 | A    |
| 10  | A     | 520 | G    |
| 10  | A     | 529 | A    |
| 10  | A     | 534 | G    |
| 10  | A     | 543 | A    |
| 10  | A     | 546 | U    |
| 10  | A     | 547 | C    |
| 10  | A     | 560 | G    |
| 10  | A     | 568 | C    |
| 10  | A     | 569 | A    |
| 10  | A     | 570 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10  | A     | 571 | G    |
| 10  | A     | 581 | G    |
| 10  | A     | 582 | U    |
| 10  | A     | 583 | U    |
| 10  | A     | 584 | A    |
| 10  | A     | 585 | A    |
| 10  | A     | 587 | G    |
| 10  | A     | 599 | G    |
| 10  | A     | 609 | G    |
| 10  | A     | 611 | A    |
| 10  | A     | 639 | A    |
| 10  | A     | 650 | A    |
| 10  | A     | 651 | A    |
| 10  | A     | 665 | A    |
| 10  | A     | 675 | A    |
| 10  | A     | 683 | U    |
| 10  | A     | 684 | A    |
| 10  | A     | 691 | A    |
| 10  | A     | 692 | U    |
| 10  | A     | 694 | A    |
| 10  | A     | 716 | A    |
| 10  | A     | 725 | U    |
| 10  | A     | 754 | A    |
| 10  | A     | 756 | A    |
| 10  | A     | 768 | G    |
| 10  | A     | 769 | A    |
| 10  | A     | 786 | U    |
| 10  | A     | 803 | A    |
| 10  | A     | 804 | G    |
| 10  | A     | 814 | G    |
| 10  | A     | 815 | C    |
| 10  | A     | 821 | A    |
| 10  | A     | 823 | U    |
| 10  | A     | 829 | A    |
| 10  | A     | 844 | G    |
| 10  | A     | 851 | C    |
| 10  | A     | 858 | A    |
| 10  | A     | 866 | U    |
| 10  | A     | 867 | U    |
| 10  | A     | 885 | U    |
| 10  | A     | 886 | G    |
| 10  | A     | 899 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 10  | A     | 922  | G    |
| 10  | A     | 923  | C    |
| 10  | A     | 926  | A    |
| 10  | A     | 928  | C    |
| 10  | A     | 929  | U    |
| 10  | A     | 930  | C    |
| 10  | A     | 931  | G    |
| 10  | A     | 933  | G    |
| 10  | A     | 934  | U    |
| 10  | A     | 935  | U    |
| 10  | A     | 936  | A    |
| 10  | A     | 937  | C    |
| 10  | A     | 950  | A    |
| 10  | A     | 952  | C    |
| 10  | A     | 954  | C    |
| 10  | A     | 957  | A    |
| 10  | A     | 965  | U    |
| 10  | A     | 966  | C    |
| 10  | A     | 972  | U    |
| 10  | A     | 974  | U    |
| 10  | A     | 984  | A    |
| 10  | A     | 985  | G    |
| 10  | A     | 1000 | G    |
| 10  | A     | 1013 | A    |
| 10  | A     | 1022 | A    |
| 10  | A     | 1035 | A    |
| 10  | A     | 1051 | U    |
| 10  | A     | 1052 | A    |
| 10  | A     | 1064 | G    |
| 10  | A     | 1065 | A    |
| 10  | A     | 1066 | A    |
| 10  | A     | 1072 | U    |
| 10  | A     | 1085 | A    |
| 10  | A     | 1086 | G    |
| 10  | A     | 1101 | G    |
| 10  | A     | 1109 | A    |
| 10  | A     | 1110 | G    |
| 10  | A     | 1111 | C    |
| 10  | A     | 1115 | C    |
| 10  | A     | 1122 | U    |
| 10  | A     | 1123 | A    |
| 10  | A     | 1126 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 10  | A     | 1127 | A    |
| 10  | A     | 1151 | G    |
| 10  | A     | 1155 | C    |
| 10  | A     | 1167 | A    |
| 10  | A     | 1171 | U    |
| 10  | A     | 1172 | A    |
| 10  | A     | 1174 | C    |
| 10  | A     | 1175 | G    |
| 10  | A     | 1181 | A    |
| 10  | A     | 1182 | A    |
| 10  | A     | 1190 | A    |
| 10  | A     | 1196 | G    |
| 10  | A     | 1212 | U    |
| 10  | A     | 1213 | U    |
| 10  | A     | 1243 | G    |
| 10  | A     | 1248 | G    |
| 10  | A     | 1272 | G    |
| 10  | A     | 1274 | G    |
| 10  | A     | 1286 | G    |
| 10  | A     | 1289 | A    |
| 10  | A     | 1292 | G    |
| 10  | A     | 1307 | G    |
| 10  | A     | 1308 | A    |
| 10  | A     | 1310 | A    |
| 10  | A     | 1311 | G    |
| 10  | A     | 1335 | U    |
| 10  | A     | 1336 | A    |
| 10  | A     | 1338 | G    |
| 10  | A     | 1341 | U    |
| 10  | A     | 1364 | U    |
| 10  | A     | 1380 | C    |
| 10  | A     | 1385 | C    |
| 10  | A     | 1387 | U    |
| 10  | A     | 1395 | G    |
| 10  | A     | 1400 | A    |
| 10  | A     | 1413 | A    |
| 10  | A     | 1414 | U    |
| 10  | A     | 1421 | C    |
| 10  | A     | 1430 | A    |
| 10  | A     | 1431 | U    |
| 10  | A     | 1451 | G    |
| 10  | A     | 1454 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 10  | A     | 1455 | G    |
| 10  | A     | 1460 | A    |
| 10  | A     | 1461 | U    |
| 10  | A     | 1468 | A    |
| 10  | A     | 1469 | C    |
| 10  | A     | 1474 | U    |
| 10  | A     | 1495 | U    |
| 10  | A     | 1496 | U    |
| 10  | A     | 1497 | G    |
| 10  | A     | 1500 | A    |
| 10  | A     | 1503 | G    |
| 10  | A     | 1509 | C    |
| 10  | A     | 1511 | A    |
| 10  | A     | 1520 | G    |
| 10  | A     | 1524 | U    |
| 10  | A     | 1530 | G    |
| 10  | A     | 1534 | U    |
| 10  | A     | 1535 | A    |
| 10  | A     | 1536 | A    |
| 10  | A     | 1537 | A    |
| 10  | A     | 1538 | U    |
| 10  | A     | 1546 | U    |
| 10  | A     | 1550 | U    |
| 10  | A     | 1551 | A    |
| 10  | A     | 1564 | G    |
| 10  | A     | 1565 | A    |
| 10  | A     | 1567 | G    |
| 10  | A     | 1575 | A    |
| 10  | A     | 1576 | A    |
| 10  | A     | 1583 | G    |
| 10  | A     | 1584 | U    |
| 10  | A     | 1600 | G    |
| 10  | A     | 1604 | C    |
| 10  | A     | 1614 | A    |
| 10  | A     | 1621 | U    |
| 10  | A     | 1623 | U    |
| 10  | A     | 1627 | G    |
| 10  | A     | 1628 | A    |
| 10  | A     | 1629 | G    |
| 10  | A     | 1649 | U    |
| 10  | A     | 1650 | A    |
| 10  | A     | 1652 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 10  | A     | 1688 | A    |
| 10  | A     | 1689 | G    |
| 10  | A     | 1690 | C    |
| 10  | A     | 1716 | G    |
| 10  | A     | 1742 | A    |
| 10  | A     | 1756 | U    |
| 10  | A     | 1757 | C    |
| 10  | A     | 1758 | G    |
| 10  | A     | 1759 | G    |
| 10  | A     | 1769 | G    |
| 10  | A     | 1775 | A    |
| 10  | A     | 1776 | G    |
| 10  | A     | 1777 | G    |
| 10  | A     | 1786 | A    |
| 10  | A     | 1795 | C    |
| 10  | A     | 1804 | A    |
| 10  | A     | 1813 | C    |
| 10  | A     | 1814 | A    |
| 10  | A     | 1828 | A    |
| 10  | A     | 1829 | A    |
| 10  | A     | 1830 | G    |
| 10  | A     | 1842 | A    |
| 10  | A     | 1860 | A    |
| 10  | A     | 1873 | U    |
| 10  | A     | 1883 | U    |
| 10  | A     | 1884 | C    |
| 10  | A     | 1885 | G    |
| 10  | A     | 1886 | G    |
| 10  | A     | 1919 | G    |
| 10  | A     | 1929 | A    |
| 10  | A     | 1935 | G    |
| 10  | A     | 1942 | G    |
| 10  | A     | 1943 | G    |
| 10  | A     | 1949 | A    |
| 10  | A     | 1951 | A    |
| 10  | A     | 1953 | U    |
| 10  | A     | 1968 | U    |
| 10  | A     | 1976 | C    |
| 10  | A     | 1980 | C    |
| 10  | A     | 1983 | A    |
| 10  | A     | 1984 | A    |
| 10  | A     | 1985 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 10  | A     | 2004 | U    |
| 10  | A     | 2006 | U    |
| 10  | A     | 2009 | C    |
| 10  | A     | 2010 | A    |
| 10  | A     | 2034 | G    |
| 10  | A     | 2036 | A    |
| 10  | A     | 2044 | A    |
| 10  | A     | 2045 | G    |
| 10  | A     | 2046 | A    |
| 10  | A     | 2056 | C    |
| 10  | A     | 2068 | C    |
| 10  | A     | 2069 | G    |
| 10  | A     | 2073 | A    |
| 10  | A     | 2074 | G    |
| 10  | A     | 2075 | A    |
| 10  | A     | 2082 | G    |
| 10  | A     | 2096 | G    |
| 10  | A     | 2106 | G    |
| 10  | A     | 2108 | G    |
| 10  | A     | 2112 | U    |
| 10  | A     | 2120 | C    |
| 10  | A     | 2121 | A    |
| 10  | A     | 2124 | U    |
| 10  | A     | 2129 | G    |
| 10  | A     | 2130 | A    |
| 10  | A     | 2145 | U    |
| 10  | A     | 2146 | G    |
| 10  | A     | 2158 | C    |
| 10  | A     | 2161 | G    |
| 10  | A     | 2171 | A    |
| 10  | A     | 2172 | G    |
| 10  | A     | 2173 | G    |
| 10  | A     | 2185 | U    |
| 10  | A     | 2186 | A    |
| 10  | A     | 2191 | C    |
| 10  | A     | 2196 | U    |
| 10  | A     | 2201 | U    |
| 10  | A     | 2207 | C    |
| 10  | A     | 2211 | A    |
| 10  | A     | 2212 | A    |
| 10  | A     | 2216 | G    |
| 10  | A     | 2217 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 10  | A     | 2224 | A    |
| 10  | A     | 2225 | A    |
| 10  | A     | 2227 | C    |
| 10  | A     | 2238 | A    |
| 10  | A     | 2251 | G    |
| 10  | A     | 2252 | G    |
| 10  | A     | 2259 | G    |
| 10  | A     | 2281 | A    |
| 10  | A     | 2292 | G    |
| 10  | A     | 2296 | C    |
| 10  | A     | 2300 | A    |
| 10  | A     | 2301 | A    |
| 10  | A     | 2312 | G    |
| 10  | A     | 2318 | U    |
| 10  | A     | 2319 | U    |
| 10  | A     | 2320 | G    |
| 10  | A     | 2321 | G    |
| 10  | A     | 2322 | A    |
| 10  | A     | 2333 | A    |
| 10  | A     | 2335 | A    |
| 10  | A     | 2338 | G    |
| 10  | A     | 2347 | G    |
| 10  | A     | 2348 | A    |
| 10  | A     | 2360 | C    |
| 10  | A     | 2363 | C    |
| 10  | A     | 2392 | G    |
| 10  | A     | 2396 | G    |
| 10  | A     | 2398 | C    |
| 10  | A     | 2415 | U    |
| 10  | A     | 2435 | C    |
| 10  | A     | 2437 | C    |
| 10  | A     | 2438 | A    |
| 10  | A     | 2442 | G    |
| 10  | A     | 2443 | A    |
| 10  | A     | 2448 | A    |
| 10  | A     | 2454 | C    |
| 10  | A     | 2461 | A    |
| 10  | A     | 2478 | C    |
| 10  | A     | 2482 | A    |
| 10  | A     | 2487 | C    |
| 10  | A     | 2489 | A    |
| 10  | A     | 2491 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 10  | A     | 2511 | C    |
| 10  | A     | 2515 | G    |
| 10  | A     | 2517 | U    |
| 10  | A     | 2518 | G    |
| 10  | A     | 2531 | A    |
| 10  | A     | 2533 | C    |
| 10  | A     | 2542 | G    |
| 10  | A     | 2548 | G    |
| 10  | A     | 2561 | G    |
| 10  | A     | 2567 | U    |
| 10  | A     | 2579 | A    |
| 10  | A     | 2580 | G    |
| 10  | A     | 2591 | G    |
| 10  | A     | 2597 | U    |
| 10  | A     | 2599 | C    |
| 10  | A     | 2615 | A    |
| 10  | A     | 2622 | U    |
| 10  | A     | 2626 | U    |
| 10  | A     | 2628 | U    |
| 10  | A     | 2642 | U    |
| 10  | A     | 2643 | G    |
| 10  | A     | 2674 | G    |
| 10  | A     | 2676 | G    |
| 10  | A     | 2702 | U    |
| 10  | A     | 2727 | G    |
| 10  | A     | 2739 | U    |
| 10  | A     | 2746 | A    |
| 10  | A     | 2747 | A    |
| 10  | A     | 2761 | A    |
| 10  | A     | 2791 | A    |
| 10  | A     | 2792 | U    |
| 10  | A     | 2793 | G    |
| 10  | A     | 2803 | A    |
| 10  | A     | 2804 | U    |
| 10  | A     | 2809 | U    |
| 10  | A     | 2810 | U    |
| 10  | A     | 2811 | A    |
| 10  | A     | 2812 | A    |
| 10  | A     | 2813 | G    |
| 10  | A     | 2816 | A    |
| 10  | A     | 2818 | U    |
| 10  | A     | 2830 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 10  | A     | 2843 | A    |
| 10  | A     | 2844 | G    |
| 10  | A     | 2871 | U    |
| 10  | A     | 2877 | G    |
| 10  | A     | 2878 | A    |
| 10  | A     | 2882 | G    |
| 10  | A     | 2890 | C    |
| 10  | A     | 2903 | G    |
| 10  | A     | 2909 | A    |
| 11  | B     | 5    | G    |
| 11  | B     | 7    | G    |
| 11  | B     | 10   | G    |
| 11  | B     | 13   | A    |
| 11  | B     | 23   | A    |
| 11  | B     | 28   | C    |
| 11  | B     | 33   | U    |
| 11  | B     | 35   | C    |
| 11  | B     | 39   | G    |
| 11  | B     | 40   | C    |
| 11  | B     | 54   | U    |
| 11  | B     | 55   | A    |
| 11  | B     | 64   | A    |
| 11  | B     | 65   | G    |
| 11  | B     | 87   | U    |
| 11  | B     | 88   | C    |
| 11  | B     | 97   | A    |
| 11  | B     | 101  | U    |
| 11  | B     | 107  | G    |
| 11  | B     | 108  | U    |
| 12  | C     | 6    | G    |
| 12  | C     | 11   | C    |
| 12  | C     | 12   | U    |
| 12  | C     | 14   | A    |
| 12  | C     | 18   | G    |
| 12  | C     | 30   | G    |
| 12  | C     | 31   | A    |
| 12  | C     | 45   | G    |
| 12  | C     | 46   | G    |
| 12  | C     | 47   | U    |
| 12  | C     | 48   | C    |
| 12  | C     | 62   | C    |
| 12  | C     | 63   | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 12  | C     | 68  | G    |
| 12  | C     | 70  | C    |
| 12  | C     | 71  | U    |
| 12  | C     | 72  | C    |
| 12  | C     | 73  | A    |
| 12  | C     | 74  | C    |
| 12  | C     | 76  | A    |
| 13  | D     | 6   | G    |
| 13  | D     | 8   | U    |
| 13  | D     | 11  | A    |
| 13  | D     | 14  | A    |
| 13  | D     | 16  | U    |
| 13  | D     | 17  | C    |
| 13  | D     | 19  | G    |
| 13  | D     | 21  | U    |
| 13  | D     | 22  | A    |
| 13  | D     | 23  | G    |
| 13  | D     | 47  | G    |
| 13  | D     | 48  | U    |
| 13  | D     | 50  | G    |
| 34  | a     | 10  | A    |
| 34  | a     | 11  | G    |
| 34  | a     | 34  | A    |
| 34  | a     | 41  | G    |
| 34  | a     | 49  | C    |
| 34  | a     | 50  | C    |
| 34  | a     | 53  | A    |
| 34  | a     | 57  | A    |
| 34  | a     | 75  | U    |
| 34  | a     | 117 | A    |
| 34  | a     | 118 | G    |
| 34  | a     | 132 | A    |
| 34  | a     | 135 | A    |
| 34  | a     | 136 | A    |
| 34  | a     | 137 | C    |
| 34  | a     | 146 | A    |
| 34  | a     | 161 | G    |
| 34  | a     | 163 | G    |
| 34  | a     | 168 | A    |
| 34  | a     | 172 | C    |
| 34  | a     | 179 | A    |
| 34  | a     | 180 | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 34  | a     | 181 | A    |
| 34  | a     | 182 | G    |
| 34  | a     | 190 | U    |
| 34  | a     | 191 | A    |
| 34  | a     | 200 | C    |
| 34  | a     | 213 | A    |
| 34  | a     | 215 | G    |
| 34  | a     | 227 | A    |
| 34  | a     | 228 | A    |
| 34  | a     | 229 | A    |
| 34  | a     | 230 | G    |
| 34  | a     | 271 | U    |
| 34  | a     | 273 | G    |
| 34  | a     | 277 | G    |
| 34  | a     | 292 | G    |
| 34  | a     | 293 | C    |
| 34  | a     | 297 | C    |
| 34  | a     | 299 | A    |
| 34  | a     | 315 | G    |
| 34  | a     | 332 | A    |
| 34  | a     | 354 | C    |
| 34  | a     | 355 | A    |
| 34  | a     | 358 | G    |
| 34  | a     | 370 | A    |
| 34  | a     | 378 | C    |
| 34  | a     | 380 | G    |
| 34  | a     | 391 | U    |
| 34  | a     | 392 | C    |
| 34  | a     | 393 | U    |
| 34  | a     | 398 | C    |
| 34  | a     | 399 | A    |
| 34  | a     | 417 | C    |
| 34  | a     | 418 | G    |
| 34  | a     | 423 | A    |
| 34  | a     | 430 | G    |
| 34  | a     | 432 | G    |
| 34  | a     | 438 | A    |
| 34  | a     | 439 | G    |
| 34  | a     | 440 | A    |
| 34  | a     | 441 | A    |
| 34  | a     | 442 | G    |
| 34  | a     | 446 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 34  | a     | 447 | U    |
| 34  | a     | 448 | C    |
| 34  | a     | 450 | G    |
| 34  | a     | 455 | U    |
| 34  | a     | 465 | U    |
| 34  | a     | 470 | A    |
| 34  | a     | 471 | G    |
| 34  | a     | 478 | A    |
| 34  | a     | 479 | C    |
| 34  | a     | 485 | C    |
| 34  | a     | 488 | U    |
| 34  | a     | 492 | A    |
| 34  | a     | 494 | C    |
| 34  | a     | 495 | U    |
| 34  | a     | 510 | G    |
| 34  | a     | 511 | G    |
| 34  | a     | 523 | A    |
| 34  | a     | 524 | A    |
| 34  | a     | 537 | C    |
| 34  | a     | 544 | C    |
| 34  | a     | 547 | G    |
| 34  | a     | 553 | G    |
| 34  | a     | 556 | G    |
| 34  | a     | 557 | U    |
| 34  | a     | 567 | G    |
| 34  | a     | 573 | A    |
| 34  | a     | 585 | A    |
| 34  | a     | 588 | U    |
| 34  | a     | 590 | U    |
| 34  | a     | 598 | A    |
| 34  | a     | 599 | A    |
| 34  | a     | 602 | C    |
| 34  | a     | 603 | G    |
| 34  | a     | 640 | C    |
| 34  | a     | 644 | C    |
| 34  | a     | 659 | U    |
| 34  | a     | 679 | U    |
| 34  | a     | 691 | A    |
| 34  | a     | 713 | A    |
| 34  | a     | 714 | G    |
| 34  | a     | 736 | G    |
| 34  | a     | 749 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 34  | a     | 750  | G    |
| 34  | a     | 757  | G    |
| 34  | a     | 787  | G    |
| 34  | a     | 818  | A    |
| 34  | a     | 819  | U    |
| 34  | a     | 820  | A    |
| 34  | a     | 841  | A    |
| 34  | a     | 843  | C    |
| 34  | a     | 846  | U    |
| 34  | a     | 854  | A    |
| 34  | a     | 862  | G    |
| 34  | a     | 866  | G    |
| 34  | a     | 870  | C    |
| 34  | a     | 873  | C    |
| 34  | a     | 882  | G    |
| 34  | a     | 899  | A    |
| 34  | a     | 929  | G    |
| 34  | a     | 941  | A    |
| 34  | a     | 953  | G    |
| 34  | a     | 954  | G    |
| 34  | a     | 961  | C    |
| 34  | a     | 962  | A    |
| 34  | a     | 972  | G    |
| 34  | a     | 987  | U    |
| 34  | a     | 995  | A    |
| 34  | a     | 996  | A    |
| 34  | a     | 998  | G    |
| 34  | a     | 1002 | A    |
| 34  | a     | 1003 | G    |
| 34  | a     | 1004 | A    |
| 34  | a     | 1019 | U    |
| 34  | a     | 1020 | G    |
| 34  | a     | 1028 | U    |
| 34  | a     | 1030 | G    |
| 34  | a     | 1031 | A    |
| 34  | a     | 1033 | C    |
| 34  | a     | 1036 | U    |
| 34  | a     | 1045 | A    |
| 34  | a     | 1050 | U    |
| 34  | a     | 1051 | U    |
| 34  | a     | 1053 | C    |
| 34  | a     | 1057 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 34  | a     | 1058 | C    |
| 34  | a     | 1060 | G    |
| 34  | a     | 1063 | A    |
| 34  | a     | 1065 | A    |
| 34  | a     | 1067 | A    |
| 34  | a     | 1073 | A    |
| 34  | a     | 1077 | G    |
| 34  | a     | 1081 | C    |
| 34  | a     | 1092 | U    |
| 34  | a     | 1121 | G    |
| 34  | a     | 1122 | U    |
| 34  | a     | 1128 | A    |
| 34  | a     | 1159 | C    |
| 34  | a     | 1161 | U    |
| 34  | a     | 1163 | U    |
| 34  | a     | 1165 | G    |
| 34  | a     | 1166 | U    |
| 34  | a     | 1171 | C    |
| 34  | a     | 1172 | A    |
| 34  | a     | 1180 | G    |
| 34  | a     | 1183 | A    |
| 34  | a     | 1185 | U    |
| 34  | a     | 1194 | C    |
| 34  | a     | 1210 | G    |
| 34  | a     | 1222 | A    |
| 34  | a     | 1223 | A    |
| 34  | a     | 1238 | U    |
| 34  | a     | 1239 | A    |
| 34  | a     | 1253 | A    |
| 34  | a     | 1264 | A    |
| 34  | a     | 1283 | C    |
| 34  | a     | 1286 | U    |
| 34  | a     | 1296 | G    |
| 34  | a     | 1306 | A    |
| 34  | a     | 1307 | U    |
| 34  | a     | 1323 | U    |
| 34  | a     | 1326 | G    |
| 34  | a     | 1328 | U    |
| 34  | a     | 1331 | G    |
| 34  | a     | 1343 | C    |
| 34  | a     | 1344 | A    |
| 34  | a     | 1348 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 34  | a     | 1364 | G    |
| 34  | a     | 1372 | A    |
| 34  | a     | 1379 | G    |
| 34  | a     | 1390 | C    |
| 34  | a     | 1420 | A    |
| 34  | a     | 1423 | C    |
| 34  | a     | 1424 | A    |
| 34  | a     | 1445 | G    |
| 34  | a     | 1449 | G    |
| 34  | a     | 1455 | C    |
| 34  | a     | 1466 | U    |
| 34  | a     | 1468 | A    |
| 34  | a     | 1472 | A    |
| 34  | a     | 1478 | U    |
| 34  | a     | 1479 | U    |
| 34  | a     | 1480 | U    |
| 34  | a     | 1481 | G    |
| 34  | a     | 1514 | G    |
| 34  | a     | 1517 | U    |
| 34  | a     | 1519 | A    |
| 34  | a     | 1524 | G    |
| 34  | a     | 1530 | A    |
| 34  | a     | 1533 | U    |
| 34  | a     | 1544 | G    |
| 34  | a     | 1556 | G    |
| 34  | a     | 1557 | G    |
| 34  | a     | 1558 | A    |
| 34  | a     | 1564 | U    |

All (23) RNA pucker outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 10  | A     | 9    | G    |
| 10  | A     | 33   | U    |
| 10  | A     | 227  | A    |
| 10  | A     | 251  | C    |
| 10  | A     | 288  | U    |
| 10  | A     | 295  | G    |
| 10  | A     | 429  | A    |
| 10  | A     | 683  | U    |
| 10  | A     | 1057 | U    |
| 10  | A     | 1189 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 10  | A     | 1413 | A    |
| 10  | A     | 1536 | A    |
| 10  | A     | 1583 | G    |
| 10  | A     | 1828 | A    |
| 10  | A     | 1927 | C    |
| 10  | A     | 2111 | U    |
| 10  | A     | 2216 | G    |
| 10  | A     | 2318 | U    |
| 10  | A     | 2598 | U    |
| 10  | A     | 2810 | U    |
| 10  | A     | 2877 | G    |
| 12  | C     | 69   | G    |
| 13  | D     | 20   | G    |

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

5 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 |
| 12  | 5MU  | C     | 54  | 12    | 19,22,23     | 7.58 | 8 (42%)  | 27,32,35    | 3.08 | 10 (37%) |
| 12  | T6A  | C     | 37  | 12    | 31,34,35     | 1.81 | 6 (19%)  | 43,49,52    | 4.24 | 16 (37%) |
| 12  | U8U  | C     | 34  | 35,12 | 20,24,25     | 2.58 | 5 (25%)  | 22,34,37    | 1.00 | 2 (9%)   |
| 12  | PSU  | C     | 39  | 12    | 18,21,22     | 4.65 | 8 (44%)  | 21,30,33    | 2.03 | 5 (23%)  |
| 12  | PSU  | C     | 55  | 12    | 18,21,22     | 4.62 | 7 (38%)  | 21,30,33    | 2.03 | 5 (23%)  |

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   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 12  | 5MU  | C     | 54  | 12   | -       | 0/7/25/26 | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link  | Chirals | Torsions   | Rings   |
|-----|------|-------|-----|-------|---------|------------|---------|
| 12  | T6A  | C     | 37  | 12    | -       | 5/23/41/42 | 0/3/3/3 |
| 12  | U8U  | C     | 34  | 35,12 | -       | 1/10/28/29 | 0/2/2/2 |
| 12  | PSU  | C     | 39  | 12    | -       | 2/7/25/26  | 0/2/2/2 |
| 12  | PSU  | C     | 55  | 12    | -       | 2/7/25/26  | 0/2/2/2 |

All (34) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 12  | C     | 54  | 5MU  | C4-C5   | 21.82  | 1.80        | 1.44     |
| 12  | C     | 54  | 5MU  | C6-N1   | 16.57  | 1.66        | 1.38     |
| 12  | C     | 39  | PSU  | C6-C5   | 12.42  | 1.49        | 1.35     |
| 12  | C     | 55  | PSU  | C6-C5   | 12.37  | 1.49        | 1.35     |
| 12  | C     | 54  | 5MU  | C6-C5   | -12.19 | 1.14        | 1.34     |
| 12  | C     | 54  | 5MU  | C4-N3   | -10.97 | 1.18        | 1.38     |
| 12  | C     | 39  | PSU  | C2-N1   | 9.76   | 1.49        | 1.36     |
| 12  | C     | 55  | PSU  | C2-N1   | 9.69   | 1.49        | 1.36     |
| 12  | C     | 39  | PSU  | C2-N3   | 8.73   | 1.51        | 1.37     |
| 12  | C     | 55  | PSU  | C2-N3   | 8.65   | 1.51        | 1.37     |
| 12  | C     | 34  | U8U  | C2-S2   | -6.72  | 1.56        | 1.67     |
| 12  | C     | 55  | PSU  | C6-N1   | 5.51   | 1.45        | 1.36     |
| 12  | C     | 39  | PSU  | C6-N1   | 5.46   | 1.45        | 1.36     |
| 12  | C     | 34  | U8U  | C6-N1   | 5.24   | 1.46        | 1.38     |
| 12  | C     | 54  | 5MU  | O2-C2   | -5.19  | 1.13        | 1.23     |
| 12  | C     | 54  | 5MU  | C2-N3   | 4.85   | 1.46        | 1.38     |
| 12  | C     | 37  | T6A  | C10-N6  | 4.73   | 1.47        | 1.37     |
| 12  | C     | 34  | U8U  | C2-N3   | 4.49   | 1.49        | 1.38     |
| 12  | C     | 34  | U8U  | C6-C5   | 4.35   | 1.47        | 1.35     |
| 12  | C     | 37  | T6A  | C10-N11 | 4.29   | 1.47        | 1.35     |
| 12  | C     | 37  | T6A  | C6-N6   | 4.27   | 1.48        | 1.39     |
| 12  | C     | 34  | U8U  | C4-N3   | 4.07   | 1.46        | 1.38     |
| 12  | C     | 55  | PSU  | C4-N3   | 3.64   | 1.45        | 1.38     |
| 12  | C     | 39  | PSU  | C4-N3   | 3.60   | 1.45        | 1.38     |
| 12  | C     | 54  | 5MU  | C5M-C5  | 3.03   | 1.58        | 1.50     |
| 12  | C     | 54  | 5MU  | C2-N1   | 2.90   | 1.43        | 1.38     |
| 12  | C     | 37  | T6A  | C5-N7   | -2.86  | 1.33        | 1.39     |
| 12  | C     | 37  | T6A  | C5-C4   | -2.56  | 1.34        | 1.39     |
| 12  | C     | 39  | PSU  | C1'-C5  | 2.29   | 1.55        | 1.50     |
| 12  | C     | 55  | PSU  | C1'-C5  | 2.24   | 1.55        | 1.50     |
| 12  | C     | 55  | PSU  | O4-C4   | -2.15  | 1.19        | 1.23     |
| 12  | C     | 39  | PSU  | O4-C4   | -2.10  | 1.19        | 1.23     |
| 12  | C     | 37  | T6A  | C8-N9   | -2.09  | 1.34        | 1.37     |
| 12  | C     | 39  | PSU  | O4'-C1' | -2.03  | 1.41        | 1.43     |

All (38) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 12  | C     | 37  | T6A  | C5-C6-N6    | 15.44  | 158.36      | 118.94   |
| 12  | C     | 37  | T6A  | N6-C6-N1    | -13.62 | 82.33       | 117.54   |
| 12  | C     | 37  | T6A  | N6-C10-N11  | 10.48  | 128.18      | 113.77   |
| 12  | C     | 54  | 5MU  | C5-C4-N3    | 9.20   | 123.32      | 115.32   |
| 12  | C     | 54  | 5MU  | C5-C6-N1    | -7.00  | 115.71      | 123.31   |
| 12  | C     | 37  | T6A  | C4-C5-C6    | 6.54   | 122.22      | 116.78   |
| 12  | C     | 37  | T6A  | C5-C4-N3    | -6.14  | 118.27      | 126.72   |
| 12  | C     | 54  | 5MU  | C4-N3-C2    | -6.04  | 119.42      | 127.34   |
| 12  | C     | 37  | T6A  | N3-C2-N1    | -4.98  | 121.05      | 128.58   |
| 12  | C     | 39  | PSU  | C4-N3-C2    | -4.86  | 119.68      | 126.37   |
| 12  | C     | 55  | PSU  | C4-N3-C2    | -4.80  | 119.76      | 126.37   |
| 12  | C     | 39  | PSU  | N1-C2-N3    | 4.54   | 119.96      | 115.17   |
| 12  | C     | 37  | T6A  | O10-C10-N6  | -4.50  | 115.64      | 123.64   |
| 12  | C     | 55  | PSU  | N1-C2-N3    | 4.44   | 119.85      | 115.17   |
| 12  | C     | 54  | 5MU  | C5M-C5-C6   | -4.38  | 116.92      | 122.85   |
| 12  | C     | 37  | T6A  | N3-C4-N9    | 4.29   | 134.46      | 127.17   |
| 12  | C     | 54  | 5MU  | N3-C2-N1    | 4.25   | 120.42      | 114.89   |
| 12  | C     | 54  | 5MU  | C5M-C5-C4   | 3.84   | 122.88      | 118.78   |
| 12  | C     | 55  | PSU  | C6-C5-C4    | 3.58   | 120.59      | 118.17   |
| 12  | C     | 39  | PSU  | C6-C5-C4    | 3.51   | 120.55      | 118.17   |
| 12  | C     | 37  | T6A  | N9-C8-N7    | -3.49  | 108.98      | 113.94   |
| 12  | C     | 54  | 5MU  | O4-C4-C5    | -3.48  | 120.94      | 124.92   |
| 12  | C     | 39  | PSU  | C6-N1-C2    | -3.28  | 119.65      | 122.69   |
| 12  | C     | 37  | T6A  | C2-N3-C4    | 3.27   | 119.83      | 111.83   |
| 12  | C     | 55  | PSU  | C6-N1-C2    | -3.18  | 119.74      | 122.69   |
| 12  | C     | 37  | T6A  | C6-C5-N7    | -3.06  | 129.09      | 132.43   |
| 12  | C     | 37  | T6A  | O10-C10-N11 | -3.04  | 116.18      | 122.67   |
| 12  | C     | 37  | T6A  | C4-N9-C1'   | -3.02  | 119.56      | 126.63   |
| 12  | C     | 37  | T6A  | C12-N11-C10 | -3.00  | 116.99      | 121.99   |
| 12  | C     | 34  | U8U  | C5-C4-N3    | 2.87   | 119.59      | 115.21   |
| 12  | C     | 37  | T6A  | C5-N7-C8    | 2.68   | 107.67      | 103.45   |
| 12  | C     | 37  | T6A  | C1'-N9-C8   | 2.68   | 133.04      | 127.09   |
| 12  | C     | 55  | PSU  | O2-C2-N1    | -2.65  | 120.06      | 122.79   |
| 12  | C     | 54  | 5MU  | C6-C5-C4    | 2.64   | 120.19      | 118.02   |
| 12  | C     | 34  | U8U  | O4-C4-C5    | -2.60  | 120.34      | 124.71   |
| 12  | C     | 39  | PSU  | O2-C2-N1    | -2.58  | 120.13      | 122.79   |
| 12  | C     | 54  | 5MU  | O2-C2-N1    | -2.45  | 119.61      | 122.80   |
| 12  | C     | 54  | 5MU  | O4-C4-N3    | -2.32  | 115.75      | 120.11   |

There are no chirality outliers.

All (10) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 12  | C     | 34  | U8U  | C5-C-N-CA       |
| 12  | C     | 37  | T6A  | N11-C12-C13-ODB |
| 12  | C     | 37  | T6A  | C14-C12-C13-ODA |
| 12  | C     | 37  | T6A  | C14-C12-C13-ODB |
| 12  | C     | 37  | T6A  | N11-C12-C13-ODA |
| 12  | C     | 39  | PSU  | C3'-C4'-C5'-O5' |
| 12  | C     | 37  | T6A  | C5-C6-N6-C10    |
| 12  | C     | 55  | PSU  | O4'-C1'-C5-C4   |
| 12  | C     | 55  | PSU  | O4'-C1'-C5-C6   |
| 12  | C     | 39  | PSU  | O4'-C4'-C5'-O5' |

There are no ring outliers.

2 monomers are involved in 3 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 12  | C     | 54  | 5MU  | 1       | 0            |
| 12  | C     | 37  | T6A  | 2       | 0            |

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 307 ligands modelled in this entry, 303 are monoatomic - leaving 4 for Mogul analysis.

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

| Mol | Type | Chain | Res  | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |      |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 60  | PUT  | a     | 1627 | -    | 5,5,5        | 0.25 | 0           | 4,4,4       | 0.43 | 0           |
| 59  | SCM  | a     | 1615 | -    | 23,25,25     | 7.21 | 13 (56%)    | 27,39,39    | 1.36 | 3 (11%)     |
| 55  | ATP  | 0     | 601  | 56   | 32,33,33     | 3.59 | 15 (46%)    | 48,52,52    | 2.17 | 14 (29%)    |
| 55  | ATP  | 0     | 602  | 56   | 32,33,33     | 3.56 | 15 (46%)    | 48,52,52    | 2.23 | 15 (31%)    |

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   |
|-----|------|-------|------|------|---------|------------|---------|
| 60  | PUT  | a     | 1627 | -    | -       | 0/3/3/3    | -       |
| 59  | SCM  | a     | 1615 | -    | -       | 0/4/57/57  | 0/3/3/3 |
| 55  | ATP  | 0     | 601  | 56   | -       | 9/22/38/38 | 0/3/3/3 |
| 55  | ATP  | 0     | 602  | 56   | -       | 6/22/38/38 | 0/3/3/3 |

All (43) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|--------|-------------|----------|
| 59  | a     | 1615 | SCM  | O2B-C12 | -27.62 | 1.01        | 1.44     |
| 59  | a     | 1615 | SCM  | O1-C2   | -16.53 | 1.15        | 1.44     |
| 55  | 0     | 601  | ATP  | C2'-C3' | -10.64 | 1.24        | 1.53     |
| 55  | 0     | 602  | ATP  | C2'-C3' | -10.57 | 1.24        | 1.53     |
| 55  | 0     | 602  | ATP  | O4'-C4' | -6.66  | 1.30        | 1.45     |
| 55  | 0     | 601  | ATP  | O4'-C4' | -6.53  | 1.30        | 1.45     |
| 55  | 0     | 601  | ATP  | PA-O3A  | 6.24   | 1.66        | 1.59     |
| 55  | 0     | 602  | ATP  | PA-O3A  | 6.21   | 1.66        | 1.59     |
| 55  | 0     | 601  | ATP  | PB-O3A  | 6.01   | 1.66        | 1.59     |
| 55  | 0     | 602  | ATP  | PB-O3A  | 5.95   | 1.65        | 1.59     |
| 55  | 0     | 601  | ATP  | PB-O3B  | 5.72   | 1.65        | 1.59     |
| 55  | 0     | 601  | ATP  | C3'-C4' | 5.71   | 1.67        | 1.53     |
| 59  | a     | 1615 | SCM  | C2M-C2  | 5.57   | 1.72        | 1.51     |
| 55  | 0     | 602  | ATP  | PB-O3B  | 5.55   | 1.65        | 1.59     |
| 55  | 0     | 602  | ATP  | C3'-C4' | 5.54   | 1.67        | 1.53     |
| 55  | 0     | 601  | ATP  | C1'-N9  | -5.01  | 1.32        | 1.46     |
| 55  | 0     | 602  | ATP  | C1'-N9  | -4.97  | 1.32        | 1.46     |
| 59  | a     | 1615 | SCM  | C9-C8   | 4.75   | 1.61        | 1.53     |
| 55  | 0     | 601  | ATP  | C6-N6   | 4.58   | 1.45        | 1.34     |
| 55  | 0     | 602  | ATP  | C6-N6   | 4.57   | 1.45        | 1.34     |
| 59  | a     | 1615 | SCM  | C8-N8   | -4.22  | 1.40        | 1.47     |
| 59  | a     | 1615 | SCM  | C11-C12 | 4.12   | 1.63        | 1.52     |
| 59  | a     | 1615 | SCM  | O1B-C7  | 4.07   | 1.50        | 1.44     |
| 55  | 0     | 602  | ATP  | O4'-C1' | 3.82   | 1.50        | 1.42     |
| 55  | 0     | 601  | ATP  | O4'-C1' | 3.81   | 1.50        | 1.42     |
| 59  | a     | 1615 | SCM  | C12-C7  | -3.55  | 1.45        | 1.52     |
| 59  | a     | 1615 | SCM  | C3-C2   | -3.39  | 1.44        | 1.51     |
| 59  | a     | 1615 | SCM  | O11-C11 | -3.31  | 1.34        | 1.43     |
| 55  | 0     | 602  | ATP  | O2'-C2' | 3.18   | 1.50        | 1.43     |
| 55  | 0     | 601  | ATP  | O2'-C2' | 3.11   | 1.50        | 1.43     |
| 55  | 0     | 601  | ATP  | C5-C4   | -3.11  | 1.33        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 55  | 0     | 602  | ATP  | C5-C4   | -2.99 | 1.33        | 1.39     |
| 55  | 0     | 601  | ATP  | C5-N7   | -2.53 | 1.34        | 1.39     |
| 55  | 0     | 602  | ATP  | C5-N7   | -2.45 | 1.34        | 1.39     |
| 55  | 0     | 602  | ATP  | C2'-C1' | 2.30  | 1.60        | 1.53     |
| 55  | 0     | 601  | ATP  | C2'-C1' | 2.28  | 1.60        | 1.53     |
| 55  | 0     | 602  | ATP  | C8-N9   | -2.12 | 1.33        | 1.37     |
| 59  | a     | 1615 | SCM  | C9-C10  | -2.11 | 1.49        | 1.53     |
| 59  | a     | 1615 | SCM  | C3-C4   | 2.11  | 1.54        | 1.50     |
| 55  | 0     | 601  | ATP  | C8-N9   | -2.07 | 1.34        | 1.37     |
| 55  | 0     | 601  | ATP  | O3'-C3' | 2.05  | 1.48        | 1.43     |
| 59  | a     | 1615 | SCM  | C7-C8   | 2.04  | 1.56        | 1.53     |
| 55  | 0     | 602  | ATP  | O3'-C3' | 2.01  | 1.47        | 1.43     |

All (32) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 55  | 0     | 602  | ATP  | C1'-N9-C8   | -5.77 | 114.29      | 127.09   |
| 55  | 0     | 601  | ATP  | C1'-N9-C8   | -5.70 | 114.45      | 127.09   |
| 55  | 0     | 602  | ATP  | N3-C2-N1    | -5.63 | 120.06      | 128.58   |
| 55  | 0     | 601  | ATP  | N3-C2-N1    | -5.62 | 120.07      | 128.58   |
| 55  | 0     | 602  | ATP  | C5-C4-N3    | -4.86 | 120.02      | 126.72   |
| 55  | 0     | 601  | ATP  | C5-C4-N3    | -4.81 | 120.10      | 126.72   |
| 55  | 0     | 601  | ATP  | C4-N9-C1'   | 4.65  | 137.51      | 126.63   |
| 55  | 0     | 602  | ATP  | C4-N9-C1'   | 4.64  | 137.49      | 126.63   |
| 55  | 0     | 602  | ATP  | N9-C8-N7    | -4.22 | 107.95      | 113.94   |
| 55  | 0     | 601  | ATP  | N9-C8-N7    | -4.17 | 108.03      | 113.94   |
| 55  | 0     | 602  | ATP  | N6-C6-N1    | -4.12 | 109.21      | 118.38   |
| 55  | 0     | 601  | ATP  | N6-C6-N1    | -4.02 | 109.43      | 118.38   |
| 59  | a     | 1615 | SCM  | C1M-N10-C10 | -3.74 | 109.40      | 114.23   |
| 55  | 0     | 602  | ATP  | C2-N3-C4    | 3.40  | 120.14      | 111.83   |
| 55  | 0     | 601  | ATP  | C2-N3-C4    | 3.34  | 120.00      | 111.83   |
| 55  | 0     | 602  | ATP  | C4'-O4'-C1' | -3.04 | 102.74      | 109.47   |
| 55  | 0     | 602  | ATP  | N3-C4-N9    | 2.93  | 132.14      | 127.17   |
| 55  | 0     | 601  | ATP  | N3-C4-N9    | 2.86  | 132.02      | 127.17   |
| 55  | 0     | 602  | ATP  | C5-C6-N6    | 2.84  | 130.32      | 123.29   |
| 55  | 0     | 602  | ATP  | C5-N7-C8    | 2.83  | 107.89      | 103.45   |
| 55  | 0     | 601  | ATP  | C2'-C3'-C4' | 2.81  | 108.04      | 102.61   |
| 55  | 0     | 601  | ATP  | C5-N7-C8    | 2.80  | 107.86      | 103.45   |
| 55  | 0     | 601  | ATP  | C5-C6-N6    | 2.79  | 130.20      | 123.29   |
| 55  | 0     | 602  | ATP  | C2'-C3'-C4' | 2.59  | 107.61      | 102.61   |
| 59  | a     | 1615 | SCM  | C2M-C2-C3   | -2.51 | 108.76      | 113.27   |
| 55  | 0     | 602  | ATP  | C3'-C2'-C1' | 2.43  | 106.05      | 101.46   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 55  | 0     | 602  | ATP  | C4-N9-C8    | 2.36  | 108.22      | 105.74   |
| 59  | a     | 1615 | SCM  | C8M-N8-C8   | -2.35 | 111.20      | 114.23   |
| 55  | 0     | 601  | ATP  | C4-N9-C8    | 2.19  | 108.03      | 105.74   |
| 55  | 0     | 602  | ATP  | C4-C5-N7    | -2.16 | 108.11      | 110.58   |
| 55  | 0     | 601  | ATP  | C4-C5-N7    | -2.08 | 108.20      | 110.58   |
| 55  | 0     | 601  | ATP  | C3'-C2'-C1' | 2.04  | 105.33      | 101.46   |

There are no chirality outliers.

All (15) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 55  | 0     | 601 | ATP  | PB-O3B-PG-O2G   |
| 55  | 0     | 601 | ATP  | C5'-O5'-PA-O1A  |
| 55  | 0     | 601 | ATP  | C5'-O5'-PA-O2A  |
| 55  | 0     | 601 | ATP  | O4'-C4'-C5'-O5' |
| 55  | 0     | 601 | ATP  | C3'-C4'-C5'-O5' |
| 55  | 0     | 601 | ATP  | C5'-O5'-PA-O3A  |
| 55  | 0     | 602 | ATP  | C5'-O5'-PA-O1A  |
| 55  | 0     | 602 | ATP  | C5'-O5'-PA-O2A  |
| 55  | 0     | 602 | ATP  | C5'-O5'-PA-O3A  |
| 55  | 0     | 601 | ATP  | PG-O3B-PB-O2B   |
| 55  | 0     | 602 | ATP  | PA-O3A-PB-O2B   |
| 55  | 0     | 601 | ATP  | PB-O3B-PG-O1G   |
| 55  | 0     | 602 | ATP  | O4'-C4'-C5'-O5' |
| 55  | 0     | 601 | ATP  | PG-O3B-PB-O1B   |
| 55  | 0     | 602 | ATP  | PA-O3A-PB-O1B   |

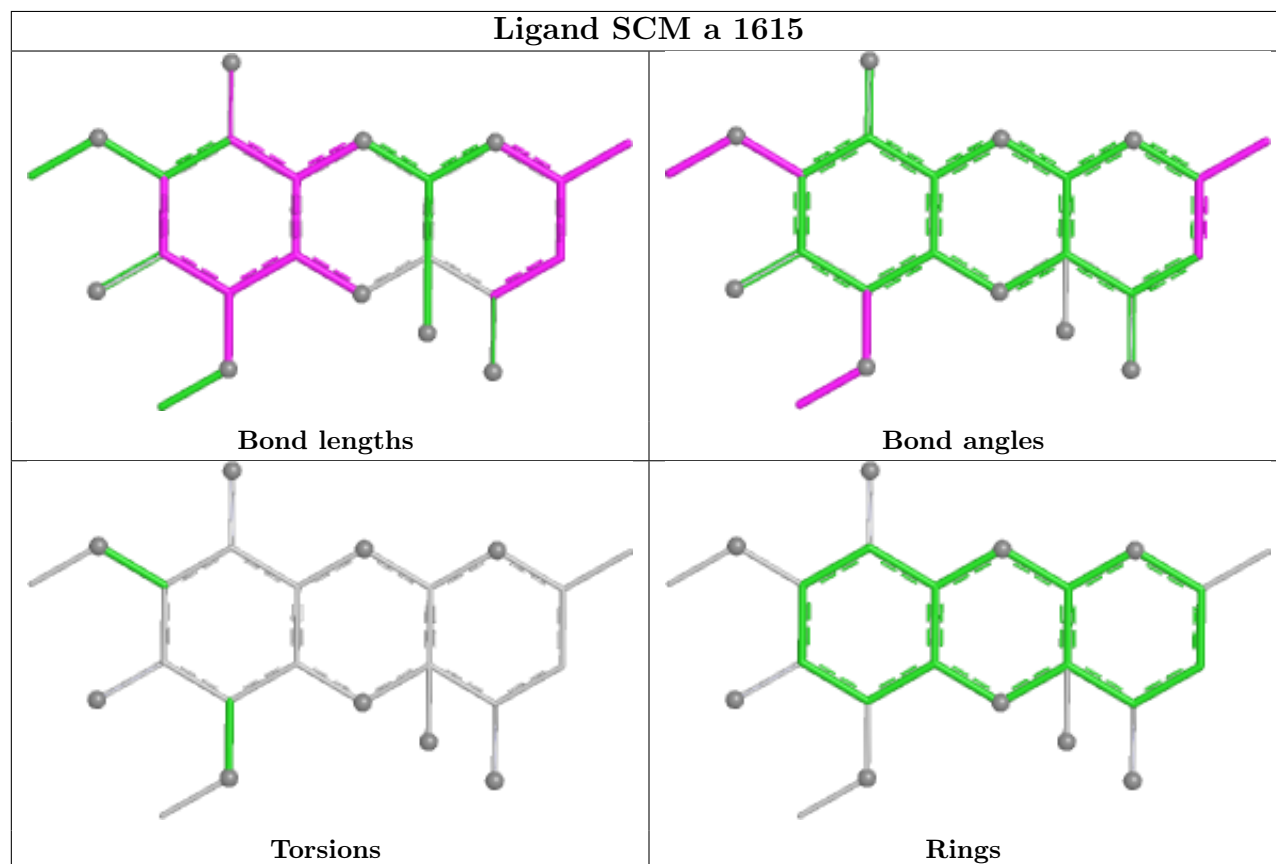
There are no ring outliers.

3 monomers are involved in 8 short contacts:

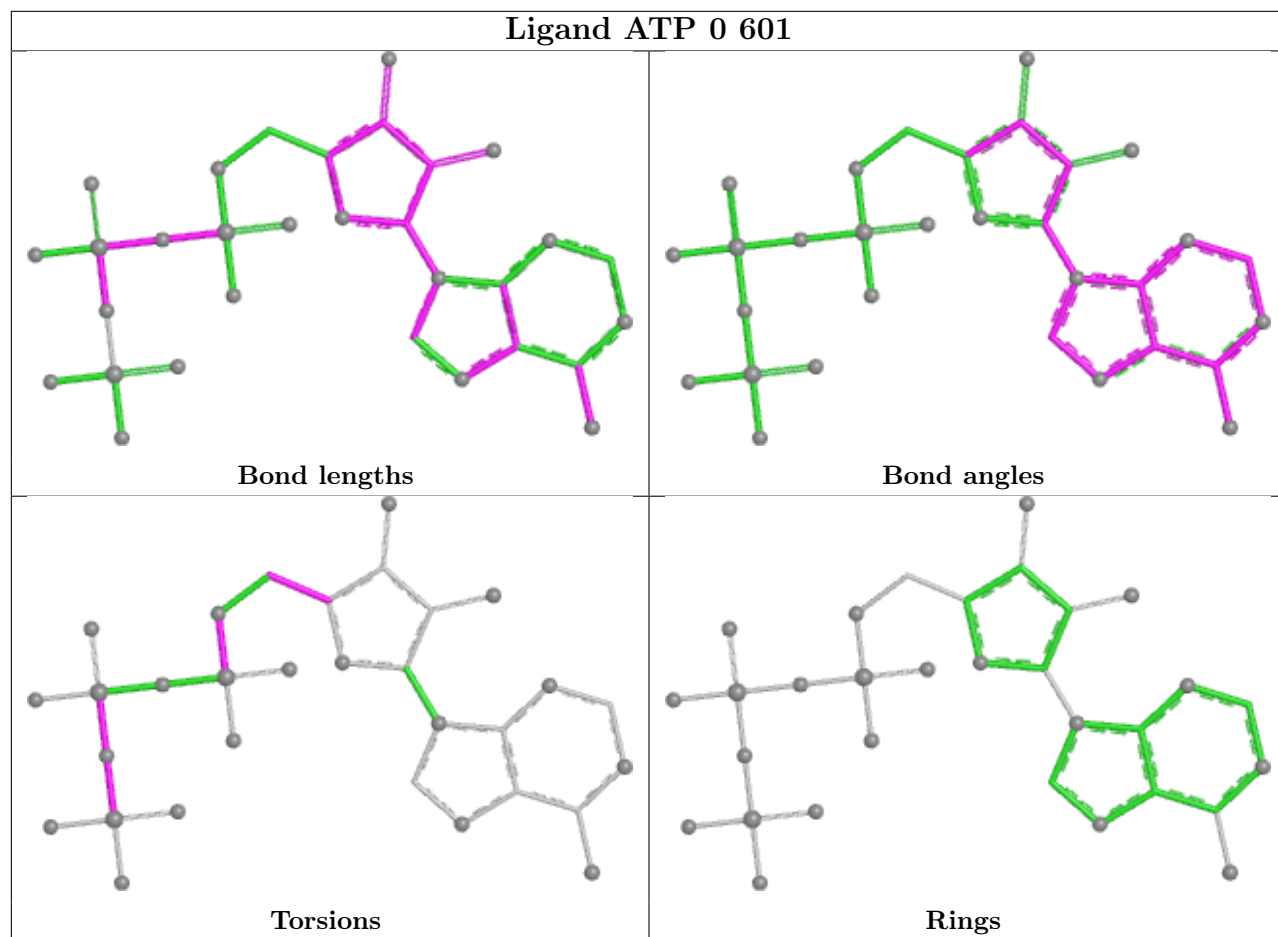
| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 59  | a     | 1615 | SCM  | 4       | 0            |
| 55  | 0     | 601  | ATP  | 1       | 0            |
| 55  | 0     | 602  | ATP  | 3       | 0            |

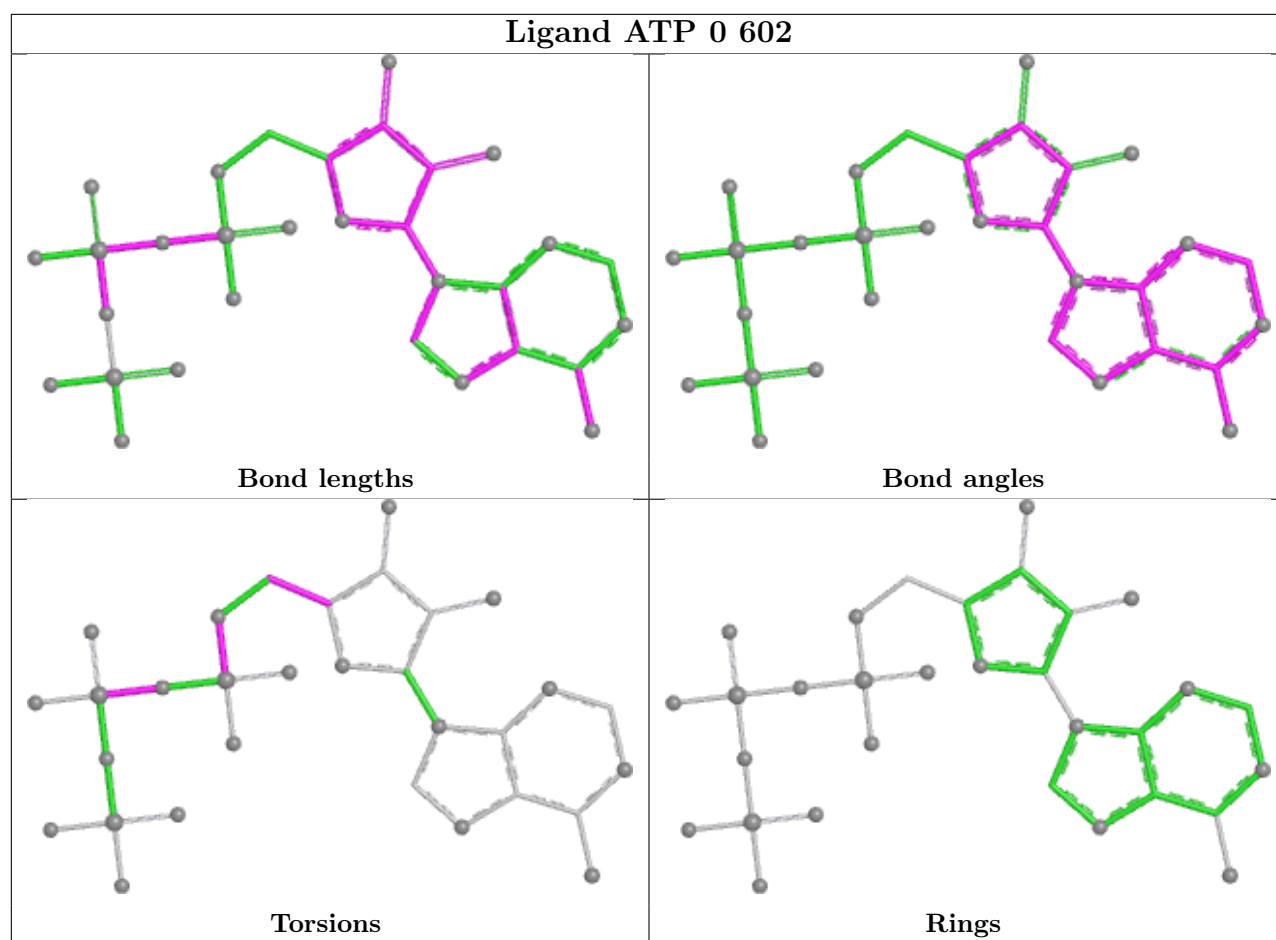
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## Ligand ATP 0 601





## 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.

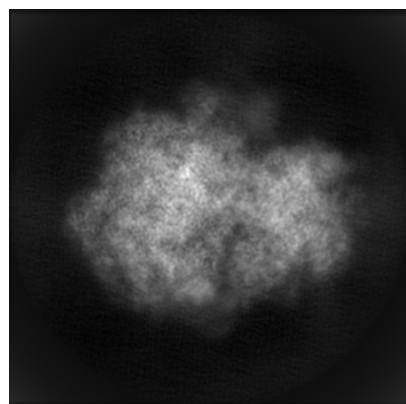
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13244. These allow visual inspection of the internal detail of the map and identification of artifacts.

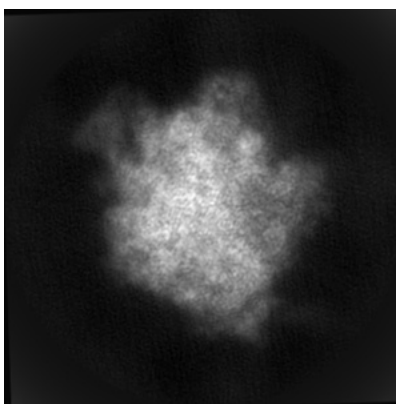
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

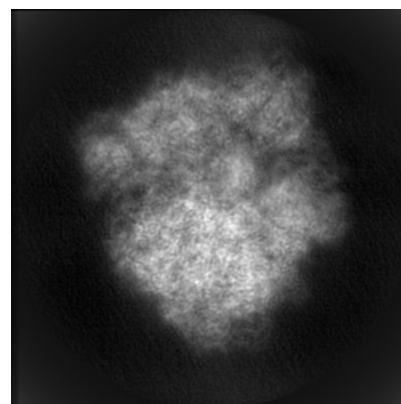
#### 6.1.1 Primary map



X

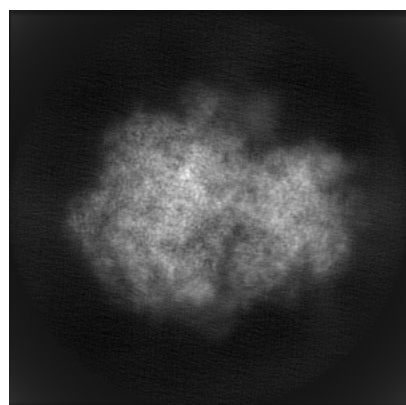


Y

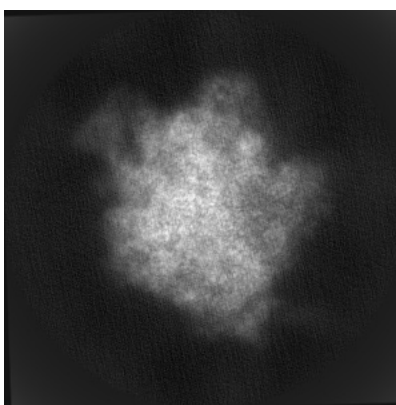


Z

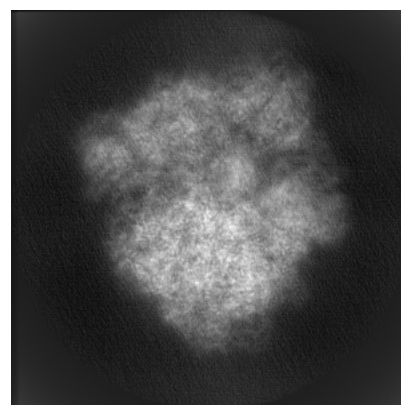
#### 6.1.2 Raw map



X



Y

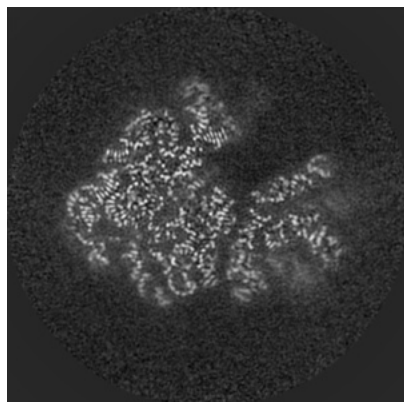


Z

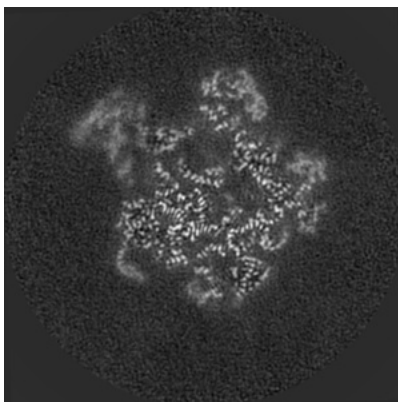
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

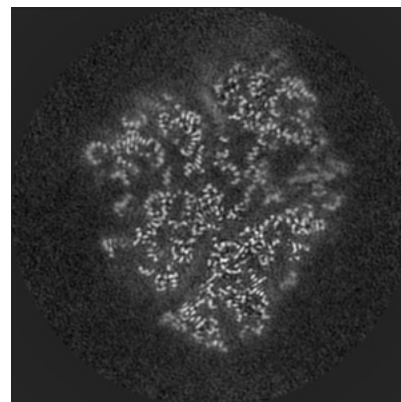
### 6.2.1 Primary map



X Index: 210

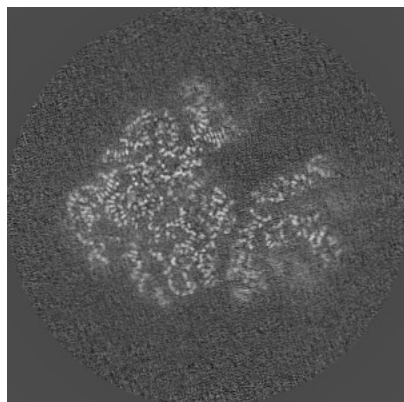


Y Index: 210

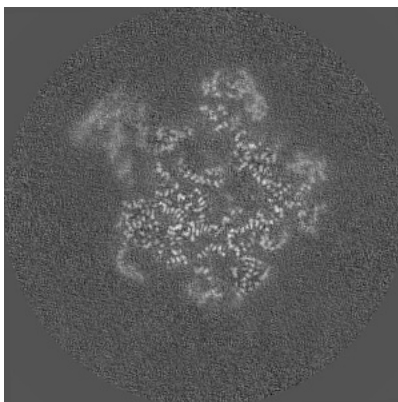


Z Index: 210

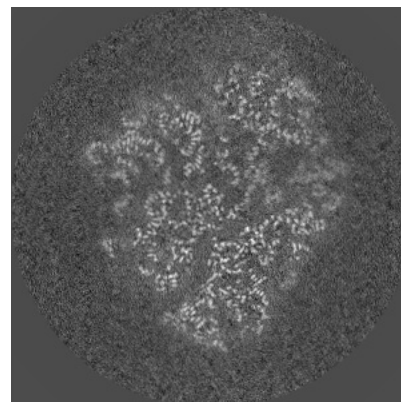
### 6.2.2 Raw map



X Index: 210



Y Index: 210

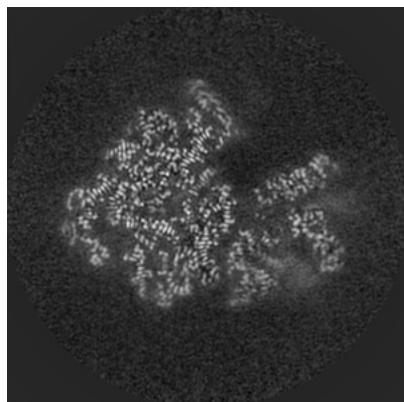


Z Index: 210

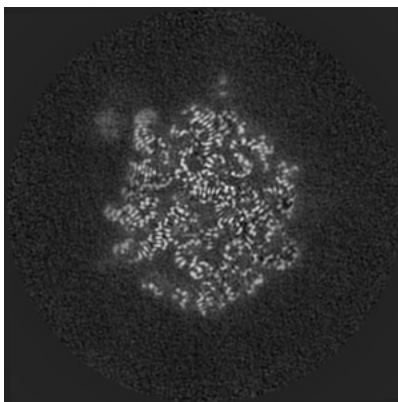
The images above show central slices of the map in three orthogonal directions.

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

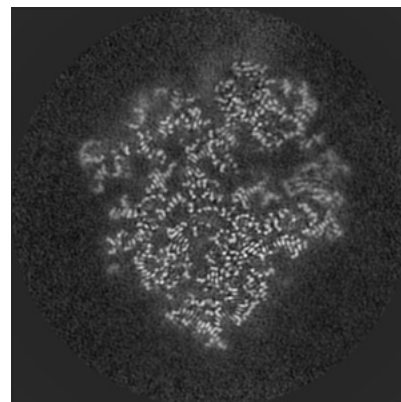
### 6.3.1 Primary map



X Index: 206

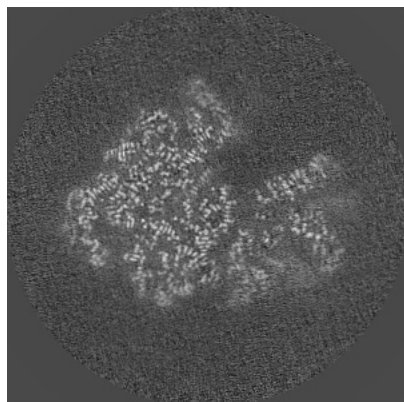


Y Index: 170

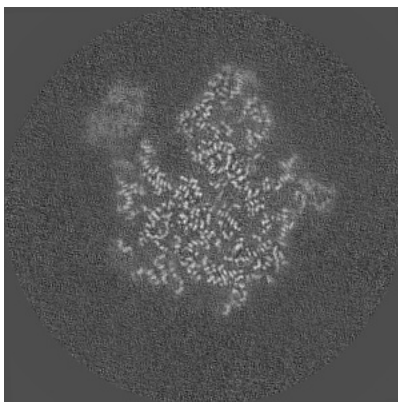


Z Index: 217

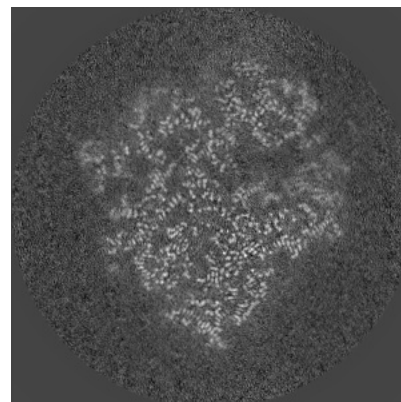
### 6.3.2 Raw map



X Index: 207



Y Index: 191

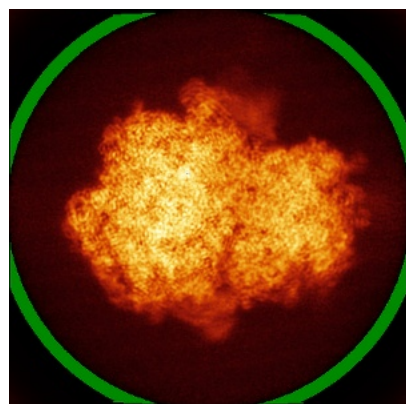


Z Index: 217

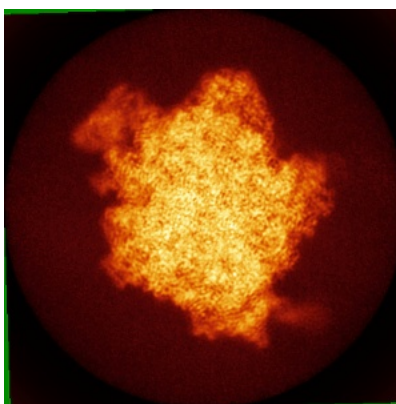
The images above show the largest variance slices of the map in three orthogonal directions.

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

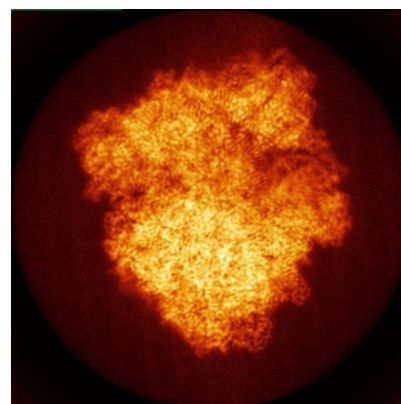
### 6.4.1 Primary map



X

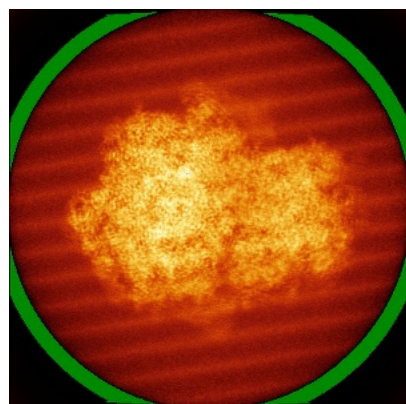


Y

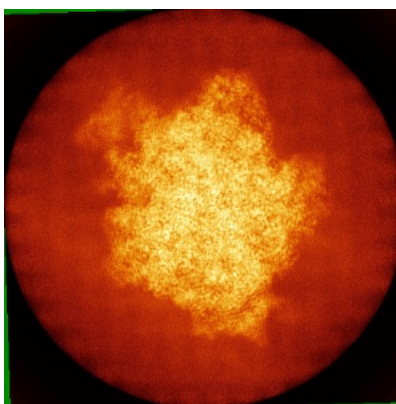


Z

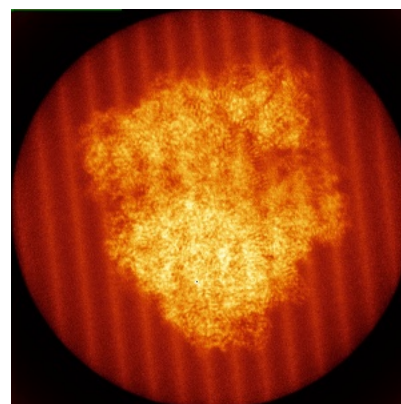
### 6.4.2 Raw map



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](#)

This section was not generated.

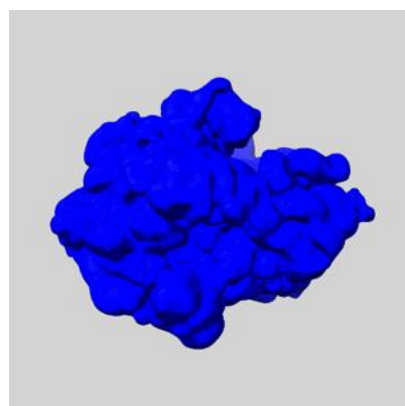
## 6.6 Mask visualisation [i](#)

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

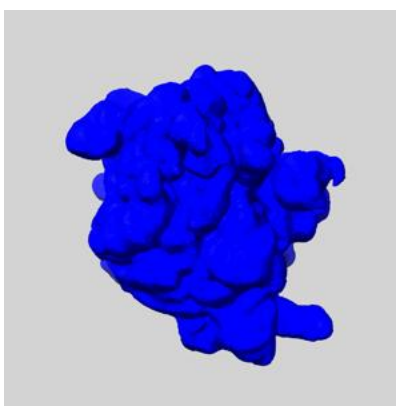
A mask typically either:

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

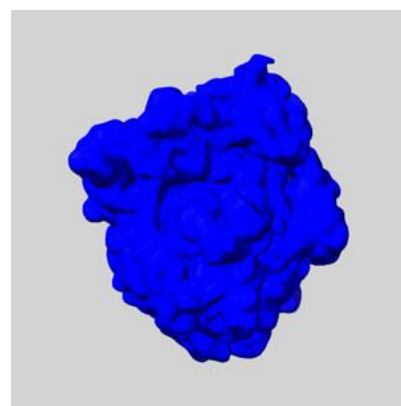
### 6.6.1 emd\_13244\_msk\_1.map [i](#)



X



Y

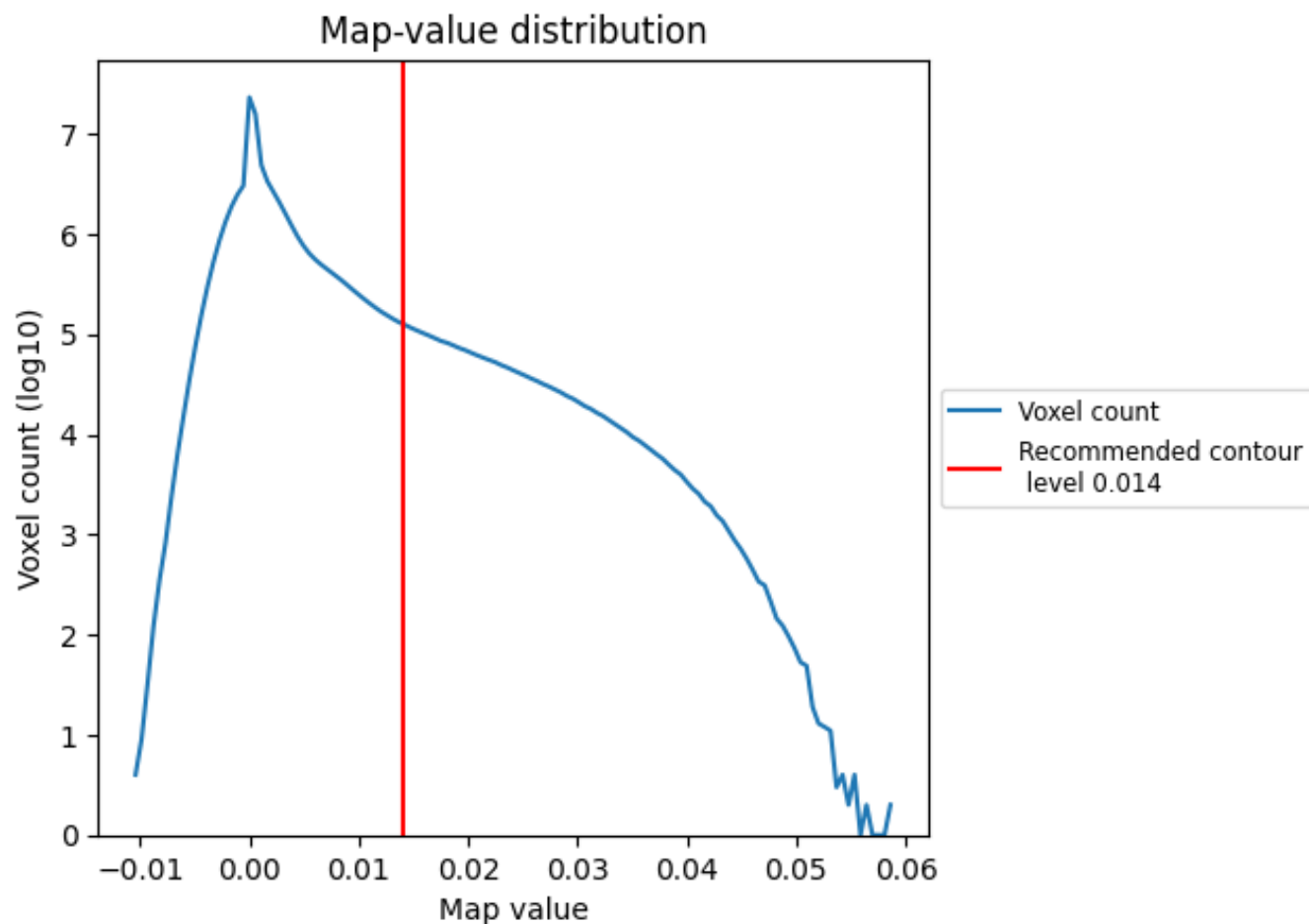


Z

## 7 Map analysis [i](#)

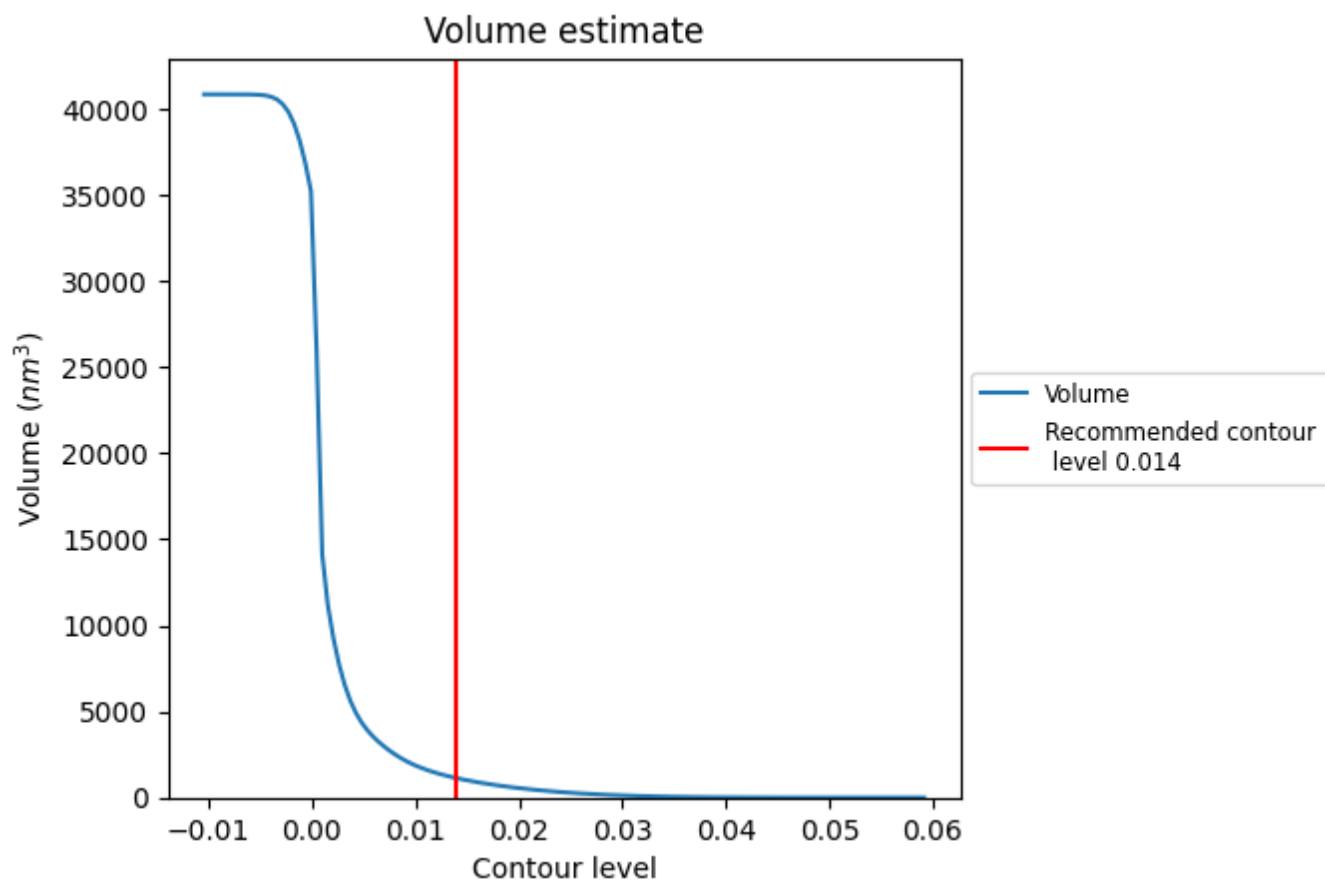
This section contains the results of statistical analysis of the map.

### 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.

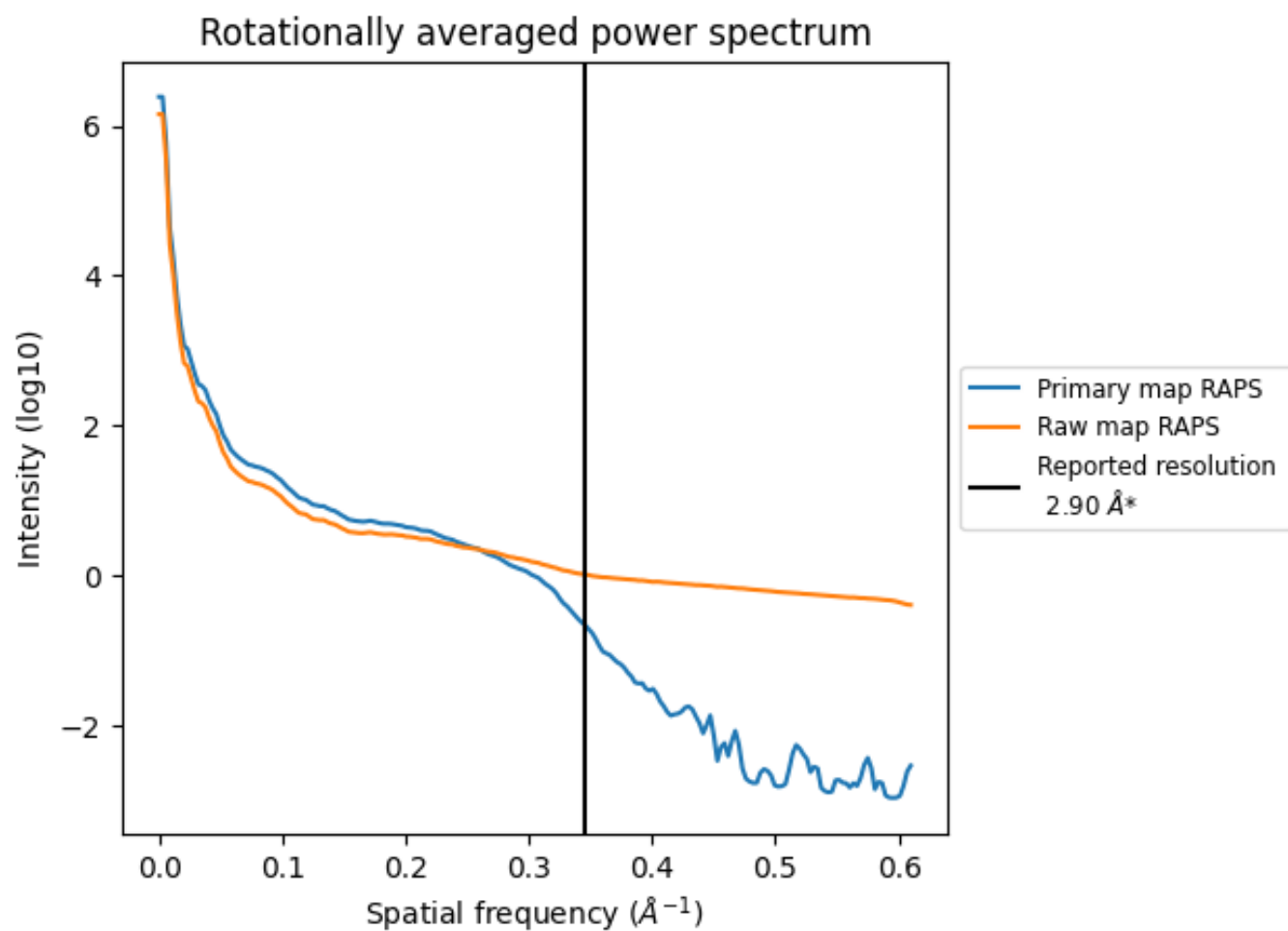
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1125 nm<sup>3</sup>; this corresponds to an approximate mass of 1016 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 ⓘ

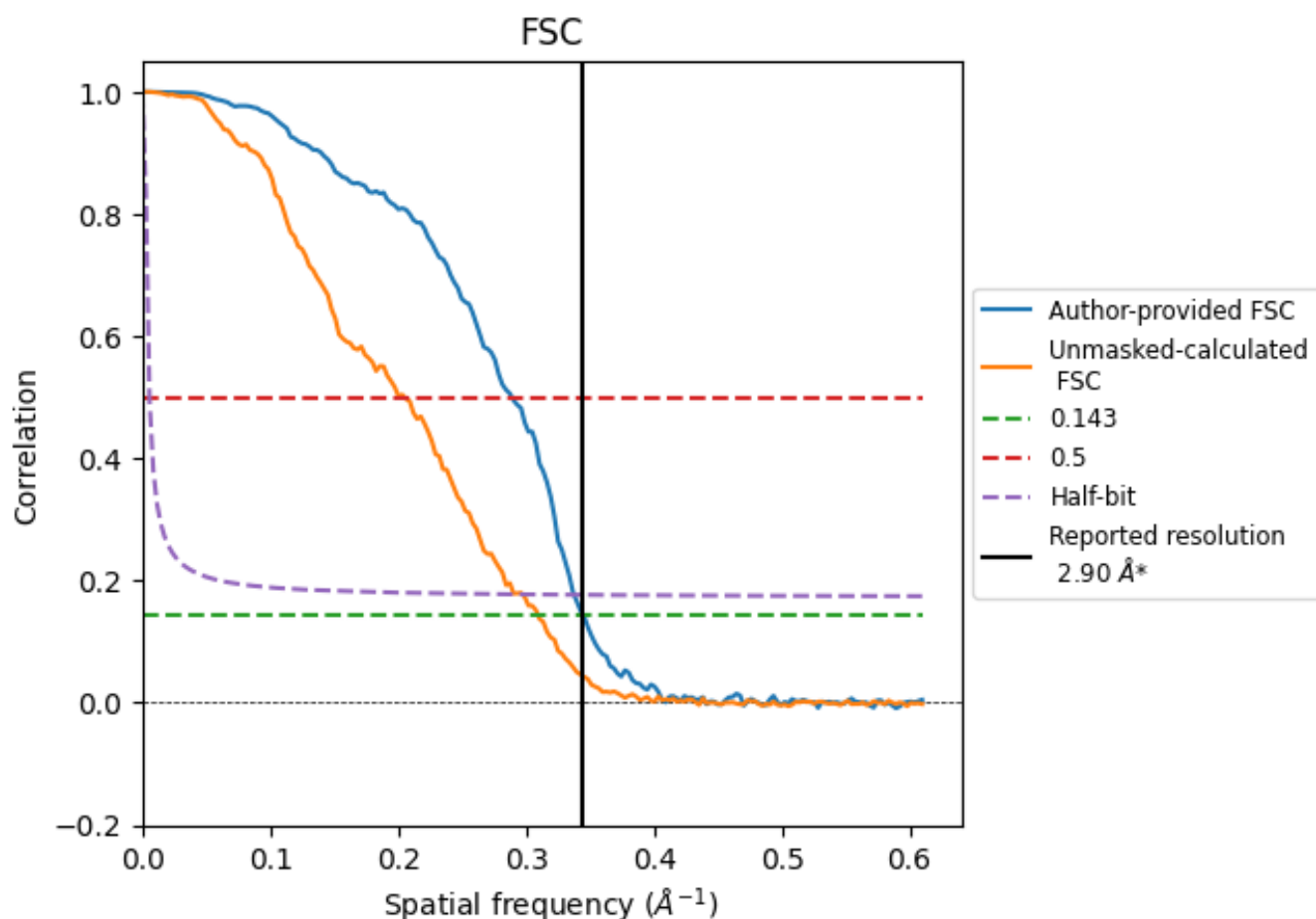


\*Reported resolution corresponds to spatial frequency of 0.345 Å<sup>-1</sup>

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

## 8.2 Resolution estimates [i](#)

| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 2.90                               | -    | -        |
| Author-provided FSC curve | 2.90                               | 3.46 | 2.96     |
| Unmasked-calculated*      | 3.23                               | 4.88 | 3.36     |

\*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 3.23 differs from the reported value 2.9 by more than 10 %

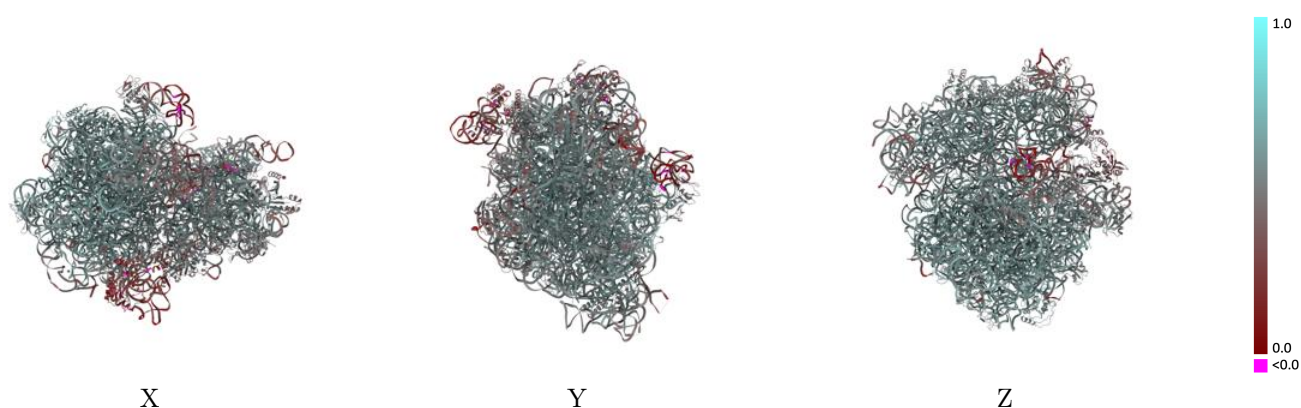
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMD map EMD-13244 and PDB model 7P7T. Per-residue inclusion information can be found in section 3 on page 18.

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

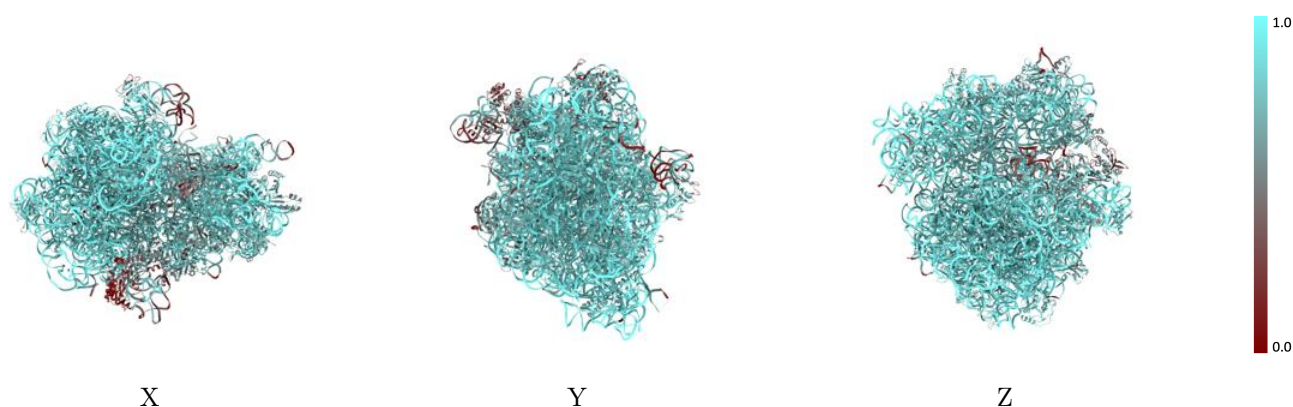
This section was not generated.

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



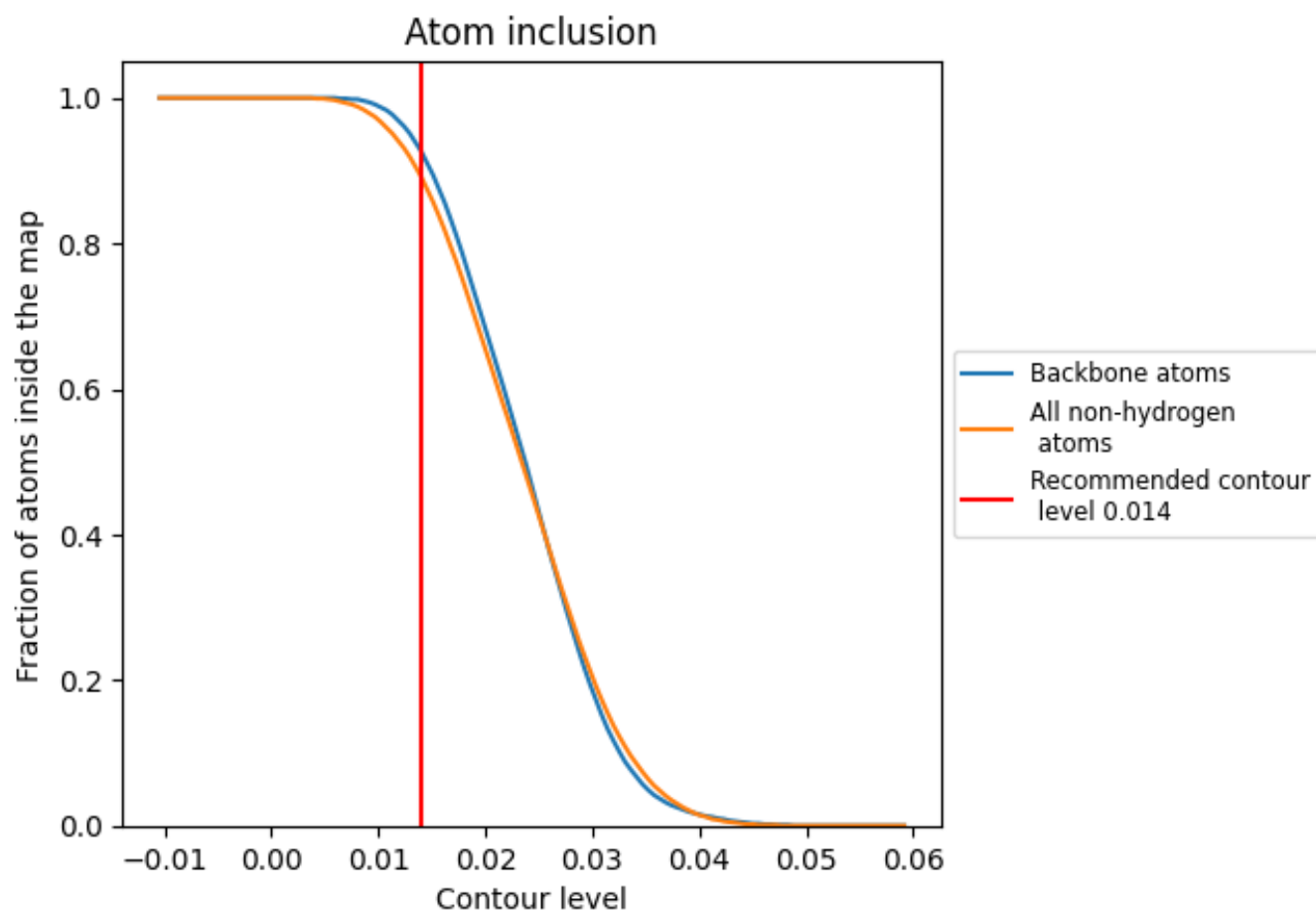
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.014).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 89% 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 (0.014) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.8920   |  0.5340   |
| 0     |  0.6110   |  0.4380   |
| 1     |  0.8120   |  0.5200   |
| 2     |  0.8560   |  0.5500   |
| 3     |  0.3670   |  0.2860   |
| 4     |  0.9140   |  0.5850   |
| 5     |  0.8760   |  0.5740   |
| 6     |  0.9540   |  0.6120   |
| 7     |  0.9640   |  0.6110   |
| 8     |  0.9260   |  0.5790   |
| A     |  0.9520   |  0.5570   |
| B     |  0.9580   |  0.4990   |
| C     |  0.8760   |  0.5050   |
| D     |  0.8960   |  0.5320   |
| F     |  0.2330  |  0.2460  |
| G     |  0.8910 |  0.5880 |
| H     |  0.8940 |  0.5870 |
| I     |  0.8960 |  0.5770 |
| J     |  0.5930 |  0.3920 |
| K     |  0.7510 |  0.4740 |
| M     |  0.9140 |  0.5830 |
| N     |  0.8500 |  0.5830 |
| O     |  0.8670 |  0.5720 |
| P     |  0.8970 |  0.5890 |
| Q     |  0.8910 |  0.5700 |
| R     |  0.8110 |  0.5070 |
| S     |  0.8230 |  0.5700 |
| T     |  0.9340 |  0.5900 |
| U     |  0.8820 |  0.5850 |
| V     |  0.9010 |  0.5740 |
| W     |  0.8750 |  0.5610 |
| X     |  0.7950 |  0.5240 |
| Y     |  0.9370 |  0.5880 |
| Z     |  0.7680 |  0.5640 |
| a     |  0.9550 |  0.5310 |



*Continued on next page...*

*Continued from previous page...*

| Chain | Atom inclusion                                                                            | Q-score                                                                                   |
|-------|-------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------|
| b     |  0.6970  |  0.4340  |
| c     |  0.7100  |  0.4550  |
| d     |  0.7840  |  0.5110  |
| e     |  0.8020  |  0.5030  |
| f     |  0.8230  |  0.5300  |
| g     |  0.6120  |  0.4300  |
| h     |  0.7060  |  0.4900  |
| i     |  0.8400  |  0.5160  |
| j     |  0.7890  |  0.5070  |
| k     |  0.7420  |  0.4890  |
| l     |  0.7350  |  0.4850  |
| m     |  0.8210  |  0.5700  |
| n     |  0.7180  |  0.4780  |
| o     |  0.8970  |  0.5460  |
| p     |  0.7620  |  0.4760  |
| q     |  0.8520  |  0.5230  |
| r     |  0.8410  |  0.5300  |
| s     |  0.7330  |  0.4610  |
| t     |  0.7110  |  0.4590  |
| u     |  0.7920 |  0.5150 |