



## Full wwPDB EM Validation Report ⓘ

Aug 5, 2026 – 09:33 am BST

PDB ID : 9RBF / pdb\_00009rbf  
EMDB ID : EMD-53892  
Title : Structure of a stalled E. coli 70S RNC-NuoK-86 in complex with the membrane protein insertase SecYEG-YidC  
Authors : Rosales-Hernandez, C.; Busch, M.; Kamel, M.; Beckmann, R.; Kedrov, A.  
Deposited on : 2025-05-22  
Resolution : 2.44 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:

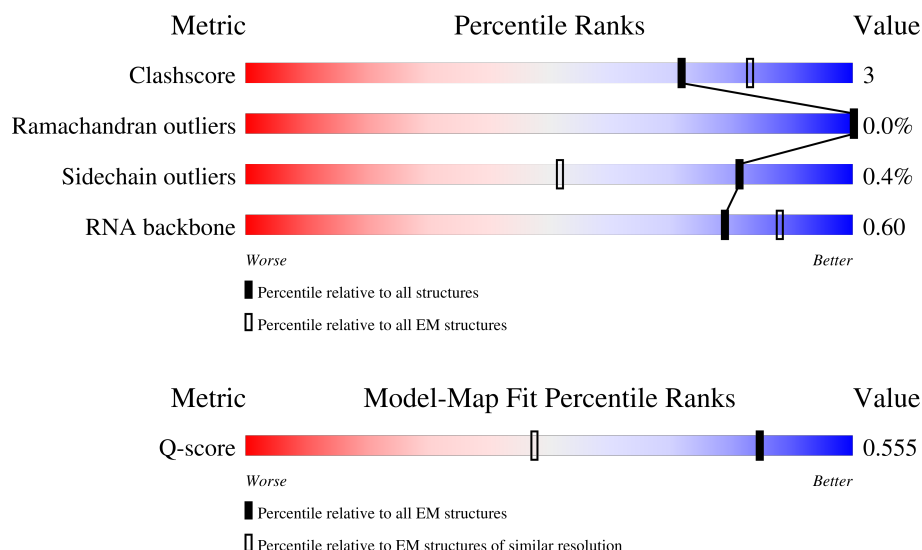
EMDB validation analysis : 0.0.1.dev133  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.50

# 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 2.44 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.



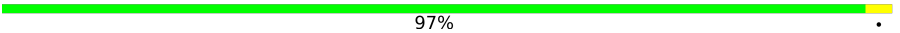
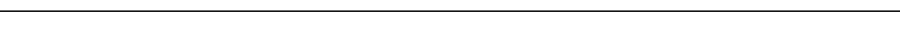
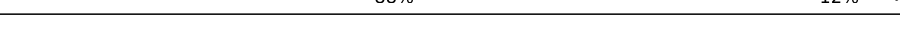
| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| RNA backbone          | 8273                        | 3508                        | -                                                        |
| Q-score               | -                           | 25397                       | 5856 ( 1.94 - 2.94 )                                     |

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     | 55     | <br>82% 11% 7%   |
| 2   | 1     | 46     | <br>96% .        |
| 3   | 2     | 65     | <br>89% 9% .     |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 4   | 3     | 38     |    |
| 5   | 4     | 70     |    |
| 6   | 5     | 2      |    |
| 7   | 6     | 443    |    |
| 8   | 7     | 127    |    |
| 9   | 8     | 110    |    |
| 10  | 9     | 548    |    |
| 11  | A     | 1542   |    |
| 12  | B     | 241    |    |
| 13  | C     | 233    |    |
| 14  | D     | 206    |    |
| 15  | E     | 167    |    |
| 16  | F     | 135    |  |
| 17  | G     | 179    |  |
| 18  | H     | 130    |  |
| 19  | I     | 130    |  |
| 20  | J     | 103    |  |
| 21  | K     | 129    |  |
| 22  | L     | 124    |  |
| 23  | M     | 118    |  |
| 24  | N     | 101    |  |
| 25  | O     | 89     |  |
| 26  | P     | 82     |  |
| 27  | Q     | 84     |  |
| 28  | R     | 75     |  |

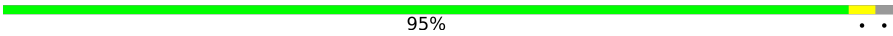
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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 29  | S     | 92     |                  |
| 30  | T     | 87     |                  |
| 31  | U     | 71     |                  |
| 32  | V     | 119    |                  |
| 33  | X     | 9      |                  |
| 34  | Y     | 77     |                  |
| 35  | Z     | 77     |                  |
| 36  | a     | 2904   |                  |
| 37  | b     | 120    |                  |
| 38  | c     | 273    |                  |
| 39  | d     | 209    |                  |
| 40  | e     | 201    |                  |
| 41  | f     | 179    |                  |
| 42  | g     | 177    |                  |
| 43  | h     | 149    |                  |
| 44  | i     | 142    |                  |
| 45  | j     | 123    |                  |
| 46  | k     | 144    |                  |
| 47  | l     | 136    |                  |
| 48  | m     | 127    |                  |
| 49  | n     | 117    |                  |
| 50  | o     | 115    |                  |
| 51  | p     | 118    |                  |
| 52  | q     | 103    |                  |
| 53  | r     | 110    |                  |

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| Mol | Chain | Length | Quality of chain                                                                             |
|-----|-------|--------|----------------------------------------------------------------------------------------------|
| 54  | s     | 100    |  89% 7%    |
| 55  | t     | 104    |  95%       |
| 56  | u     | 94     |  81% 19%   |
| 57  | v     | 85     |  86% 6% 8% |
| 58  | w     | 78     |  91% 8%    |
| 59  | x     | 63     |  87% 11%   |
| 60  | y     | 59     |  90% 8%    |
| 61  | z     | 57     |  91% 7%    |

## 2 Entry composition

There are 65 unique types of molecules in this entry. The entry contains 150736 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 Large ribosomal subunit protein bL33.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 1   | 0     | 51       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 417   | 269 | 76 | 72 |         |       |

- Molecule 2 is a protein called Large ribosomal subunit protein bL34.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 2   | 1     | 46       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 377   | 228 | 90 | 57 | 2 |         |       |

- Molecule 3 is a protein called Large ribosomal subunit protein bL35.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 3   | 2     | 64       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 504   | 323 | 105 | 74 | 2 |         |       |

- Molecule 4 is a protein called Large ribosomal subunit protein bL36A.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 4   | 3     | 38       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 302   | 185 | 65 | 48 | 4 |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 5   | 4     | 60       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 480   | 299 | 90 | 85 | 6 |         |       |

- Molecule 6 is a RNA chain called E-site tRNA.

| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf | Trace |
|-----|-------|----------|-------|----|---|----|---|---------|-------|
| 6   | 5     | 2        | Total | C  | N | O  | P | 0       | 0     |
|     |       |          | 42    | 19 | 8 | 13 | 2 |         |       |

- Molecule 7 is a protein called Protein translocase subunit SecY.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 7   | 6     | 421      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3260  | 2158 | 535 | 550 | 17 |         |       |

- Molecule 8 is a protein called Protein translocase subunit SecE.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 8   | 7     | 114      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 873   | 579 | 149 | 142 | 3 |         |       |

- Molecule 9 is a protein called Protein-export membrane protein SecG.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 9   | 8     | 56       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 431   | 287 | 68 | 72 | 4 |         |       |

- Molecule 10 is a protein called Membrane protein insertase YidC.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 10  | 9     | 467      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3716  | 2419 | 606 | 670 | 21 |         |       |

- Molecule 11 is a RNA chain called 16S rRNA.

| Mol | Chain | Residues | Atoms |       |      |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|-------|
| 11  | A     | 1519     | Total | C     | N    | O     | P    | 0       | 0     |
|     |       |          | 32612 | 14552 | 5986 | 10555 | 1519 |         |       |

- Molecule 12 is a protein called Small ribosomal subunit protein uS2.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 12  | B     | 224      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1753  | 1109 | 315 | 321 | 8 |         |       |

- Molecule 13 is a protein called Small ribosomal subunit protein uS3.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 13  | C     | 206      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1624  | 1028 | 305 | 288 | 3 |         |       |

- Molecule 14 is a protein called Small ribosomal subunit protein uS4.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 14  | D     | 205      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1643  | 1026 | 315 | 298 | 4 |         |       |

- Molecule 15 is a protein called Small ribosomal subunit protein uS5.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 15  | E     | 156      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1152  | 717 | 217 | 212 | 6 |         |       |

- Molecule 16 is a protein called Small ribosomal subunit protein bS6, fully modified isoform.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 16  | F     | 103      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 839   | 530 | 151 | 151 | 7 |         |       |

- Molecule 17 is a protein called Small ribosomal subunit protein uS7.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 17  | G     | 153      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1203  | 750 | 231 | 218 | 4 |         |       |

- Molecule 18 is a protein called Small ribosomal subunit protein uS8.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 18  | H     | 129      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 979   | 616 | 173 | 184 | 6 |         |       |

- Molecule 19 is a protein called Small ribosomal subunit protein uS9.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 19  | I     | 127      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1022  | 634 | 206 | 179 | 3 |         |       |

- Molecule 20 is a protein called Small ribosomal subunit protein uS10.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 20  | J     | 98       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 786   | 493 | 150 | 142 | 1 |         |       |

- Molecule 21 is a protein called Small ribosomal subunit protein uS11.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 21  | K     | 117      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 877   | 540 | 174 | 160 | 3 |         |       |

- Molecule 22 is a protein called Small ribosomal subunit protein uS12.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 22  | L     | 123      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 957   | 591 | 196 | 165 | 5 |         |       |

- Molecule 23 is a protein called Small ribosomal subunit protein uS13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 23  | M     | 115      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 891   | 552 | 179 | 157 | 3 |         |       |

- Molecule 24 is a protein called Small ribosomal subunit protein uS14.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 24  | N     | 100      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 805   | 499 | 164 | 139 | 3 |         |       |

- Molecule 25 is a protein called Small ribosomal subunit protein uS15.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 25  | O     | 88       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 714   | 439 | 144 | 130 | 1 |         |       |

- Molecule 26 is a protein called Small ribosomal subunit protein bS16.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 26  | P     | 81       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 643   | 403 | 127 | 112 | 1 |         |       |

- Molecule 27 is a protein called Small ribosomal subunit protein uS17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 27  | Q     | 79       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 641   | 406 | 120 | 112 | 3 |         |       |

- Molecule 28 is a protein called Small ribosomal subunit protein bS18.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 28  | R     | 66       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 544   | 345 | 102 | 96 | 1 |         |       |

- Molecule 29 is a protein called Small ribosomal subunit protein uS19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 29  | S     | 84       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 668   | 427 | 127 | 112 | 2 |         |       |

- Molecule 30 is a protein called Small ribosomal subunit protein bS20.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 30  | T     | 86       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 670   | 414 | 138 | 115 | 3 |         |       |

- Molecule 31 is a protein called Small ribosomal subunit protein bS21.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 31  | U     | 70       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 589   | 366 | 125 | 97 | 1 |         |       |

- Molecule 32 is a protein called NuoK-86 nascent peptide.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 32  | V     | 89       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 542   | 344 | 99 | 99 |         |       |

- Molecule 33 is a RNA chain called mRNA.

| Mol | Chain | Residues | Atoms |    |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---|---------|-------|
| 33  | X     | 9        | Total | C  | N  | O  | P | 0       | 0     |
|     |       |          | 189   | 84 | 31 | 65 | 9 |         |       |

- Molecule 34 is a RNA chain called A-site tRNA-Pro.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 34  | Y     | 77       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 1646  | 734 | 297 | 539 | 76 |         |       |

- Molecule 35 is a RNA chain called P-site tRNA-Pro.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 35  | Z     | 77       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 1644  | 733 | 295 | 540 | 76 |         |       |

- Molecule 36 is a RNA chain called 23S rRNA.

| Mol | Chain | Residues | Atoms |       |       |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|-------|
| 36  | a     | 2753     | Total | C     | N     | O     | P    | 0       | 0     |
|     |       |          | 59127 | 26381 | 10897 | 19096 | 2753 |         |       |

- Molecule 37 is a RNA chain called 5S rRNA.

| Mol | Chain | Residues | Atoms |      |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|-------|
| 37  | b     | 119      | Total | C    | N   | O   | P   | 0       | 0     |
|     |       |          | 2549  | 1135 | 466 | 829 | 119 |         |       |

- Molecule 38 is a protein called Large ribosomal subunit protein uL2.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 38  | c     | 271      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2082  | 1288 | 423 | 364 | 7 |         |       |

- Molecule 39 is a protein called Large ribosomal subunit protein uL3.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 39  | d     | 209      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1566  | 980 | 288 | 294 | 4 |         |       |

- Molecule 40 is a protein called Large ribosomal subunit protein uL4.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 40  | e     | 201      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1552  | 974 | 283 | 290 | 5 |         |       |

- Molecule 41 is a protein called Large ribosomal subunit protein uL5.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 41  | f     | 177      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1410  | 899 | 249 | 256 | 6 |         |       |

- Molecule 42 is a protein called Large ribosomal subunit protein uL6.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 42  | g     | 176      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1323  | 832 | 243 | 246 | 2 |         |       |

- Molecule 43 is a protein called Large ribosomal subunit protein bL9.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 43  | h     | 41       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 303   | 194 | 54 | 54 | 1 |         |       |

- Molecule 44 is a protein called Large ribosomal subunit protein uL13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 44  | i     | 142      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1129  | 714 | 212 | 199 | 4 |         |       |

- Molecule 45 is a protein called Large ribosomal subunit protein uL14.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 45  | j     | 123      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 946   | 593 | 181 | 166 | 6 |         |       |

- Molecule 46 is a protein called Large ribosomal subunit protein uL15.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 46  | k     | 144      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1053  | 654 | 207 | 190 | 2 |         |       |

- Molecule 47 is a protein called 50S ribosomal protein L16.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 47  | l     | 136      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1074  | 686 | 205 | 177 | 6 |         |       |

- Molecule 48 is a protein called Large ribosomal subunit protein bL17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 48  | m     | 118      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 945   | 585 | 194 | 161 | 5 |         |       |

- Molecule 49 is a protein called Large ribosomal subunit protein uL18.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 49  | n     | 116      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 892   | 552 | 178 | 162 |         |       |

- Molecule 50 is a protein called Large ribosomal subunit protein bL19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 50  | o     | 114      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 917   | 574 | 179 | 163 | 1 |         |       |

- Molecule 51 is a protein called Large ribosomal subunit protein bL20.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 51  | p     | 117      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 947   | 604 | 192 | 151 |         |       |

- Molecule 52 is a protein called Large ribosomal subunit protein bL21.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 52  | q     | 103      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 816   | 516 | 153 | 145 | 2 |         |       |

- Molecule 53 is a protein called Large ribosomal subunit protein uL22.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 53  | r     | 110      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 857   | 532 | 166 | 156 | 3 |         |       |

- Molecule 54 is a protein called Large ribosomal subunit protein uL23.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 54  | s     | 93       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 738   | 466 | 139 | 131 | 2 |         |       |

- Molecule 55 is a protein called Large ribosomal subunit protein uL24.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 55  | t     | 102      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 779   | 492 | 146 | 141 |         |       |

- Molecule 56 is a protein called Large ribosomal subunit protein bL25.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 56  | u     | 94       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 753   | 479 | 137 | 134 | 3 |         |       |

- Molecule 57 is a protein called Large ribosomal subunit protein bL27.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 57  | v     | 78       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 592   | 365 | 119 | 107 | 1 |         |       |

- Molecule 58 is a protein called Large ribosomal subunit protein bL28.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 58  | w     | 77       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 625   | 388 | 129 | 106 | 2 |         |       |

- Molecule 59 is a protein called Large ribosomal subunit protein uL29.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 59  | x     | 62       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 501   | 308 | 98 | 94 | 1 |         |       |

- Molecule 60 is a protein called Large ribosomal subunit protein uL30.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 60  | y     | 58       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 449   | 281 | 87 | 79 | 2 |         |       |

- Molecule 61 is a protein called Large ribosomal subunit protein bL32.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 61  | z     | 56       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 444   | 269 | 94 | 80 | 1 |         |       |

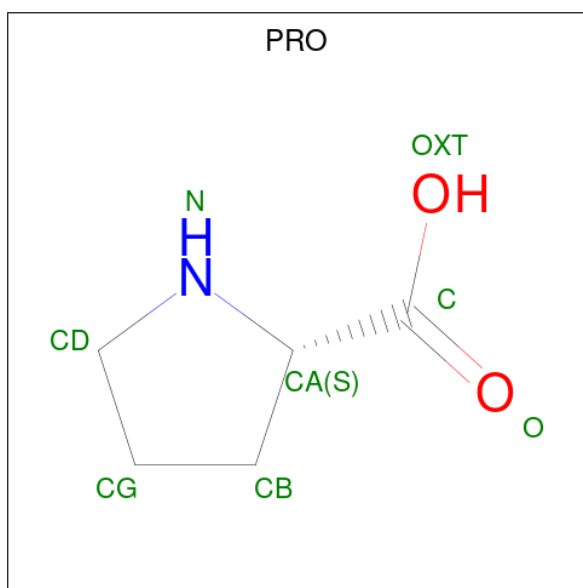
- Molecule 62 is ZINC ION (CCD ID: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 62  | 3     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 62  | 4     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |

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

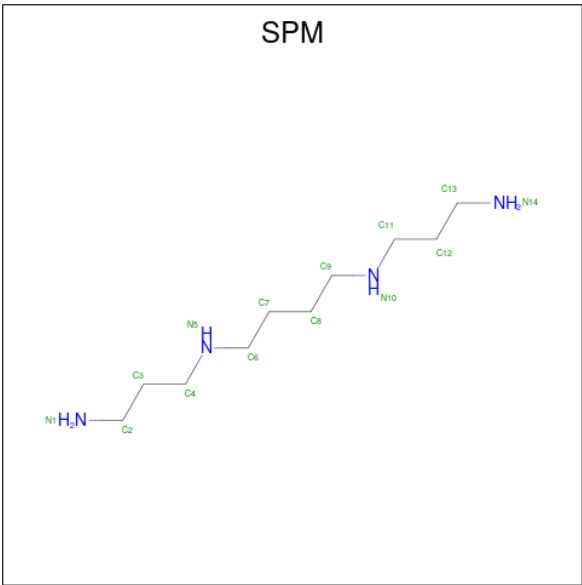
| Mol | Chain | Residues | Atoms |     | AltConf |
|-----|-------|----------|-------|-----|---------|
| 63  | A     | 91       | Total | Mg  | 0       |
|     |       |          | 91    | 91  |         |
| 63  | N     | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |
| 63  | Q     | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |
| 63  | a     | 208      | Total | Mg  | 0       |
|     |       |          | 208   | 208 |         |
| 63  | b     | 5        | Total | Mg  | 0       |
|     |       |          | 5     | 5   |         |
| 63  | c     | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |
| 63  | d     | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |
| 63  | z     | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |

- Molecule 64 is PROLINE (CCD ID: PRO) (formula:  $C_5H_9NO_2$ ).



| Mol | Chain | Residues | Atoms |   |   |   | AltConf |
|-----|-------|----------|-------|---|---|---|---------|
| 64  | Y     | 1        | Total | C | N | O | 0       |
|     |       |          | 7     | 5 | 1 | 1 |         |

- Molecule 65 is SPERMINE (CCD ID: SPM) (formula:  $C_{10}H_{26}N_4$ ).



| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 65  | a     | 1        | Total | C  | N | 0       |
|     |       |          | 14    | 10 | 4 |         |

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

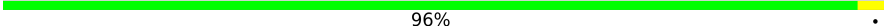
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

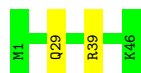
- Molecule 1: Large ribosomal subunit protein bL33

Chain 0: 



- Molecule 2: Large ribosomal subunit protein bL34

Chain 1: 

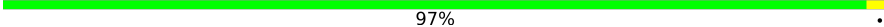


- Molecule 3: Large ribosomal subunit protein bL35

Chain 2: 



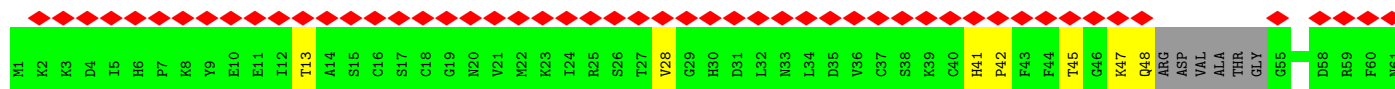
- Molecule 4: Large ribosomal subunit protein bL36A

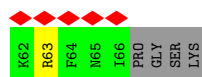
Chain 3: 



- Molecule 5: Large ribosomal subunit protein bL31A

Chain 4: 





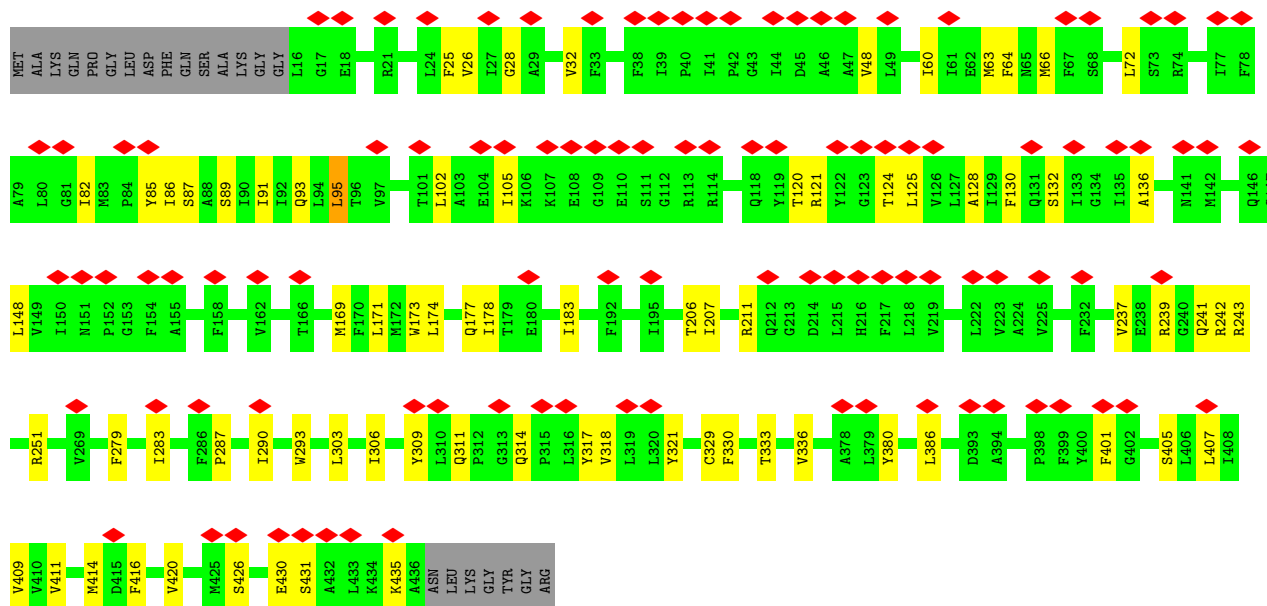
• Molecule 6: E-site tRNA

Chain 5: 50% 50%



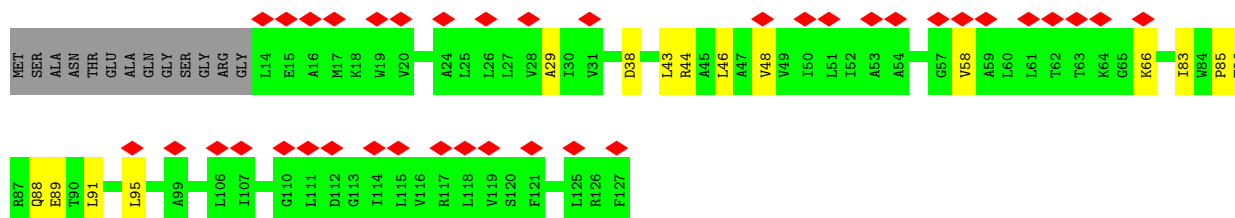
• Molecule 7: Protein translocase subunit SecY

Chain 6: 24% 78% 17% 5%



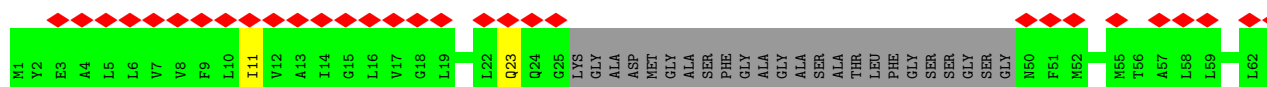
• Molecule 8: Protein translocase subunit SecE

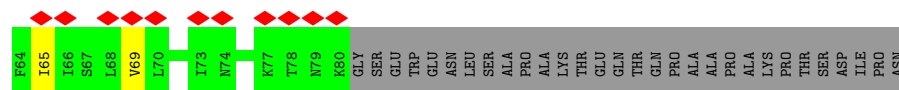
Chain 7: 30% 78% 12% 10%



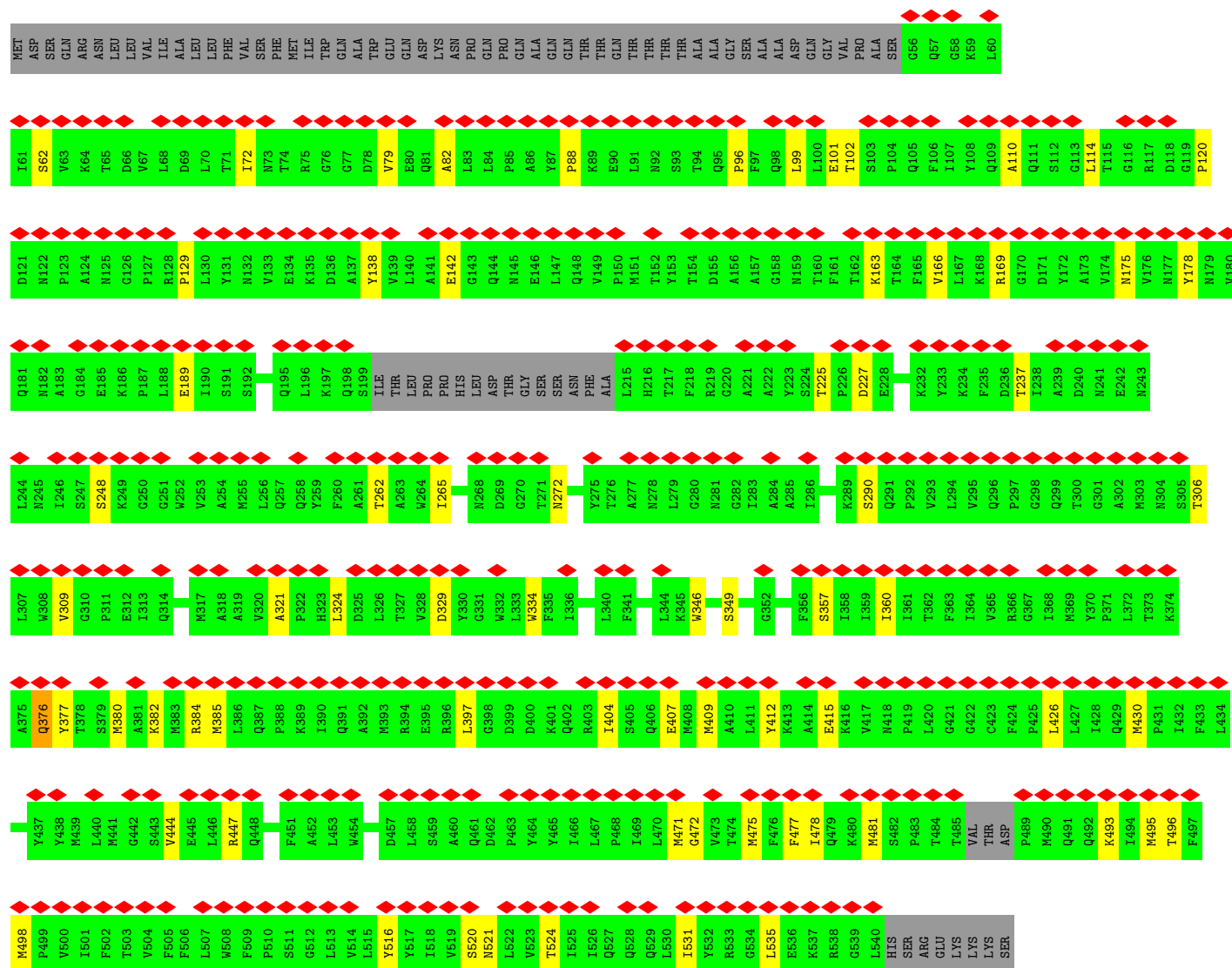
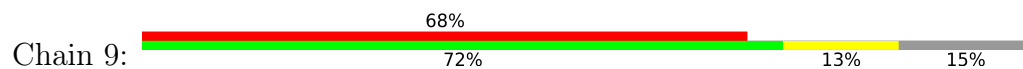
• Molecule 9: Protein-export membrane protein SecG

Chain 8: 37% 47% 49%

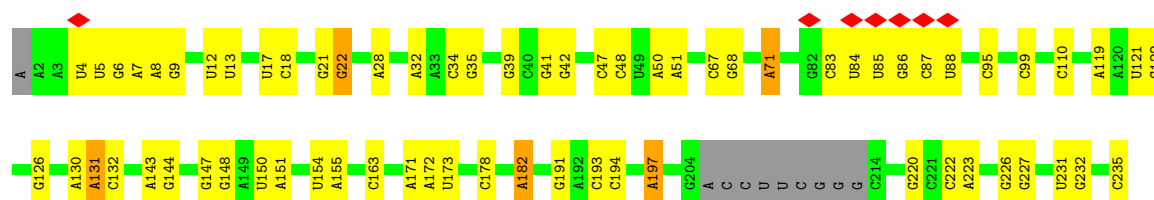


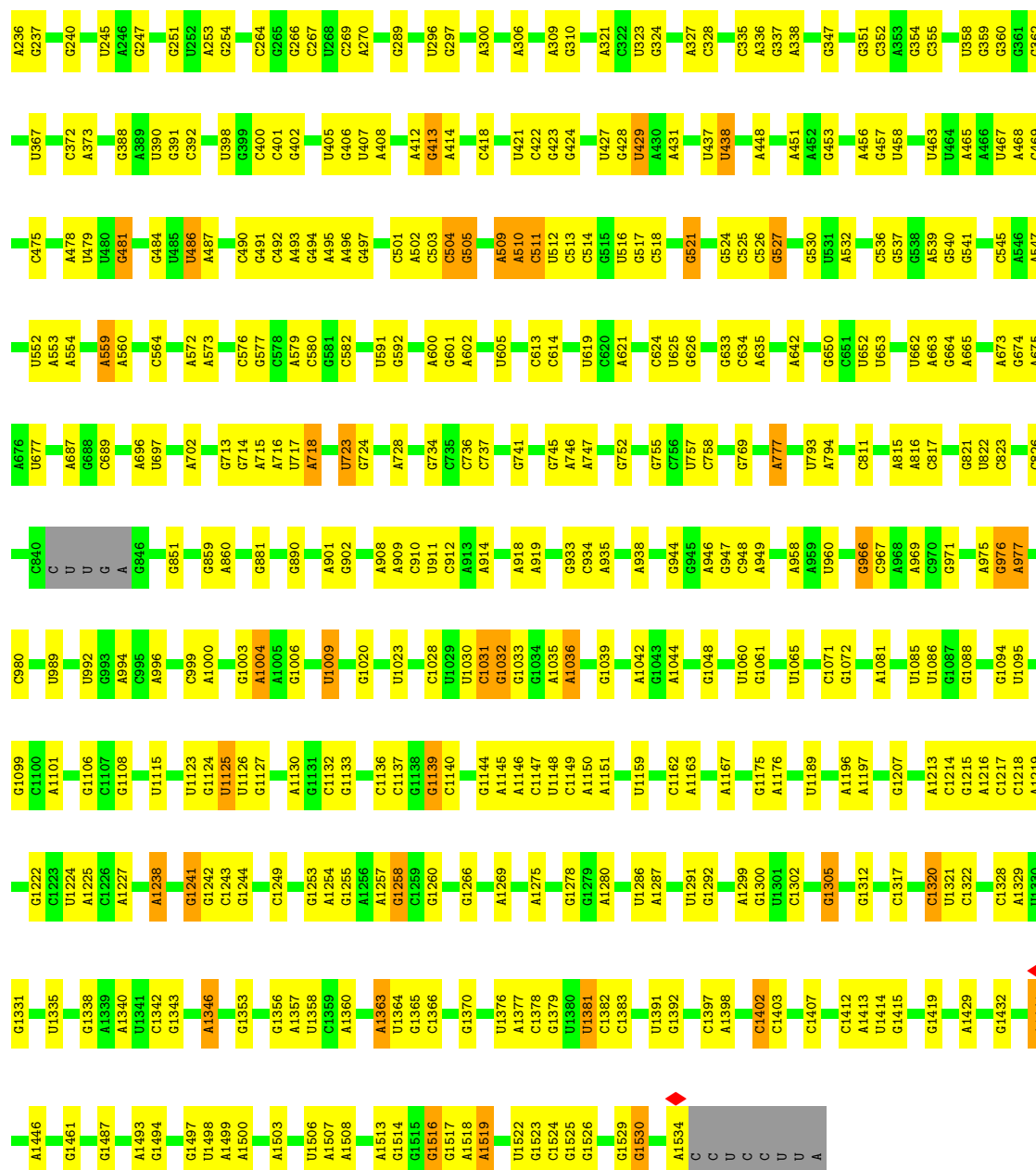


• Molecule 10: Membrane protein insertase YidC



• Molecule 11: 16S rRNA





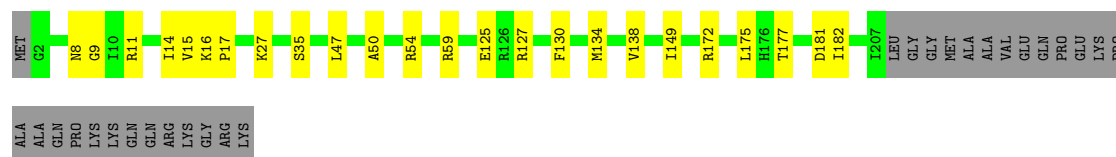
- Molecule 12: Small ribosomal subunit protein uS2

Chain B: 87% 6% 7%

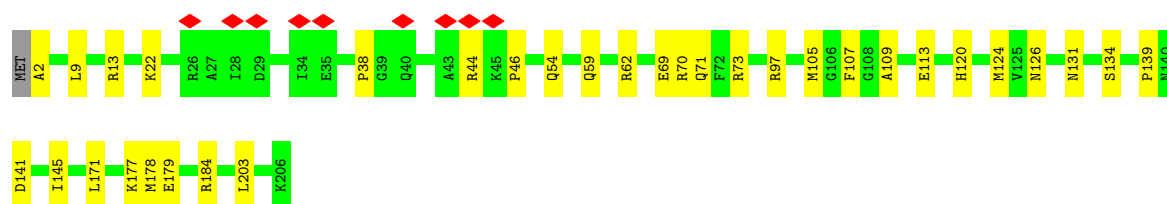
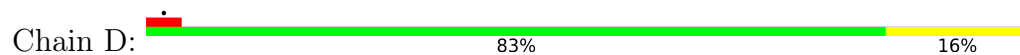


- Molecule 13: Small ribosomal subunit protein uS3

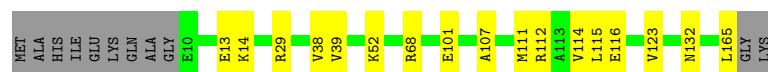
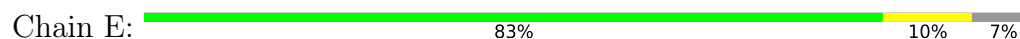
Chain C: 78% 10% 12%



- Molecule 14: Small ribosomal subunit protein uS4



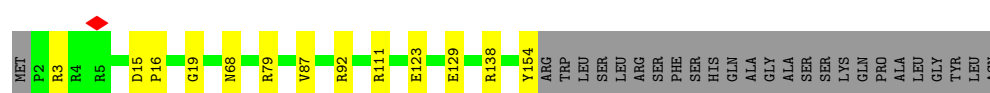
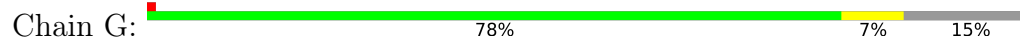
- Molecule 15: Small ribosomal subunit protein uS5



- Molecule 16: Small ribosomal subunit protein bS6, fully modified isoform



- Molecule 17: Small ribosomal subunit protein uS7

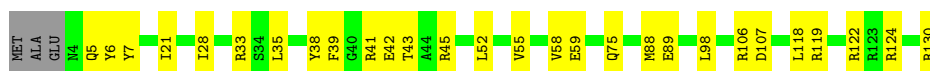


- Molecule 18: Small ribosomal subunit protein uS8



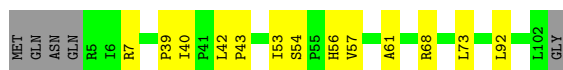
- Molecule 19: Small ribosomal subunit protein uS9





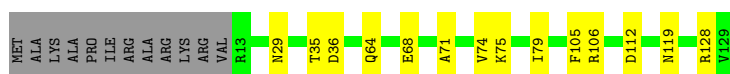
- Molecule 20: Small ribosomal subunit protein uS10

Chain J: 83% 13% 5%



- Molecule 21: Small ribosomal subunit protein uS11

Chain K: 80% 11% 9%



- Molecule 22: Small ribosomal subunit protein uS12

Chain L: 86% 13% .



- Molecule 23: Small ribosomal subunit protein uS13

Chain M: 82% 15% .



- Molecule 24: Small ribosomal subunit protein uS14

Chain N: 82% 16% ..



- Molecule 25: Small ribosomal subunit protein uS15

Chain O: 91% 8% .

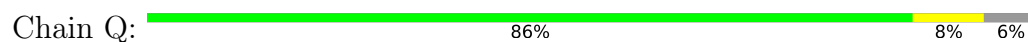


- Molecule 26: Small ribosomal subunit protein bS16

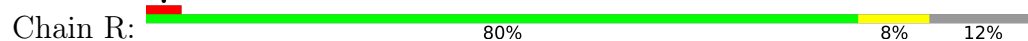
Chain P: 90% 9% .



- Molecule 27: Small ribosomal subunit protein uS17



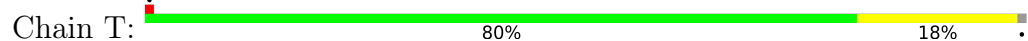
- Molecule 28: Small ribosomal subunit protein bS18



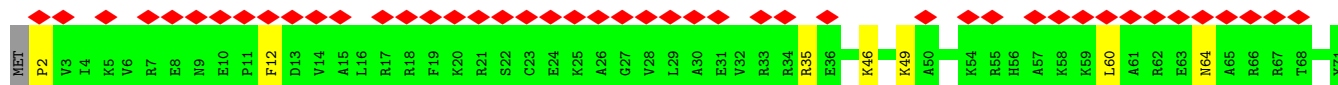
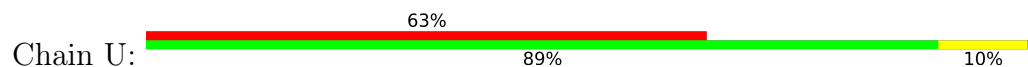
- Molecule 29: Small ribosomal subunit protein uS19



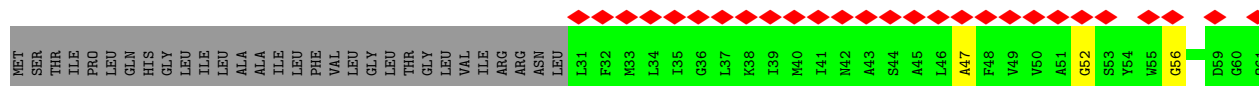
- Molecule 30: Small ribosomal subunit protein bS20

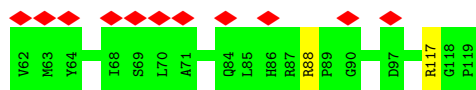


- Molecule 31: Small ribosomal subunit protein bS21



- Molecule 32: NuoK-86 nascent peptide





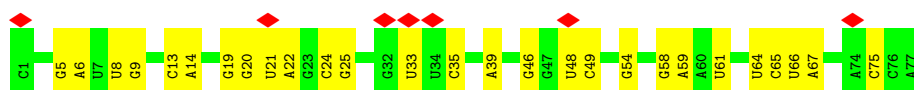
• Molecule 33: mRNA

Chain X: 89% 11%



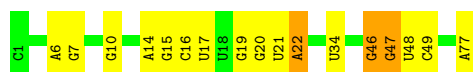
• Molecule 34: A-site tRNA-Pro

Chain Y: 9% 65% 35%



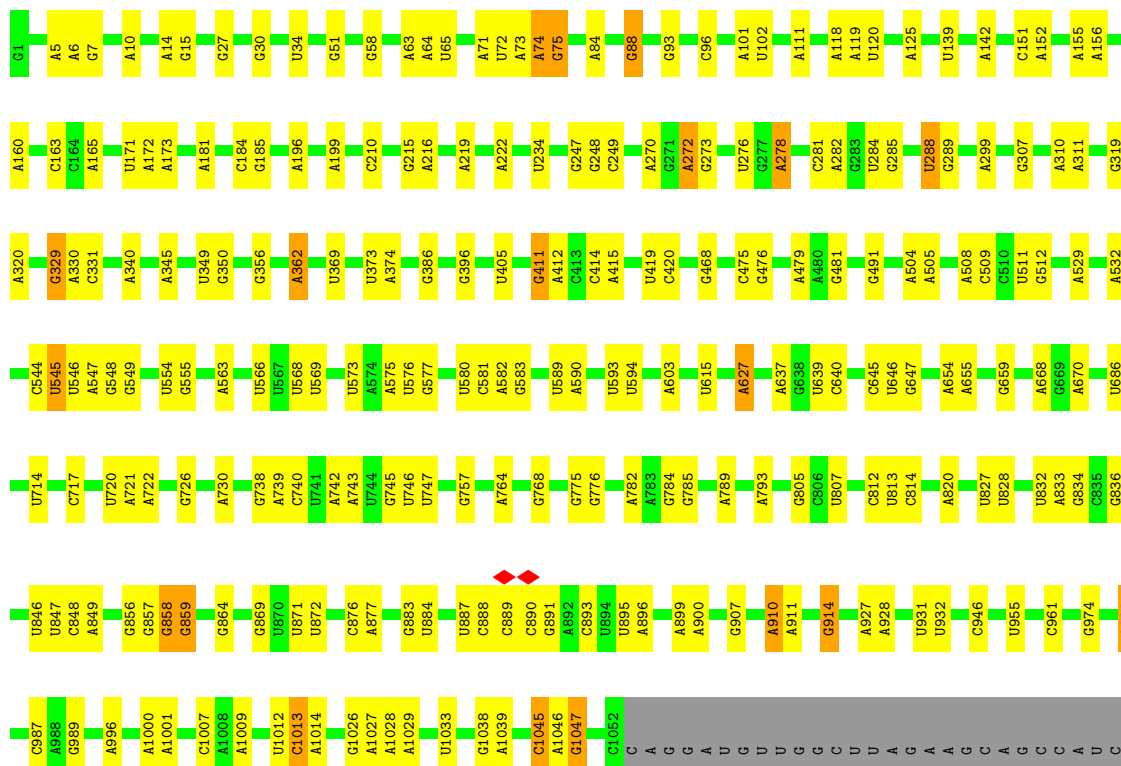
• Molecule 35: P-site tRNA-Pro

Chain Z: 78% 18%

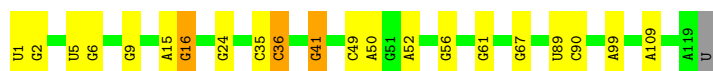


• Molecule 36: 23S rRNA

Chain a: 73% 21% 5%







- Molecule 38: Large ribosomal subunit protein uL2

Chain c: 91% 8%



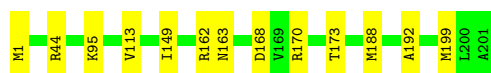
- Molecule 39: Large ribosomal subunit protein uL3

Chain d: 94% 6%



- Molecule 40: Large ribosomal subunit protein uL4

Chain e: 94% 6%



- Molecule 41: Large ribosomal subunit protein uL5

Chain f: 84% 15%



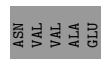
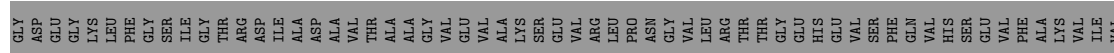
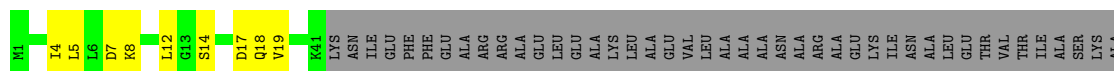
- Molecule 42: Large ribosomal subunit protein uL6

Chain g: 95% 5%

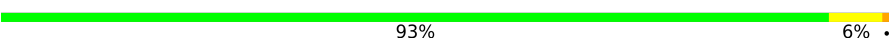


- Molecule 43: Large ribosomal subunit protein bL9

Chain h: 21% 6% 72%

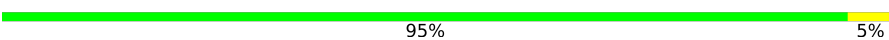


- Molecule 44: Large ribosomal subunit protein uL13

Chain i:  93% 6%

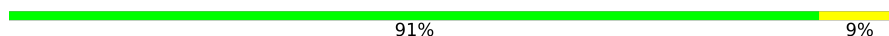


- Molecule 45: Large ribosomal subunit protein uL14

Chain j:  95% 5%



- Molecule 46: Large ribosomal subunit protein uL15

Chain k:  91% 9%



- Molecule 47: 50S ribosomal protein L16

Chain l:  90% 10%

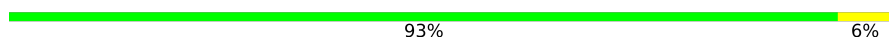


- Molecule 48: Large ribosomal subunit protein bL17

Chain m:  88% 5% 7%



- Molecule 49: Large ribosomal subunit protein uL18

Chain n:  93% 6%

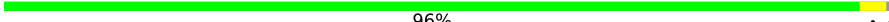


- Molecule 50: Large ribosomal subunit protein bL19

Chain o:  89% 10%



- Molecule 51: Large ribosomal subunit protein bL20

Chain p:  96%



- Molecule 52: Large ribosomal subunit protein bL21

Chain q:  93% 7%



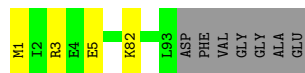
- Molecule 53: Large ribosomal subunit protein uL22

Chain r:  91% 9%



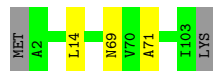
- Molecule 54: Large ribosomal subunit protein uL23

Chain s:  89% 7%



- Molecule 55: Large ribosomal subunit protein uL24

Chain t:  95%



- Molecule 56: Large ribosomal subunit protein bL25

Chain u:  81% 19%



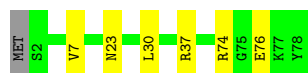
- Molecule 57: Large ribosomal subunit protein bL27

Chain v:  86% 6% 8%



- Molecule 58: Large ribosomal subunit protein bL28

Chain w:  91% 8%



- Molecule 59: Large ribosomal subunit protein uL29

Chain x:  87% 11%



- Molecule 60: Large ribosomal subunit protein uL30

Chain y:  90% 8%



- Molecule 61: Large ribosomal subunit protein bL32

Chain z:  91% 7%



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 113368                                  | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | TFS KRIOS                               | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 40                                      | Depositor |
| Minimum defocus (nm)                 | 500                                     | Depositor |
| Maximum defocus (nm)                 | 3500                                    | Depositor |
| Magnification                        | Not provided                            |           |
| Image detector                       | FEI FALCON IV (4k x 4k)                 | Depositor |
| Maximum map value                    | 2.073                                   | Depositor |
| Minimum map value                    | -0.651                                  | Depositor |
| Average map value                    | 0.001                                   | Depositor |
| Map value standard deviation         | 0.061                                   | Depositor |
| Recommended contour level            | 0.15                                    | Depositor |
| Map size (Å)                         | 494.36, 494.36, 494.36                  | wwPDB     |
| Map dimensions                       | 680, 680, 680                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 0.727, 0.727, 0.727                     | Depositor |

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MEQ, D2T, G7M, PSU, 5MC, H2U, MA6, OMC, OMG, 1MG, UR3, MG, 4OC, 6MZ, OMU, SPM, 2MA, 2MG, ZN

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     | 0.17         | 0/424   | 0.38        | 0/565         |
| 2   | 1     | 0.21         | 0/380   | 0.31        | 0/498         |
| 3   | 2     | 0.22         | 0/513   | 0.37        | 0/676         |
| 4   | 3     | 0.21         | 0/303   | 0.37        | 0/397         |
| 5   | 4     | 0.16         | 0/488   | 0.38        | 0/649         |
| 6   | 5     | 0.11         | 0/46    | 0.12        | 0/69          |
| 7   | 6     | 0.23         | 0/3335  | 0.59        | 0/4526        |
| 8   | 7     | 0.21         | 0/886   | 0.57        | 0/1209        |
| 9   | 8     | 0.20         | 0/434   | 0.46        | 0/584         |
| 10  | 9     | 0.21         | 0/3813  | 0.50        | 0/5179        |
| 11  | A     | 0.16         | 0/36236 | 0.29        | 0/56520       |
| 12  | B     | 0.18         | 0/1784  | 0.43        | 0/2403        |
| 13  | C     | 0.17         | 0/1651  | 0.38        | 0/2225        |
| 14  | D     | 0.16         | 0/1665  | 0.38        | 0/2227        |
| 15  | E     | 0.20         | 0/1165  | 0.44        | 0/1568        |
| 16  | F     | 0.22         | 0/858   | 0.53        | 0/1160        |
| 17  | G     | 0.19         | 0/1219  | 0.47        | 0/1635        |
| 18  | H     | 0.17         | 0/989   | 0.39        | 0/1326        |
| 19  | I     | 0.18         | 0/1034  | 0.50        | 0/1375        |
| 20  | J     | 0.22         | 0/796   | 0.54        | 0/1077        |
| 21  | K     | 0.19         | 0/893   | 0.48        | 0/1205        |
| 22  | L     | 0.17         | 0/960   | 0.42        | 0/1286        |
| 23  | M     | 0.17         | 0/900   | 0.49        | 0/1204        |
| 24  | N     | 0.17         | 0/817   | 0.43        | 1/1088 (0.1%) |
| 25  | O     | 0.15         | 0/722   | 0.34        | 0/964         |
| 26  | P     | 0.19         | 0/653   | 0.43        | 0/877         |
| 27  | Q     | 0.20         | 0/650   | 0.53        | 0/871         |
| 28  | R     | 0.18         | 0/553   | 0.45        | 0/742         |
| 29  | S     | 0.15         | 0/685   | 0.40        | 0/922         |
| 30  | T     | 0.24         | 0/676   | 0.48        | 0/895         |
| 31  | U     | 0.16         | 0/597   | 0.40        | 0/792         |

| Mol | Chain | Bond lengths |          | Bond angles |                 |
|-----|-------|--------------|----------|-------------|-----------------|
|     |       | RMSZ         | # Z  >5  | RMSZ        | # Z  >5         |
| 32  | V     | 0.19         | 0/559    | 0.48        | 0/777           |
| 33  | X     | 0.15         | 0/209    | 0.26        | 0/323           |
| 34  | Y     | 0.13         | 0/1840   | 0.30        | 0/2869          |
| 35  | Z     | 0.13         | 0/1837   | 0.25        | 0/2864          |
| 36  | a     | 0.24         | 0/65718  | 0.31        | 0/102519        |
| 37  | b     | 0.19         | 0/2850   | 0.27        | 0/4444          |
| 38  | c     | 0.23         | 0/2121   | 0.38        | 0/2852          |
| 39  | d     | 0.23         | 0/1576   | 0.37        | 0/2119          |
| 40  | e     | 0.21         | 0/1571   | 0.35        | 0/2113          |
| 41  | f     | 0.21         | 0/1434   | 0.51        | 0/1926          |
| 42  | g     | 0.21         | 0/1343   | 0.50        | 0/1816          |
| 43  | h     | 0.22         | 0/306    | 0.62        | 0/413           |
| 44  | i     | 0.21         | 0/1152   | 0.35        | 0/1551          |
| 45  | j     | 0.23         | 0/955    | 0.37        | 0/1279          |
| 46  | k     | 0.21         | 0/1062   | 0.37        | 0/1413          |
| 47  | l     | 0.24         | 0/1093   | 0.37        | 0/1460          |
| 48  | m     | 0.22         | 0/958    | 0.40        | 0/1281          |
| 49  | n     | 0.18         | 0/902    | 0.40        | 0/1209          |
| 50  | o     | 0.21         | 0/929    | 0.32        | 0/1242          |
| 51  | p     | 0.23         | 0/960    | 0.36        | 0/1278          |
| 52  | q     | 0.23         | 0/829    | 0.46        | 0/1107          |
| 53  | r     | 0.22         | 0/864    | 0.37        | 0/1156          |
| 54  | s     | 0.21         | 0/744    | 0.37        | 0/994           |
| 55  | t     | 0.20         | 0/787    | 0.38        | 0/1051          |
| 56  | u     | 0.19         | 0/766    | 0.39        | 0/1025          |
| 57  | v     | 0.20         | 0/599    | 0.36        | 0/792           |
| 58  | w     | 0.21         | 0/635    | 0.35        | 0/848           |
| 59  | x     | 0.19         | 0/502    | 0.38        | 0/667           |
| 60  | y     | 0.22         | 0/453    | 0.47        | 0/605           |
| 61  | z     | 0.21         | 0/450    | 0.37        | 0/599           |
| All | All   | 0.21         | 0/162129 | 0.35        | 1/241306 (0.0%) |

There are no bond length outliers.

All (1) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|------|-------------|----------|
| 24  | N     | 89  | MET  | CB-CG-SD | 5.52 | 129.27      | 112.70   |

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     | 417   | 0        | 451      | 4       | 0            |
| 2   | 1     | 377   | 0        | 418      | 2       | 0            |
| 3   | 2     | 504   | 0        | 572      | 6       | 0            |
| 4   | 3     | 302   | 0        | 340      | 1       | 0            |
| 5   | 4     | 480   | 0        | 478      | 8       | 0            |
| 6   | 5     | 42    | 0        | 23       | 0       | 0            |
| 7   | 6     | 3260  | 0        | 3416     | 47      | 0            |
| 8   | 7     | 873   | 0        | 966      | 9       | 0            |
| 9   | 8     | 431   | 0        | 475      | 2       | 0            |
| 10  | 9     | 3716  | 0        | 3720     | 41      | 0            |
| 11  | A     | 32612 | 0        | 16428    | 216     | 0            |
| 12  | B     | 1753  | 0        | 1780     | 8       | 0            |
| 13  | C     | 1624  | 0        | 1696     | 14      | 0            |
| 14  | D     | 1643  | 0        | 1707     | 23      | 0            |
| 15  | E     | 1152  | 0        | 1196     | 12      | 0            |
| 16  | F     | 839   | 0        | 833      | 5       | 0            |
| 17  | G     | 1203  | 0        | 1254     | 9       | 0            |
| 18  | H     | 979   | 0        | 1031     | 10      | 0            |
| 19  | I     | 1022  | 0        | 1070     | 18      | 0            |
| 20  | J     | 786   | 0        | 828      | 9       | 0            |
| 21  | K     | 877   | 0        | 887      | 12      | 0            |
| 22  | L     | 957   | 0        | 1017     | 10      | 0            |
| 23  | M     | 891   | 0        | 952      | 12      | 0            |
| 24  | N     | 805   | 0        | 844      | 15      | 0            |
| 25  | O     | 714   | 0        | 734      | 5       | 0            |
| 26  | P     | 643   | 0        | 661      | 5       | 0            |
| 27  | Q     | 641   | 0        | 682      | 5       | 0            |
| 28  | R     | 544   | 0        | 565      | 4       | 0            |
| 29  | S     | 668   | 0        | 693      | 13      | 0            |
| 30  | T     | 670   | 0        | 719      | 11      | 0            |
| 31  | U     | 589   | 0        | 629      | 6       | 0            |
| 32  | V     | 542   | 0        | 379      | 3       | 0            |
| 33  | X     | 189   | 0        | 98       | 0       | 0            |
| 34  | Y     | 1646  | 0        | 832      | 8       | 0            |
| 35  | Z     | 1644  | 0        | 832      | 6       | 0            |
| 36  | a     | 59127 | 0        | 29762    | 256     | 0            |
| 37  | b     | 2549  | 0        | 1291     | 10      | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 38  | c     | 2082   | 0        | 2154     | 13      | 0            |
| 39  | d     | 1566   | 0        | 1618     | 9       | 0            |
| 40  | e     | 1552   | 0        | 1619     | 9       | 0            |
| 41  | f     | 1410   | 0        | 1444     | 15      | 0            |
| 42  | g     | 1323   | 0        | 1371     | 4       | 0            |
| 43  | h     | 303    | 0        | 327      | 5       | 0            |
| 44  | i     | 1129   | 0        | 1162     | 8       | 0            |
| 45  | j     | 946    | 0        | 1023     | 5       | 0            |
| 46  | k     | 1053   | 0        | 1129     | 10      | 0            |
| 47  | l     | 1074   | 0        | 1157     | 10      | 0            |
| 48  | m     | 945    | 0        | 989      | 3       | 0            |
| 49  | n     | 892    | 0        | 923      | 5       | 0            |
| 50  | o     | 917    | 0        | 962      | 9       | 0            |
| 51  | p     | 947    | 0        | 1019     | 3       | 0            |
| 52  | q     | 816    | 0        | 839      | 6       | 0            |
| 53  | r     | 857    | 0        | 922      | 5       | 0            |
| 54  | s     | 738    | 0        | 807      | 3       | 0            |
| 55  | t     | 779    | 0        | 831      | 2       | 0            |
| 56  | u     | 753    | 0        | 780      | 10      | 0            |
| 57  | v     | 592    | 0        | 607      | 4       | 0            |
| 58  | w     | 625    | 0        | 652      | 5       | 0            |
| 59  | x     | 501    | 0        | 531      | 5       | 0            |
| 60  | y     | 449    | 0        | 488      | 3       | 0            |
| 61  | z     | 444    | 0        | 458      | 3       | 0            |
| 62  | 3     | 1      | 0        | 0        | 0       | 0            |
| 62  | 4     | 1      | 0        | 0        | 0       | 0            |
| 63  | A     | 91     | 0        | 0        | 0       | 0            |
| 63  | N     | 1      | 0        | 0        | 0       | 0            |
| 63  | Q     | 1      | 0        | 0        | 0       | 0            |
| 63  | a     | 208    | 0        | 0        | 0       | 0            |
| 63  | b     | 5      | 0        | 0        | 0       | 0            |
| 63  | c     | 1      | 0        | 0        | 0       | 0            |
| 63  | d     | 1      | 0        | 0        | 0       | 0            |
| 63  | z     | 1      | 0        | 0        | 0       | 0            |
| 64  | Y     | 7      | 0        | 7        | 0       | 0            |
| 65  | a     | 14     | 0        | 26       | 1       | 0            |
| All | All   | 150736 | 0        | 104104   | 838     | 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 3.

All (838) 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) |
|-------------------|--------------------|--------------------------|-------------------|
| 11:A:1441:A:N6    | 11:A:1461:G:H21    | 1.54                     | 1.03              |
| 11:A:1441:A:H62   | 11:A:1461:G:N2     | 1.59                     | 1.01              |
| 11:A:1009:U:H3    | 11:A:1020:G:H1     | 1.29                     | 0.79              |
| 11:A:1441:A:H62   | 11:A:1461:G:H21    | 0.83                     | 0.76              |
| 34:Y:33:U:H3      | 34:Y:39:A:H61      | 1.38                     | 0.71              |
| 11:A:1127:G:H1    | 11:A:1145:A:H61    | 1.40                     | 0.69              |
| 11:A:664:G:H22    | 11:A:741:G:H1      | 1.41                     | 0.68              |
| 7:6:306:ILE:HA    | 7:6:309:TYR:HB3    | 1.76                     | 0.67              |
| 36:a:2343:U:HO2'  | 36:a:2373:G:HO2'   | 1.41                     | 0.67              |
| 19:I:58:VAL:HG13  | 19:I:59:GLU:HG3    | 1.78                     | 0.65              |
| 43:h:14:SER:HB2   | 43:h:17:ASP:HB2    | 1.79                     | 0.65              |
| 11:A:1088:G:H21   | 11:A:1167:A:H61    | 1.45                     | 0.64              |
| 11:A:1031:C:O2'   | 11:A:1032:G:N2     | 2.31                     | 0.64              |
| 11:A:1086:U:H3    | 11:A:1099:G:H22    | 1.46                     | 0.63              |
| 21:K:119:ASN:OD1  | 31:U:35:ARG:NH2    | 2.32                     | 0.63              |
| 36:a:2469:A:H4'   | 47:l:55:ARG:HD3    | 1.80                     | 0.63              |
| 36:a:1724:G:O6    | 36:a:1737:G:N2     | 2.31                     | 0.63              |
| 11:A:958:A:N6     | 29:S:77:THR:O      | 2.32                     | 0.63              |
| 11:A:71:A:H61     | 11:A:99:C:H1'      | 1.65                     | 0.62              |
| 35:Z:22:A:N6      | 35:Z:47:G:O2'      | 2.33                     | 0.62              |
| 19:I:28:ILE:HG21  | 19:I:35:LEU:HD22   | 1.81                     | 0.62              |
| 36:a:568:U:H1'    | 36:a:2030:6MZ:H9C1 | 1.81                     | 0.62              |
| 7:6:329:CYS:SG    | 7:6:330:PHE:N      | 2.73                     | 0.62              |
| 11:A:823:C:HO2'   | 18:H:2:SER:N       | 1.98                     | 0.61              |
| 11:A:407:U:O2'    | 14:D:113:GLU:OE1   | 2.16                     | 0.61              |
| 10:9:426:LEU:HD21 | 32:V:47:ALA:HB1    | 1.81                     | 0.61              |
| 36:a:848:C:H2'    | 36:a:849:A:H8      | 1.65                     | 0.61              |
| 10:9:380:MET:HE1  | 10:9:481:MET:HE2   | 1.81                     | 0.61              |
| 11:A:1150:A:H4'   | 20:J:43:PRO:HG3    | 1.82                     | 0.61              |
| 11:A:1081:A:OP2   | 15:E:52:LYS:NZ     | 2.32                     | 0.61              |
| 36:a:768:G:N7     | 65:a:6209:SPM:N14  | 2.48                     | 0.61              |
| 35:Z:10:G:O6      | 35:Z:46:G:N2       | 2.27                     | 0.61              |
| 36:a:1434:A:H2'   | 36:a:1435:G:H8     | 1.64                     | 0.60              |
| 11:A:335:C:H2'    | 11:A:336:A:H8      | 1.65                     | 0.60              |
| 11:A:910:C:OP2    | 22:L:18:LYS:NZ     | 2.33                     | 0.60              |
| 19:I:130:ARG:NH2  | 35:Z:34:U:OP2      | 2.34                     | 0.60              |
| 36:a:2848:G:O2'   | 36:a:2867:G:N2     | 2.31                     | 0.59              |
| 3:2:31:HIS:NE2    | 36:a:2421:G:N7     | 2.50                     | 0.59              |
| 51:p:97:ASP:OD2   | 52:q:13:ARG:NH1    | 2.36                     | 0.59              |
| 7:6:121:ARG:NH1   | 9:8:23:GLN:O       | 2.36                     | 0.59              |
| 11:A:1149:C:H2'   | 11:A:1150:A:H8     | 1.67                     | 0.59              |
| 47:l:66:ARG:NH1   | 47:l:104:GLU:OE2   | 2.36                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:2:39:LYS:NZ     | 36:a:2365:G:N7    | 2.49                     | 0.58              |
| 11:A:362:G:H5''   | 22:L:58:THR:HG21  | 1.85                     | 0.58              |
| 11:A:826:C:O2     | 18:H:16:ASN:ND2   | 2.36                     | 0.58              |
| 16:F:38:ARG:NH1   | 16:F:99:ALA:O     | 2.36                     | 0.58              |
| 11:A:1071:C:H2'   | 11:A:1072:G:H8    | 1.69                     | 0.58              |
| 47:l:64:TRP:HB2   | 47:l:104:GLU:HB2  | 1.84                     | 0.58              |
| 13:C:16:LYS:NZ    | 13:C:181:ASP:OD1  | 2.36                     | 0.58              |
| 11:A:674:G:H2'    | 11:A:675:A:H8     | 1.67                     | 0.57              |
| 53:r:37:THR:OG1   | 53:r:48:LYS:NZ    | 2.36                     | 0.57              |
| 36:a:1590:A:H2'   | 36:a:1591:A:H8    | 1.69                     | 0.57              |
| 47:l:53:MET:HG3   | 47:l:120:ALA:HB2  | 1.85                     | 0.57              |
| 24:N:92:GLU:N     | 24:N:92:GLU:OE1   | 2.37                     | 0.57              |
| 39:d:46:ARG:NH1   | 39:d:85:ALA:O     | 2.36                     | 0.57              |
| 11:A:1144:G:H21   | 11:A:1146:A:H62   | 1.51                     | 0.57              |
| 19:I:39:PHE:O     | 19:I:45:ARG:NH1   | 2.37                     | 0.57              |
| 11:A:1397:C:OP2   | 15:E:29:ARG:NH2   | 2.37                     | 0.57              |
| 17:G:111:ARG:NH2  | 17:G:123:GLU:OE1  | 2.37                     | 0.57              |
| 50:o:88:ARG:NH2   | 50:o:110:ILE:O    | 2.36                     | 0.57              |
| 19:I:52:LEU:HG    | 19:I:58:VAL:HG23  | 1.87                     | 0.57              |
| 46:k:108:ALA:HB3  | 46:k:125:LEU:HD22 | 1.86                     | 0.57              |
| 11:A:405:U:O4     | 14:D:2:ALA:N      | 2.37                     | 0.57              |
| 11:A:501:C:H2'    | 11:A:502:A:H8     | 1.70                     | 0.57              |
| 5:4:42:PRO:HB3    | 5:4:47:LYS:HB3    | 1.85                     | 0.57              |
| 7:6:251:ARG:NH2   | 36:a:1335:C:O3'   | 2.38                     | 0.57              |
| 11:A:401:C:O2'    | 11:A:621:A:N3     | 2.36                     | 0.57              |
| 22:L:83:ARG:NH1   | 22:L:84:GLY:O     | 2.38                     | 0.57              |
| 36:a:2469:A:N6    | 36:a:2481:G:O2'   | 2.36                     | 0.57              |
| 36:a:284:U:H3     | 36:a:356:G:H1     | 1.51                     | 0.56              |
| 11:A:1106:G:H5''  | 13:C:172:ARG:HG2  | 1.87                     | 0.56              |
| 15:E:14:LYS:NZ    | 15:E:116:GLU:OE2  | 2.37                     | 0.56              |
| 30:T:17:ALA:O     | 30:T:21:ASN:ND2   | 2.39                     | 0.56              |
| 36:a:1007:C:OP1   | 44:i:37:ARG:NH1   | 2.37                     | 0.56              |
| 11:A:677:U:H3     | 11:A:713:G:H22    | 1.52                     | 0.56              |
| 15:E:115:LEU:HD13 | 15:E:123:VAL:HG11 | 1.88                     | 0.56              |
| 41:f:58:ALA:HB2   | 41:f:65:PRO:HD3   | 1.87                     | 0.56              |
| 7:6:333:THR:HA    | 7:6:336:VAL:HG12  | 1.88                     | 0.56              |
| 11:A:517:G:N2     | 11:A:530:G:OP1    | 2.38                     | 0.56              |
| 5:4:42:PRO:O      | 5:4:45:THR:C      | 2.49                     | 0.56              |
| 11:A:1088:G:N2    | 11:A:1167:A:H61   | 2.03                     | 0.56              |
| 36:a:1434:A:H2'   | 36:a:1435:G:C8    | 2.40                     | 0.56              |
| 11:A:451:A:H61    | 11:A:481:G:H5'    | 1.71                     | 0.56              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 12:B:43:LEU:HA   | 12:B:46:THR:HG22  | 1.87                     | 0.56              |
| 15:E:38:VAL:HG11 | 15:E:114:VAL:HG22 | 1.88                     | 0.56              |
| 11:A:110:C:O2'   | 26:P:25:ARG:O     | 2.23                     | 0.55              |
| 11:A:178:C:OP2   | 30:T:60:ARG:NH1   | 2.39                     | 0.55              |
| 12:B:104:TRP:HA  | 12:B:107:VAL:HG22 | 1.88                     | 0.55              |
| 23:M:87:ARG:NH2  | 29:S:73:GLU:OE1   | 2.39                     | 0.55              |
| 36:a:1432:G:H2'  | 36:a:1433:A:C8    | 2.40                     | 0.55              |
| 36:a:1796:U:H2'  | 36:a:1797:G:H8    | 1.70                     | 0.55              |
| 60:y:6:LYS:HD3   | 60:y:37:GLU:HG3   | 1.86                     | 0.55              |
| 44:i:19:ASP:O    | 44:i:23:LYS:NZ    | 2.37                     | 0.55              |
| 10:9:79:VAL:HB   | 10:9:110:ALA:HB3  | 1.88                     | 0.55              |
| 10:9:321:ALA:HB3 | 10:9:324:LEU:HD13 | 1.88                     | 0.55              |
| 10:9:376:GLN:HG2 | 10:9:377:TYR:HD1  | 1.71                     | 0.55              |
| 11:A:264:C:O2'   | 27:Q:66:PRO:O     | 2.24                     | 0.55              |
| 11:A:559:A:H4'   | 11:A:560:A:H3'    | 1.88                     | 0.55              |
| 14:D:59:GLN:OE1  | 14:D:62:ARG:NH1   | 2.39                     | 0.55              |
| 11:A:552:U:H2'   | 11:A:553:A:H8     | 1.72                     | 0.55              |
| 11:A:933:G:O6    | 17:G:3:ARG:NH2    | 2.38                     | 0.55              |
| 3:2:54:ASP:HB3   | 46:k:57:LEU:HD22  | 1.89                     | 0.55              |
| 7:6:130:PHE:HZ   | 7:6:290:ILE:HG23  | 1.72                     | 0.55              |
| 11:A:713:G:H2'   | 11:A:714:G:C8     | 2.42                     | 0.55              |
| 50:o:9:GLU:OE2   | 50:o:56:HIS:NE2   | 2.40                     | 0.55              |
| 56:u:35:GLU:N    | 56:u:35:GLU:OE1   | 2.39                     | 0.55              |
| 14:D:97:ARG:HH21 | 14:D:134:SER:HB3  | 1.72                     | 0.55              |
| 36:a:1045:C:O2   | 36:a:1111:A:N6    | 2.39                     | 0.55              |
| 51:p:49:ASP:HA   | 51:p:52:GLN:HB2   | 1.89                     | 0.55              |
| 19:I:106:ARG:NH1 | 19:I:107:ASP:O    | 2.41                     | 0.54              |
| 7:6:85:TYR:HA    | 7:6:124:THR:HG22  | 1.89                     | 0.54              |
| 54:s:3:ARG:NH1   | 54:s:5:GLU:OE2    | 2.40                     | 0.54              |
| 47:l:20:LEU:HD13 | 56:u:81:PRO:HG2   | 1.89                     | 0.54              |
| 7:6:125:LEU:HA   | 7:6:169:MET:HE1   | 1.89                     | 0.54              |
| 11:A:946:A:H2'   | 11:A:947:G:C8     | 2.42                     | 0.54              |
| 11:A:1060:U:H2'  | 11:A:1061:G:H8    | 1.71                     | 0.54              |
| 43:h:5:LEU:HD23  | 43:h:17:ASP:HB3   | 1.90                     | 0.54              |
| 11:A:1530:G:N7   | 31:U:46:LYS:NZ    | 2.56                     | 0.54              |
| 27:Q:47:HIS:HB3  | 27:Q:74:THR:HG22  | 1.89                     | 0.54              |
| 56:u:1:MET:SD    | 56:u:53:LYS:NZ    | 2.81                     | 0.54              |
| 7:6:293:TRP:HE1  | 7:6:303:LEU:HD21  | 1.73                     | 0.54              |
| 56:u:51:GLN:OE1  | 56:u:57:TYR:OH    | 2.26                     | 0.54              |
| 5:4:28:VAL:HG22  | 41:f:140:GLU:HA   | 1.89                     | 0.54              |
| 17:G:15:ASP:OD1  | 17:G:19:GLY:N     | 2.40                     | 0.54              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 18:H:77:ARG:NH1  | 18:H:79:SER:O     | 2.41                     | 0.54              |
| 26:P:69:ASP:OD1  | 26:P:70:ARG:N     | 2.40                     | 0.54              |
| 7:6:242:ARG:NH2  | 7:6:243:ARG:O     | 2.41                     | 0.54              |
| 11:A:980:C:O2'   | 24:N:13:ARG:NH1   | 2.40                     | 0.54              |
| 11:A:1127:G:H1   | 11:A:1145:A:N6    | 2.05                     | 0.54              |
| 45:j:121:GLU:OE1 | 50:o:65:SER:OG    | 2.26                     | 0.54              |
| 11:A:402:G:OP2   | 14:D:71:GLN:NE2   | 2.37                     | 0.54              |
| 13:C:35:SER:OG   | 13:C:59:ARG:NH2   | 2.41                     | 0.54              |
| 36:a:1386:C:H2'  | 36:a:1387:A:C8    | 2.43                     | 0.54              |
| 11:A:227:G:O2'   | 26:P:63:GLN:OE1   | 2.26                     | 0.53              |
| 11:A:717:U:H4'   | 21:K:119:ASN:HD22 | 1.73                     | 0.53              |
| 38:c:29:PRO:HG2  | 38:c:34:LEU:HD11  | 1.91                     | 0.53              |
| 5:4:42:PRO:O     | 5:4:45:THR:O      | 2.27                     | 0.53              |
| 36:a:864:G:O2'   | 36:a:914:G:O6     | 2.26                     | 0.53              |
| 21:K:64:GLN:NE2  | 21:K:68:GLU:OE2   | 2.40                     | 0.53              |
| 36:a:1278:C:H2'  | 36:a:1279:G:H8    | 1.73                     | 0.53              |
| 36:a:1590:A:H2'  | 36:a:1591:A:C8    | 2.43                     | 0.53              |
| 11:A:1218:C:H2'  | 11:A:1219:A:H8    | 1.73                     | 0.53              |
| 11:A:1278:G:N7   | 13:C:27:LYS:NZ    | 2.57                     | 0.53              |
| 37:b:1:U:H2'     | 37:b:2:G:H8       | 1.74                     | 0.53              |
| 12:B:58:ASN:ND2  | 12:B:220:THR:O    | 2.41                     | 0.53              |
| 25:O:88:ARG:NH2  | 36:a:714:U:OP2    | 2.39                     | 0.53              |
| 11:A:673:A:H2'   | 11:A:674:G:C8     | 2.43                     | 0.53              |
| 11:A:323:U:OP1   | 30:T:25:ARG:NH2   | 2.38                     | 0.52              |
| 11:A:335:C:H2'   | 11:A:336:A:C8     | 2.42                     | 0.52              |
| 30:T:55:GLN:HG3  | 30:T:76:LYS:HD3   | 1.91                     | 0.52              |
| 36:a:93:G:N2     | 36:a:93:G:OP2     | 2.42                     | 0.52              |
| 38:c:107:PRO:HD2 | 38:c:110:LEU:HD22 | 1.90                     | 0.52              |
| 38:c:144:VAL:HB  | 38:c:154:LEU:HB2  | 1.90                     | 0.52              |
| 11:A:1124:G:N2   | 11:A:1125:U:O4    | 2.37                     | 0.52              |
| 17:G:68:ASN:O    | 17:G:138:ARG:NH2  | 2.43                     | 0.52              |
| 8:7:86:THR:HG23  | 8:7:89:GLU:H      | 1.73                     | 0.52              |
| 36:a:270:A:N1    | 36:a:369:U:O2'    | 2.32                     | 0.52              |
| 36:a:807:U:OP2   | 46:k:41:ARG:NH2   | 2.42                     | 0.52              |
| 11:A:811:C:O2'   | 11:A:901:A:N1     | 2.42                     | 0.52              |
| 7:6:26:VAL:HG21  | 7:6:183:ILE:HG13  | 1.90                     | 0.52              |
| 11:A:1360:A:OP2  | 24:N:75:ARG:NH2   | 2.42                     | 0.52              |
| 24:N:52:PRO:O    | 24:N:55:SER:OG    | 2.28                     | 0.52              |
| 36:a:627:A:OP1   | 46:k:78:ARG:NH1   | 2.43                     | 0.52              |
| 36:a:1248:G:OP1  | 40:e:44:ARG:NH1   | 2.42                     | 0.52              |
| 11:A:946:A:OP1   | 23:M:113:ARG:NH1  | 2.40                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:E:107:ALA:O    | 15:E:112:ARG:NH1  | 2.43                     | 0.52              |
| 36:a:577:G:O2'    | 36:a:1254:A:OP1   | 2.28                     | 0.52              |
| 36:a:832:U:H2'    | 36:a:833:A:H8     | 1.74                     | 0.52              |
| 11:A:1218:C:H2'   | 11:A:1219:A:C8    | 2.45                     | 0.52              |
| 11:A:1381:U:H2'   | 17:G:79:ARG:HE    | 1.74                     | 0.52              |
| 30:T:39:ILE:HG23  | 30:T:86:LEU:HD12  | 1.91                     | 0.52              |
| 36:a:411:G:OP2    | 36:a:2406:A:O2'   | 2.26                     | 0.52              |
| 41:f:162:SER:OG   | 41:f:165:GLU:OE1  | 2.28                     | 0.52              |
| 11:A:1088:G:H21   | 11:A:1167:A:N6    | 2.07                     | 0.52              |
| 20:J:53:ILE:HD11  | 20:J:61:ALA:HB1   | 1.92                     | 0.52              |
| 58:w:74:ARG:NH1   | 58:w:76:GLU:OE2   | 2.43                     | 0.52              |
| 10:9:225:THR:HG23 | 10:9:248:SER:HB2  | 1.92                     | 0.52              |
| 10:9:272:ASN:HA   | 10:9:290:SER:HA   | 1.91                     | 0.52              |
| 11:A:1222:G:OP2   | 11:A:1322:C:N4    | 2.40                     | 0.52              |
| 11:A:1377:A:OP1   | 17:G:92:ARG:NH2   | 2.43                     | 0.52              |
| 7:6:237:VAL:HG21  | 7:6:380:TYR:CZ    | 2.45                     | 0.51              |
| 10:9:88:PRO:HA    | 10:9:96:PRO:HA    | 1.90                     | 0.51              |
| 10:9:397:LEU:HB3  | 10:9:404:ILE:HG23 | 1.92                     | 0.51              |
| 11:A:714:G:H2'    | 11:A:715:A:C8     | 2.45                     | 0.51              |
| 13:C:130:PHE:O    | 13:C:134:MET:HG2  | 2.10                     | 0.51              |
| 20:J:40:ILE:HB    | 20:J:73:LEU:HD23  | 1.92                     | 0.51              |
| 23:M:17:ILE:O     | 23:M:20:THR:OG1   | 2.28                     | 0.51              |
| 11:A:41:G:H2'     | 11:A:42:G:H8      | 1.74                     | 0.51              |
| 11:A:946:A:H2'    | 11:A:947:G:H8     | 1.75                     | 0.51              |
| 11:A:1522:U:H2'   | 11:A:1523:G:H8    | 1.74                     | 0.51              |
| 35:Z:15:G:H22     | 35:Z:49:C:H42     | 1.58                     | 0.51              |
| 36:a:476:G:N1     | 36:a:479:A:OP2    | 2.40                     | 0.51              |
| 36:a:2200:C:OP2   | 58:w:37:ARG:NH1   | 2.42                     | 0.51              |
| 51:p:89:GLU:O     | 52:q:11:GLN:NE2   | 2.40                     | 0.51              |
| 36:a:1819:A:H5''  | 38:c:160:THR:HG21 | 1.91                     | 0.51              |
| 36:a:2303:G:O2'   | 41:f:121:SER:O    | 2.28                     | 0.51              |
| 46:k:143:GLU:OE1  | 46:k:143:GLU:N    | 2.44                     | 0.51              |
| 49:n:69:ASP:OD1   | 49:n:69:ASP:N     | 2.37                     | 0.51              |
| 5:4:63:ARG:NH1    | 11:A:1312:G:OP2   | 2.44                     | 0.51              |
| 10:9:521:ASN:HA   | 10:9:524:THR:HB   | 1.93                     | 0.51              |
| 36:a:887:U:O2'    | 36:a:889:C:OP2    | 2.29                     | 0.51              |
| 37:b:15:A:H3'     | 37:b:16:G:H8      | 1.75                     | 0.51              |
| 11:A:501:C:H2'    | 11:A:502:A:C8     | 2.46                     | 0.51              |
| 13:C:125:GLU:O    | 13:C:127:ARG:NH1  | 2.42                     | 0.51              |
| 13:C:138:VAL:HG23 | 13:C:149:ILE:HG23 | 1.91                     | 0.51              |
| 36:a:1800:C:OP2   | 38:c:182:ARG:NH2  | 2.44                     | 0.51              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 41:f:2:ALA:N     | 41:f:98:GLU:OE2   | 2.43                     | 0.51              |
| 56:u:76:ASP:H    | 56:u:90:ASP:HB2   | 1.75                     | 0.51              |
| 10:9:265:ILE:HB  | 10:9:306:THR:HB   | 1.91                     | 0.51              |
| 15:E:13:GLU:OE2  | 15:E:68:ARG:NH1   | 2.39                     | 0.51              |
| 15:E:101:GLU:N   | 15:E:101:GLU:OE1  | 2.43                     | 0.51              |
| 18:H:91:GLU:N    | 18:H:91:GLU:OE1   | 2.44                     | 0.51              |
| 23:M:87:ARG:HH22 | 29:S:69:HIS:CE1   | 2.28                     | 0.51              |
| 36:a:2831:G:OP2  | 39:d:59:ARG:NH1   | 2.41                     | 0.51              |
| 11:A:723:U:O2    | 31:U:49:LYS:NZ    | 2.44                     | 0.51              |
| 11:A:1366:C:OP1  | 19:I:119:ARG:NH1  | 2.44                     | 0.51              |
| 11:A:309:A:H2'   | 11:A:310:G:H8     | 1.74                     | 0.51              |
| 11:A:1305:G:N2   | 11:A:1331:G:O2'   | 2.43                     | 0.51              |
| 36:a:340:A:O2'   | 40:e:162:ARG:NH2  | 2.44                     | 0.51              |
| 36:a:568:U:O4    | 52:q:81:LYS:NZ    | 2.44                     | 0.51              |
| 36:a:2515:C:H2'  | 36:a:2516:A:H8    | 1.75                     | 0.51              |
| 44:i:9:GLU:OE1   | 44:i:9:GLU:N      | 2.44                     | 0.51              |
| 11:A:126:G:OP1   | 11:A:605:U:O2'    | 2.24                     | 0.50              |
| 11:A:437:U:O2'   | 14:D:120:HIS:ND1  | 2.40                     | 0.50              |
| 12:B:11:LYS:O    | 12:B:208:ARG:NH1  | 2.43                     | 0.50              |
| 29:S:44:MET:HG3  | 29:S:62:VAL:HG11  | 1.92                     | 0.50              |
| 36:a:545:U:O2'   | 36:a:548:G:N2     | 2.45                     | 0.50              |
| 36:a:2372:U:H2'  | 36:a:2373:G:H8    | 1.77                     | 0.50              |
| 48:m:24:MET:HE1  | 48:m:40:LYS:HB3   | 1.93                     | 0.50              |
| 10:9:382:LYS:NZ  | 10:9:415:GLU:O    | 2.40                     | 0.50              |
| 2:l:29:GLN:NE2   | 36:a:210:C:OP1    | 2.45                     | 0.50              |
| 7:6:239:ARG:HG3  | 8:7:85:PRO:HG3    | 1.92                     | 0.50              |
| 10:9:516:TYR:O   | 10:9:520:SER:OG   | 2.19                     | 0.50              |
| 36:a:581:C:H2'   | 36:a:582:A:C8     | 2.46                     | 0.50              |
| 36:a:793:A:OP2   | 36:a:2071:A:O2'   | 2.27                     | 0.50              |
| 59:x:49:ASP:OD1  | 59:x:52:ARG:NH1   | 2.44                     | 0.50              |
| 11:A:50:A:O2'    | 11:A:360:G:N2     | 2.44                     | 0.50              |
| 7:6:86:ILE:HD11  | 7:6:279:PHE:HA    | 1.94                     | 0.50              |
| 11:A:1321:U:O2'  | 29:S:78:ARG:NH1   | 2.44                     | 0.50              |
| 34:Y:59:A:O2'    | 34:Y:61:U:OP2     | 2.29                     | 0.50              |
| 36:a:151:C:H2'   | 36:a:152:A:H8     | 1.76                     | 0.50              |
| 1:0:29:THR:HG22  | 1:0:30:LYS:HD3    | 1.93                     | 0.50              |
| 7:6:318:VAL:HG12 | 7:6:386:LEU:HD12  | 1.92                     | 0.50              |
| 10:9:82:ALA:HB3  | 10:9:99:LEU:HD12  | 1.94                     | 0.50              |
| 24:N:66:GLN:HG3  | 24:N:79:LEU:HD22  | 1.94                     | 0.50              |
| 7:6:407:LEU:O    | 7:6:411:VAL:HG22  | 2.12                     | 0.50              |
| 14:D:105:MET:HG3 | 14:D:171:LEU:HD13 | 1.93                     | 0.50              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 19:I:6:TYR:HB2    | 19:I:21:ILE:HG23 | 1.93                     | 0.50              |
| 36:a:1796:U:H2'   | 36:a:1797:G:C8   | 2.46                     | 0.50              |
| 52:q:46:GLU:OE1   | 52:q:46:GLU:N    | 2.44                     | 0.50              |
| 36:a:2229:U:H2'   | 36:a:2230:G:H8   | 1.77                     | 0.50              |
| 36:a:2484:G:OP1   | 47:l:44:ARG:NH1  | 2.39                     | 0.50              |
| 53:r:20:VAL:HG11  | 53:r:44:ALA:HA   | 1.94                     | 0.50              |
| 7:6:26:VAL:HG22   | 7:6:178:ILE:HD11 | 1.94                     | 0.49              |
| 8:7:43:LEU:HD13   | 8:7:46:LEU:HD12  | 1.93                     | 0.49              |
| 11:A:938:A:N3     | 11:A:1376:U:O2'  | 2.39                     | 0.49              |
| 11:A:1255:G:O2'   | 11:A:1258:G:N3   | 2.38                     | 0.49              |
| 11:A:1507:A:H2'   | 11:A:1508:A:C8   | 2.47                     | 0.49              |
| 22:L:86:ARG:HG2   | 22:L:94:ARG:HA   | 1.93                     | 0.49              |
| 36:a:75:G:H22     | 36:a:111:A:H2    | 1.59                     | 0.49              |
| 36:a:475:C:O2     | 36:a:479:A:N6    | 2.40                     | 0.49              |
| 11:A:1253:G:H2'   | 11:A:1254:A:H8   | 1.77                     | 0.49              |
| 14:D:126:ASN:ND2  | 14:D:141:ASP:OD1 | 2.44                     | 0.49              |
| 17:G:87:VAL:HG21  | 17:G:154:TYR:HB2 | 1.93                     | 0.49              |
| 36:a:2898:U:H2'   | 36:a:2899:A:H8   | 1.78                     | 0.49              |
| 11:A:34:C:H2'     | 11:A:35:G:H8     | 1.77                     | 0.49              |
| 36:a:1476:U:H2'   | 36:a:1477:A:H8   | 1.77                     | 0.49              |
| 36:a:2313:C:O4'   | 41:f:37:ASN:ND2  | 2.32                     | 0.49              |
| 36:a:2571:U:O2'   | 39:d:151:THR:O   | 2.29                     | 0.49              |
| 7:6:89:SER:O      | 7:6:93:GLN:NE2   | 2.46                     | 0.49              |
| 7:6:207:ILE:HD11  | 10:9:334:TRP:H   | 1.78                     | 0.49              |
| 11:A:634:C:H2'    | 11:A:635:A:H8    | 1.78                     | 0.49              |
| 11:A:1414:U:H2'   | 11:A:1415:G:H8   | 1.77                     | 0.49              |
| 13:C:17:PRO:HG2   | 13:C:54:ARG:HH22 | 1.78                     | 0.49              |
| 36:a:2314:A:OP1   | 41:f:88:LYS:NZ   | 2.44                     | 0.49              |
| 45:j:43:ILE:HD12  | 45:j:56:ASP:HB2  | 1.94                     | 0.49              |
| 12:B:15:HIS:HB3   | 12:B:43:LEU:HD11 | 1.94                     | 0.49              |
| 14:D:145:ILE:HD13 | 14:D:178:MET:HB3 | 1.95                     | 0.49              |
| 36:a:1028:A:N3    | 36:a:2486:C:O2'  | 2.40                     | 0.49              |
| 36:a:1433:A:H2'   | 36:a:1434:A:C8   | 2.47                     | 0.49              |
| 11:A:150:U:H2'    | 11:A:151:A:H8    | 1.78                     | 0.49              |
| 11:A:231:U:H2'    | 11:A:232:G:H8    | 1.77                     | 0.49              |
| 23:M:58:ASP:OD1   | 23:M:58:ASP:N    | 2.45                     | 0.49              |
| 7:6:173:TRP:HD1   | 7:6:174:LEU:HD23 | 1.76                     | 0.49              |
| 11:A:1004:A:O2'   | 11:A:1036:A:N6   | 2.46                     | 0.49              |
| 11:A:1241:G:H2'   | 11:A:1242:G:H8   | 1.77                     | 0.49              |
| 36:a:742:A:H2'    | 36:a:743:A:C8    | 2.48                     | 0.49              |
| 36:a:832:U:H2'    | 36:a:833:A:C8    | 2.47                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 36:a:2564:A:OP1   | 36:a:2648:G:O2'   | 2.26                     | 0.49              |
| 11:A:413:G:N2     | 11:A:429:U:OP2    | 2.44                     | 0.49              |
| 11:A:490:C:H2'    | 11:A:491:G:H8     | 1.78                     | 0.49              |
| 11:A:1356:G:H2'   | 11:A:1357:A:C8    | 2.47                     | 0.49              |
| 48:m:28:LEU:HD23  | 48:m:48:VAL:HG21  | 1.94                     | 0.49              |
| 11:A:147:G:H2'    | 11:A:148:G:C8     | 2.48                     | 0.49              |
| 11:A:521:G:HO2'   | 11:A:536:C:HO2'   | 1.60                     | 0.49              |
| 11:A:1402:4OC:H2' | 11:A:1403:C:O4'   | 2.12                     | 0.49              |
| 29:S:36:ARG:NH2   | 29:S:75:ALA:O     | 2.45                     | 0.49              |
| 36:a:5:A:H2'      | 36:a:6:A:C8       | 2.48                     | 0.49              |
| 36:a:1319:C:O2'   | 36:a:1321:A:N6    | 2.46                     | 0.49              |
| 8:7:88:GLN:HA     | 8:7:91:LEU:HD12   | 1.94                     | 0.49              |
| 10:9:409:MET:HA   | 10:9:412:TYR:HB2  | 1.95                     | 0.49              |
| 36:a:856:G:H2'    | 36:a:857:G:C8     | 2.47                     | 0.49              |
| 56:u:40:ILE:HD12  | 56:u:42:LEU:HD21  | 1.94                     | 0.49              |
| 11:A:222:C:H2'    | 11:A:223:A:H8     | 1.78                     | 0.48              |
| 11:A:1139:G:H4'   | 11:A:1140:C:H5'   | 1.95                     | 0.48              |
| 12:B:46:THR:HB    | 12:B:201:PRO:HG2  | 1.93                     | 0.48              |
| 18:H:29:SER:HB2   | 18:H:59:LEU:HB2   | 1.95                     | 0.48              |
| 43:h:12:LEU:HD22  | 43:h:19:VAL:HG21  | 1.94                     | 0.48              |
| 46:k:132:ARG:O    | 46:k:136:GLU:HG2  | 2.13                     | 0.48              |
| 1:0:37:LYS:HE3    | 1:0:37:LYS:HB2    | 1.69                     | 0.48              |
| 37:b:49:C:H2'     | 37:b:50:A:H8      | 1.76                     | 0.48              |
| 41:f:136:ILE:HA   | 41:f:141:ILE:HD11 | 1.95                     | 0.48              |
| 11:A:624:C:H4'    | 26:P:10:GLY:HA2   | 1.96                     | 0.48              |
| 36:a:74:A:O2'     | 36:a:88:G:OP2     | 2.30                     | 0.48              |
| 36:a:1028:A:H2'   | 36:a:1029:A:C8    | 2.48                     | 0.48              |
| 36:a:1406:U:H2'   | 36:a:1407:G:H8    | 1.78                     | 0.48              |
| 60:y:9:GLN:NE2    | 60:y:11:ARG:O     | 2.40                     | 0.48              |
| 7:6:317:TYR:O     | 7:6:321:TYR:HB2   | 2.13                     | 0.48              |
| 11:A:1513:A:H2'   | 11:A:1514:G:C8    | 2.48                     | 0.48              |
| 36:a:2640:G:OP1   | 44:i:96:ARG:NH1   | 2.45                     | 0.48              |
| 49:n:99:TYR:OH    | 49:n:111:ARG:NH2  | 2.46                     | 0.48              |
| 7:6:64:PHE:HD1    | 7:6:72:LEU:HD23   | 1.77                     | 0.48              |
| 59:x:20:ASN:O     | 59:x:24:GLU:HG3   | 2.13                     | 0.48              |
| 7:6:431:SER:O     | 7:6:435:LYS:NZ    | 2.40                     | 0.48              |
| 11:A:545:C:H5'    | 14:D:69:GLU:HB2   | 1.95                     | 0.48              |
| 11:A:662:U:H2'    | 11:A:663:A:C8     | 2.49                     | 0.48              |
| 36:a:219:A:N3     | 36:a:234:U:O2'    | 2.40                     | 0.48              |
| 36:a:987:C:O2'    | 36:a:1000:A:N3    | 2.39                     | 0.48              |
| 14:D:13:ARG:HG3   | 14:D:38:PRO:HD3   | 1.95                     | 0.48              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 19:I:118:LEU:HD22 | 19:I:124:ARG:HG2 | 1.95                     | 0.48              |
| 36:a:581:C:H2'    | 36:a:582:A:H8    | 1.79                     | 0.48              |
| 42:g:2:SER:OG     | 42:g:3:ARG:N     | 2.47                     | 0.48              |
| 5:4:48:GLN:NE2    | 41:f:114:PHE:O   | 2.46                     | 0.48              |
| 35:Z:15:G:O6      | 35:Z:49:C:O2     | 2.31                     | 0.48              |
| 36:a:1047:G:O2'   | 36:a:1110:G:N1   | 2.38                     | 0.48              |
| 36:a:1429:G:H2'   | 36:a:1430:G:H8   | 1.79                     | 0.48              |
| 11:A:816:A:OP1    | 11:A:1526:G:O2'  | 2.28                     | 0.48              |
| 13:C:11:ARG:NH2   | 13:C:177:THR:O   | 2.42                     | 0.48              |
| 15:E:13:GLU:HG2   | 15:E:39:VAL:HG12 | 1.96                     | 0.48              |
| 11:A:1147:C:O2'   | 19:I:7:TYR:OH    | 2.24                     | 0.48              |
| 18:H:102:ALA:HB3  | 18:H:113:ASP:HB3 | 1.96                     | 0.48              |
| 36:a:307:G:N1     | 36:a:310:A:OP2   | 2.39                     | 0.48              |
| 36:a:1385:A:O2'   | 36:a:1396:U:O2   | 2.32                     | 0.48              |
| 36:a:1386:C:H2'   | 36:a:1387:A:H8   | 1.78                     | 0.48              |
| 36:a:1419:A:O2'   | 36:a:1421:G:N7   | 2.44                     | 0.48              |
| 19:I:52:LEU:HA    | 19:I:55:VAL:HG22 | 1.96                     | 0.47              |
| 28:R:72:ASP:OD1   | 28:R:73:ARG:N    | 2.47                     | 0.47              |
| 36:a:668:A:H2'    | 36:a:670:A:H62   | 1.78                     | 0.47              |
| 36:a:1296:G:OP1   | 36:a:2709:G:O2'  | 2.30                     | 0.47              |
| 56:u:55:GLU:OE1   | 56:u:55:GLU:N    | 2.38                     | 0.47              |
| 11:A:537:G:OP1    | 22:L:110:ARG:NH2 | 2.47                     | 0.47              |
| 11:A:1071:C:H2'   | 11:A:1072:G:C8   | 2.49                     | 0.47              |
| 36:a:2339:C:O2'   | 37:b:41:G:N2     | 2.47                     | 0.47              |
| 10:9:531:ILE:O    | 10:9:535:LEU:N   | 2.42                     | 0.47              |
| 11:A:652:U:O4     | 11:A:752:G:O2'   | 2.25                     | 0.47              |
| 11:A:689:C:OP1    | 21:K:29:ASN:ND2  | 2.44                     | 0.47              |
| 11:A:715:A:H2'    | 11:A:716:A:C8    | 2.49                     | 0.47              |
| 11:A:999:C:H2'    | 11:A:1000:A:H8   | 1.78                     | 0.47              |
| 11:A:1243:C:H2'   | 11:A:1244:G:H8   | 1.79                     | 0.47              |
| 36:a:721:A:H2'    | 36:a:722:A:C8    | 2.50                     | 0.47              |
| 36:a:1406:U:H2'   | 36:a:1407:G:C8   | 2.49                     | 0.47              |
| 36:a:1469:A:H2'   | 36:a:1470:A:C8   | 2.49                     | 0.47              |
| 36:a:2547:A:H2'   | 36:a:2548:U:C6   | 2.49                     | 0.47              |
| 43:h:4:ILE:HG22   | 43:h:18:GLN:HG2  | 1.97                     | 0.47              |
| 13:C:47:LEU:HB3   | 13:C:50:ALA:HB3  | 1.95                     | 0.47              |
| 21:K:71:ALA:O     | 21:K:75:LYS:HG3  | 2.14                     | 0.47              |
| 36:a:2246:G:H2'   | 36:a:2247:A:C8   | 2.49                     | 0.47              |
| 36:a:2305:U:H5''  | 41:f:131:GLY:HA3 | 1.96                     | 0.47              |
| 59:x:5:GLU:OE1    | 59:x:5:GLU:N     | 2.42                     | 0.47              |
| 7:6:128:ALA:O     | 7:6:132:SER:OG   | 2.23                     | 0.47              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 36:a:155:A:H2'   | 36:a:156:A:C8     | 2.50                     | 0.47              |
| 36:a:877:A:O2'   | 36:a:900:A:N6     | 2.48                     | 0.47              |
| 36:a:2233:U:H2'  | 36:a:2234:G:C8    | 2.50                     | 0.47              |
| 36:a:2676:C:OP1  | 45:j:31:ARG:NH2   | 2.48                     | 0.47              |
| 43:h:7:ASP:OD1   | 43:h:8:LYS:N      | 2.48                     | 0.47              |
| 11:A:154:U:O4    | 11:A:155:A:N6     | 2.48                     | 0.47              |
| 23:M:24:GLY:O    | 23:M:29:ARG:NH1   | 2.47                     | 0.47              |
| 36:a:72:U:O4     | 59:x:58:ASN:ND2   | 2.47                     | 0.47              |
| 36:a:2245:U:H5'' | 36:a:2246:G:H5'   | 1.97                     | 0.47              |
| 7:6:287:PRO:HA   | 7:6:290:ILE:HD12  | 1.97                     | 0.47              |
| 8:7:29:ALA:HB2   | 8:7:48:VAL:HG11   | 1.96                     | 0.47              |
| 11:A:1516:2MG:N2 | 11:A:1519:MA6:OP2 | 2.45                     | 0.47              |
| 18:H:11:LEU:HD22 | 18:H:75:ILE:HD11  | 1.96                     | 0.47              |
| 30:T:35:VAL:O    | 30:T:39:ILE:HG13  | 2.15                     | 0.47              |
| 36:a:1417:C:HO2' | 36:a:1587:G:HO2'  | 1.48                     | 0.47              |
| 36:a:2328:A:H2'  | 36:a:2329:U:C6    | 2.50                     | 0.47              |
| 36:a:2698:U:H2'  | 36:a:2699:C:C6    | 2.50                     | 0.47              |
| 42:g:73:ASN:O    | 42:g:77:ILE:HG13  | 2.15                     | 0.47              |
| 44:i:9:GLU:HG2   | 44:i:10:THR:HG23  | 1.97                     | 0.47              |
| 52:q:16:GLU:OE2  | 52:q:101:ILE:N    | 2.45                     | 0.47              |
| 11:A:253:A:O2'   | 27:Q:17:MET:SD    | 2.73                     | 0.47              |
| 36:a:1791:A:N6   | 36:a:1828:G:O2'   | 2.43                     | 0.47              |
| 36:a:2618:G:H21  | 39:d:155:VAL:HG21 | 1.80                     | 0.47              |
| 56:u:73:LYS:HG3  | 56:u:94:ALA:HB2   | 1.97                     | 0.47              |
| 21:K:64:GLN:O    | 21:K:68:GLU:HG3   | 2.15                     | 0.47              |
| 36:a:833:A:H2'   | 36:a:834:G:C8     | 2.50                     | 0.47              |
| 36:a:2540:C:O2'  | 36:a:2740:A:N3    | 2.46                     | 0.47              |
| 36:a:2788:C:O2'  | 36:a:2809:A:N3    | 2.42                     | 0.47              |
| 7:6:120:THR:O    | 7:6:124:THR:HG23  | 2.15                     | 0.47              |
| 14:D:70:ARG:HD2  | 14:D:73:ARG:HH21  | 1.80                     | 0.47              |
| 36:a:743:A:O2'   | 36:a:1659:G:OP1   | 2.28                     | 0.47              |
| 11:A:745:G:H2'   | 11:A:746:A:H8     | 1.80                     | 0.46              |
| 13:C:14:ILE:HG22 | 13:C:15:VAL:HG13  | 1.97                     | 0.46              |
| 36:a:329:G:OP2   | 55:t:69:ASN:ND2   | 2.47                     | 0.46              |
| 36:a:1266:G:O2'  | 36:a:2012:G:O6    | 2.30                     | 0.46              |
| 36:a:2012:G:N7   | 53:r:16:LYS:NZ    | 2.59                     | 0.46              |
| 36:a:2241:A:H2'  | 36:a:2242:G:C8    | 2.50                     | 0.46              |
| 37:b:1:U:H2'     | 37:b:2:G:C8       | 2.50                     | 0.46              |
| 56:u:55:GLU:HB2  | 56:u:59:GLU:HG3   | 1.98                     | 0.46              |
| 10:9:189:GLU:N   | 10:9:189:GLU:OE1  | 2.48                     | 0.46              |
| 14:D:107:PHE:CG  | 14:D:145:ILE:HD11 | 2.50                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 17:G:16:PRO:HB3  | 19:I:42:GLU:HG3  | 1.96                     | 0.46              |
| 21:K:106:ARG:HG2 | 31:U:12:PHE:HZ   | 1.80                     | 0.46              |
| 36:a:807:U:O2'   | 36:a:2060:A:N1   | 2.46                     | 0.46              |
| 36:a:1047:G:N2   | 36:a:1110:G:O2'  | 2.44                     | 0.46              |
| 36:a:1340:U:OP2  | 54:s:82:LYS:NZ   | 2.45                     | 0.46              |
| 36:a:2039:U:H2'  | 36:a:2040:G:C8   | 2.50                     | 0.46              |
| 11:A:486:U:H2'   | 11:A:487:A:H8    | 1.80                     | 0.46              |
| 12:B:19:GLN:OE1  | 12:B:19:GLN:N    | 2.45                     | 0.46              |
| 20:J:54:SER:OG   | 20:J:56:HIS:O    | 2.32                     | 0.46              |
| 36:a:576:U:H2'   | 36:a:577:G:C8    | 2.51                     | 0.46              |
| 36:a:2079:U:O2'  | 58:w:23:ASN:OD1  | 2.30                     | 0.46              |
| 8:7:91:LEU:O     | 8:7:95:LEU:HD22  | 2.15                     | 0.46              |
| 14:D:9:LEU:HG    | 14:D:22:LYS:HE3  | 1.98                     | 0.46              |
| 27:Q:15:ASP:HA   | 27:Q:21:ILE:HG22 | 1.97                     | 0.46              |
| 34:Y:19:G:O2'    | 34:Y:58:G:N2     | 2.31                     | 0.46              |
| 36:a:1734:G:H2'  | 36:a:1735:A:H8   | 1.81                     | 0.46              |
| 36:a:2291:U:H2'  | 36:a:2292:U:C6   | 2.49                     | 0.46              |
| 11:A:503:C:O2'   | 11:A:509:A:N6    | 2.49                     | 0.46              |
| 11:A:674:G:H2'   | 11:A:675:A:C8    | 2.49                     | 0.46              |
| 25:O:71:LYS:HB2  | 25:O:71:LYS:HE3  | 1.66                     | 0.46              |
| 26:P:50:THR:HG23 | 26:P:74:LEU:HD13 | 1.97                     | 0.46              |
| 34:Y:66:U:H2'    | 34:Y:67:A:H8     | 1.80                     | 0.46              |
| 38:c:142:HIS:ND1 | 38:c:193:GLY:O   | 2.38                     | 0.46              |
| 11:A:21:G:H2'    | 11:A:22:G:C8     | 2.49                     | 0.46              |
| 36:a:1278:C:H2'  | 36:a:1279:G:C8   | 2.51                     | 0.46              |
| 36:a:1667:G:O2'  | 36:a:1991:U:O4   | 2.28                     | 0.46              |
| 36:a:2246:G:H2'  | 36:a:2247:A:H8   | 1.80                     | 0.46              |
| 5:4:41:HIS:O     | 5:4:45:THR:OG1   | 2.31                     | 0.46              |
| 7:6:28:GLY:O     | 7:6:32:VAL:HG23  | 2.16                     | 0.46              |
| 11:A:1253:G:H2'  | 11:A:1254:A:C8   | 2.51                     | 0.46              |
| 14:D:109:ALA:HB3 | 14:D:113:GLU:HG3 | 1.98                     | 0.46              |
| 23:M:3:ARG:NH2   | 41:f:110:ARG:O   | 2.48                     | 0.46              |
| 36:a:2070:A:H2'  | 36:a:2071:A:C8   | 2.51                     | 0.46              |
| 36:a:2258:C:O2'  | 36:a:2427:C:OP2  | 2.29                     | 0.46              |
| 47:l:75:GLU:HB2  | 47:l:90:GLU:HG3  | 1.97                     | 0.46              |
| 10:9:101:GLU:OE1 | 10:9:102:THR:N   | 2.49                     | 0.46              |
| 11:A:324:G:N1    | 11:A:327:A:OP2   | 2.46                     | 0.46              |
| 11:A:769:G:H4'   | 11:A:1513:A:H4'  | 1.98                     | 0.46              |
| 18:H:52:GLU:OE1  | 18:H:52:GLU:N    | 2.49                     | 0.46              |
| 36:a:1799:G:O2'  | 38:c:180:GLU:OE2 | 2.32                     | 0.46              |
| 41:f:4:LEU:N     | 41:f:101:GLU:OE2 | 2.45                     | 0.46              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 61:z:46:ASP:OD1  | 61:z:46:ASP:N     | 2.39                     | 0.46              |
| 7:6:95:LEU:HD11  | 7:6:102:LEU:HD12  | 1.97                     | 0.46              |
| 20:J:42:LEU:HD21 | 20:J:73:LEU:HD22  | 1.98                     | 0.46              |
| 36:a:1306:C:H41  | 36:a:1606:C:H2'   | 1.81                     | 0.46              |
| 36:a:1802:A:H2'  | 36:a:1803:A:C8    | 2.50                     | 0.46              |
| 38:c:133:ARG:NH1 | 38:c:187:ASP:OD1  | 2.40                     | 0.46              |
| 49:n:76:LYS:NZ   | 49:n:80:GLU:OE2   | 2.45                     | 0.46              |
| 10:9:72:ILE:HG22 | 10:9:79:VAL:HG13  | 1.97                     | 0.46              |
| 36:a:414:C:H2'   | 36:a:415:A:C8     | 2.51                     | 0.46              |
| 36:a:910:A:H2'   | 36:a:911:A:C8     | 2.51                     | 0.46              |
| 36:a:2591:C:H2'  | 36:a:2592:G:C8    | 2.50                     | 0.46              |
| 36:a:2788:C:H2'  | 36:a:2789:C:C6    | 2.51                     | 0.46              |
| 11:A:634:C:H2'   | 11:A:635:A:C8     | 2.52                     | 0.45              |
| 36:a:1115:G:O2'  | 36:a:1116:G:O5'   | 2.34                     | 0.45              |
| 36:a:2273:A:H2'  | 36:a:2274:A:C8    | 2.51                     | 0.45              |
| 40:e:173:THR:HA  | 40:e:199:MET:HE1  | 1.97                     | 0.45              |
| 59:x:12:GLU:OE1  | 59:x:12:GLU:N     | 2.45                     | 0.45              |
| 10:9:357:SER:HA  | 10:9:360:ILE:HG22 | 1.97                     | 0.45              |
| 11:A:197:A:N1    | 11:A:220:G:O2'    | 2.47                     | 0.45              |
| 11:A:1291:U:H2'  | 11:A:1292:G:H8    | 1.82                     | 0.45              |
| 23:M:89:LEU:HD13 | 23:M:92:ARG:HD2   | 1.98                     | 0.45              |
| 36:a:1114:C:H2'  | 36:a:1115:G:C8    | 2.51                     | 0.45              |
| 2:1:39:ARG:NH2   | 36:a:468:G:N7     | 2.57                     | 0.45              |
| 11:A:235:C:H2'   | 11:A:236:A:C8     | 2.52                     | 0.45              |
| 11:A:1048:G:H5'' | 24:N:3:LYS:HD2    | 1.98                     | 0.45              |
| 14:D:44:ARG:HG3  | 14:D:46:PRO:HD3   | 1.97                     | 0.45              |
| 22:L:50:ARG:HG3  | 22:L:90:LEU:HD21  | 1.99                     | 0.45              |
| 36:a:1447:C:H2'  | 36:a:1448:G:H8    | 1.82                     | 0.45              |
| 36:a:2087:G:H2'  | 36:a:2088:A:H8    | 1.81                     | 0.45              |
| 36:a:2230:G:H5'' | 58:w:30:LEU:HD12  | 1.98                     | 0.45              |
| 36:a:2514:U:H2'  | 36:a:2515:C:C6    | 2.51                     | 0.45              |
| 39:d:39:ASP:N    | 39:d:39:ASP:OD1   | 2.49                     | 0.45              |
| 61:z:38:HIS:ND1  | 61:z:39:LEU:O     | 2.49                     | 0.45              |
| 11:A:171:A:H2'   | 11:A:172:A:C8     | 2.52                     | 0.45              |
| 11:A:1391:U:H2'  | 11:A:1392:G:C8    | 2.52                     | 0.45              |
| 36:a:349:U:H2'   | 36:a:350:G:H8     | 1.81                     | 0.45              |
| 36:a:589:U:H2'   | 36:a:590:A:C8     | 2.52                     | 0.45              |
| 36:a:2333:A:OP2  | 57:v:77:ARG:NH2   | 2.47                     | 0.45              |
| 10:9:114:LEU:HB2 | 10:9:120:PRO:HD2  | 1.97                     | 0.45              |
| 10:9:493:LYS:HA  | 10:9:496:THR:HG22 | 1.98                     | 0.45              |
| 11:A:1500:A:H5'' | 11:A:1508:A:H5''  | 1.99                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 13:C:175:LEU:HD23 | 13:C:182:ILE:HD13 | 1.97                     | 0.45              |
| 36:a:272:A:H2'    | 36:a:273:G:C8     | 2.52                     | 0.45              |
| 36:a:639:U:H2'    | 36:a:640:C:C6     | 2.52                     | 0.45              |
| 36:a:1794:A:H2'   | 36:a:1795:C:C6    | 2.52                     | 0.45              |
| 36:a:1853:A:H2'   | 36:a:1854:A:C8    | 2.52                     | 0.45              |
| 56:u:77:VAL:HG23  | 56:u:89:ILE:HG12  | 1.98                     | 0.45              |
| 7:6:63:MET:SD     | 7:6:63:MET:N      | 2.89                     | 0.45              |
| 10:9:163:LYS:HD3  | 10:9:178:TYR:HB3  | 1.98                     | 0.45              |
| 47:l:42:THR:HG22  | 47:l:93:VAL:HG12  | 1.97                     | 0.45              |
| 11:A:17:U:H2'     | 11:A:18:C:C6      | 2.52                     | 0.45              |
| 11:A:1126:U:OP1   | 20:J:7:ARG:NH1    | 2.38                     | 0.45              |
| 36:a:1469:A:H2'   | 36:a:1470:A:H8    | 1.82                     | 0.45              |
| 7:6:132:SER:O     | 7:6:136:ALA:HB2   | 2.16                     | 0.45              |
| 11:A:41:G:H2'     | 11:A:42:G:C8      | 2.51                     | 0.45              |
| 16:F:72:ASP:O     | 16:F:76:THR:HG23  | 2.17                     | 0.45              |
| 32:V:117:ARG:O    | 36:a:2061:G:N2    | 2.46                     | 0.45              |
| 36:a:2243:U:H2'   | 36:a:2244:U:C6    | 2.52                     | 0.45              |
| 53:r:17:VAL:HG11  | 53:r:103:ILE:HG12 | 1.98                     | 0.45              |
| 54:s:5:GLU:OE1    | 54:s:5:GLU:N      | 2.42                     | 0.45              |
| 1:0:23:THR:OG1    | 1:0:24:THR:N      | 2.50                     | 0.45              |
| 11:A:1320:C:N3    | 29:S:36:ARG:NH1   | 2.65                     | 0.45              |
| 23:M:90:ARG:HD3   | 23:M:95:LEU:HB2   | 1.98                     | 0.45              |
| 34:Y:24:C:H2'     | 34:Y:25:G:C8      | 2.52                     | 0.45              |
| 36:a:2291:U:OP1   | 36:a:2380:C:O2'   | 2.35                     | 0.45              |
| 36:a:2591:C:H2'   | 36:a:2592:G:H8    | 1.82                     | 0.45              |
| 46:k:82:LEU:HD22  | 46:k:90:VAL:HG21  | 1.98                     | 0.45              |
| 9:8:65:ILE:O      | 9:8:69:VAL:HG23   | 2.17                     | 0.45              |
| 36:a:320:A:N3     | 40:e:163:ASN:ND2  | 2.51                     | 0.45              |
| 47:l:35:ALA:HA    | 47:l:128:THR:HG22 | 1.99                     | 0.45              |
| 7:6:63:MET:HA     | 7:6:66:MET:HG2    | 1.99                     | 0.44              |
| 36:a:1799:G:OP1   | 38:c:258:ARG:NH1  | 2.38                     | 0.44              |
| 7:6:102:LEU:HD23  | 7:6:105:ILE:HD12  | 1.99                     | 0.44              |
| 7:6:311:GLN:O     | 7:6:314:GLN:NE2   | 2.50                     | 0.44              |
| 10:9:346:TRP:O    | 10:9:349:SER:OG   | 2.33                     | 0.44              |
| 11:A:757:U:OP1    | 11:A:822:U:O2'    | 2.33                     | 0.44              |
| 42:g:17:VAL:HG11  | 42:g:50:LEU:HD21  | 1.99                     | 0.44              |
| 48:m:86:ARG:NE    | 48:m:117:ASP:OD2  | 2.42                     | 0.44              |
| 11:A:1123:U:O2'   | 20:J:39:PRO:O     | 2.27                     | 0.44              |
| 11:A:1342:C:H2'   | 11:A:1343:G:C8    | 2.52                     | 0.44              |
| 36:a:593:U:H2'    | 36:a:594:U:C6     | 2.52                     | 0.44              |
| 36:a:1864:U:OP1   | 36:a:2410:G:O2'   | 2.33                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 11:A:1149:C:H2'  | 11:A:1150:A:C8   | 2.50                     | 0.44              |
| 22:L:34:CYS:HB2  | 22:L:78:SER:H    | 1.82                     | 0.44              |
| 24:N:82:ILE:O    | 24:N:86:GLU:HG3  | 2.17                     | 0.44              |
| 36:a:2047:C:H2'  | 36:a:2048:G:H8   | 1.82                     | 0.44              |
| 10:9:384:ARG:HG3 | 10:9:385:MET:HG3 | 2.00                     | 0.44              |
| 11:A:1162:C:H2'  | 11:A:1163:A:H8   | 1.82                     | 0.44              |
| 36:a:1353:A:H2'  | 36:a:1354:A:C8   | 2.53                     | 0.44              |
| 37:b:5:U:OP1     | 37:b:61:G:O2'    | 2.25                     | 0.44              |
| 10:9:477:PHE:O   | 10:9:481:MET:HG2 | 2.18                     | 0.44              |
| 11:A:539:A:H2'   | 11:A:540:G:C8    | 2.53                     | 0.44              |
| 11:A:1305:G:H22  | 11:A:1331:G:HO2' | 1.66                     | 0.44              |
| 36:a:1438:U:H2'  | 36:a:1439:A:H8   | 1.83                     | 0.44              |
| 36:a:2845:U:H5'' | 50:o:52:ASN:O    | 2.17                     | 0.44              |
| 11:A:947:G:O3'   | 23:M:108:THR:OG1 | 2.36                     | 0.44              |
| 25:O:74:ASP:OD1  | 25:O:74:ASP:N    | 2.49                     | 0.44              |
| 34:Y:54:G:O3'    | 47:l:55:ARG:NH2  | 2.48                     | 0.44              |
| 36:a:58:G:O2'    | 36:a:73:A:N1     | 2.50                     | 0.44              |
| 36:a:582:A:H2'   | 36:a:583:G:C8    | 2.53                     | 0.44              |
| 36:a:1009:A:N3   | 36:a:1153:C:O2'  | 2.47                     | 0.44              |
| 36:a:1754:A:C8   | 50:o:94:LYS:HE2  | 2.53                     | 0.44              |
| 36:a:2405:G:O2'  | 36:a:2411:A:N6   | 2.50                     | 0.44              |
| 37:b:49:C:H2'    | 37:b:50:A:C8     | 2.52                     | 0.44              |
| 7:6:60:ILE:HA    | 7:6:63:MET:HG2   | 2.00                     | 0.44              |
| 36:a:1744:A:H3'  | 36:a:1745:A:H8   | 1.83                     | 0.44              |
| 11:A:677:U:O2    | 11:A:777:A:O2'   | 2.28                     | 0.44              |
| 11:A:1147:C:H2'  | 11:A:1148:U:C6   | 2.53                     | 0.44              |
| 36:a:580:U:H2'   | 36:a:581:C:C6    | 2.53                     | 0.44              |
| 36:a:1734:G:H2'  | 36:a:1735:A:C8   | 2.53                     | 0.44              |
| 36:a:2014:A:H2'  | 36:a:2015:A:C8   | 2.53                     | 0.44              |
| 11:A:976:G:OP2   | 11:A:1358:U:O2'  | 2.35                     | 0.43              |
| 57:v:44:LYS:HB2  | 57:v:44:LYS:HE2  | 1.79                     | 0.43              |
| 11:A:490:C:H2'   | 11:A:491:G:C8    | 2.54                     | 0.43              |
| 58:w:7:VAL:O     | 58:w:74:ARG:NH2  | 2.51                     | 0.43              |
| 11:A:505:G:OP1   | 11:A:510:A:N6    | 2.51                     | 0.43              |
| 23:M:15:ALA:HB3  | 23:M:34:LEU:HD21 | 2.00                     | 0.43              |
| 36:a:278:A:N6    | 36:a:362:A:N7    | 2.67                     | 0.43              |
| 36:a:589:U:H2'   | 36:a:590:A:H8    | 1.83                     | 0.43              |
| 36:a:1013:C:H2'  | 36:a:1014:A:H8   | 1.84                     | 0.43              |
| 36:a:1808:A:H3'  | 36:a:1809:A:C8   | 2.54                     | 0.43              |
| 4:3:1:MET:HE2    | 4:3:1:MET:HB2    | 1.93                     | 0.43              |
| 36:a:151:C:H2'   | 36:a:152:A:C8    | 2.53                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 36:a:288:U:H2'    | 36:a:289:G:H8     | 1.82                     | 0.43              |
| 36:a:1563:U:H2'   | 36:a:1564:C:C6    | 2.53                     | 0.43              |
| 40:e:1:MET:HE1    | 40:e:113:VAL:HG11 | 2.00                     | 0.43              |
| 11:A:1144:G:N2    | 11:A:1146:A:H62   | 2.15                     | 0.43              |
| 11:A:1382:C:H2'   | 11:A:1383:C:H6    | 1.84                     | 0.43              |
| 36:a:1571:A:H2'   | 36:a:1572:A:C8    | 2.53                     | 0.43              |
| 36:a:1604:C:H2'   | 36:a:1605:C:H6    | 1.83                     | 0.43              |
| 36:a:1654:A:O2'   | 39:d:118:PHE:O    | 2.28                     | 0.43              |
| 36:a:2087:G:H2'   | 36:a:2088:A:C8    | 2.54                     | 0.43              |
| 10:9:471:MET:HE3  | 10:9:471:MET:HB3  | 1.91                     | 0.43              |
| 11:A:337:G:H2'    | 11:A:338:A:H8     | 1.83                     | 0.43              |
| 11:A:552:U:H2'    | 11:A:553:A:C8     | 2.53                     | 0.43              |
| 11:A:1249:C:O3'   | 19:I:75:GLN:NE2   | 2.51                     | 0.43              |
| 36:a:5:A:H2'      | 36:a:6:A:H8       | 1.82                     | 0.43              |
| 36:a:1000:A:H2'   | 36:a:1001:A:C8    | 2.54                     | 0.43              |
| 36:a:2836:U:H2'   | 36:a:2837:A:C8    | 2.54                     | 0.43              |
| 11:A:358:U:H2'    | 11:A:359:G:H8     | 1.82                     | 0.43              |
| 11:A:390:U:H2'    | 11:A:391:G:C8     | 2.54                     | 0.43              |
| 11:A:1189:U:OP1   | 24:N:98:LYS:NZ    | 2.52                     | 0.43              |
| 11:A:1291:U:H2'   | 11:A:1292:G:C8    | 2.54                     | 0.43              |
| 11:A:1412:C:H2'   | 11:A:1413:A:C8    | 2.53                     | 0.43              |
| 12:B:97:LEU:H     | 12:B:100:MET:HE3  | 1.84                     | 0.43              |
| 30:T:31:PHE:O     | 30:T:35:VAL:HG23  | 2.17                     | 0.43              |
| 36:a:171:U:H2'    | 36:a:172:A:H8     | 1.82                     | 0.43              |
| 36:a:414:C:H2'    | 36:a:415:A:H8     | 1.84                     | 0.43              |
| 36:a:582:A:H2'    | 36:a:583:G:H8     | 1.84                     | 0.43              |
| 36:a:659:G:O2'    | 40:e:95:LYS:O     | 2.35                     | 0.43              |
| 7:6:121:ARG:O     | 7:6:124:THR:OG1   | 2.28                     | 0.43              |
| 11:A:400:C:OP1    | 14:D:70:ARG:NH2   | 2.51                     | 0.43              |
| 24:N:54:ASP:OD1   | 24:N:59:ARG:NH2   | 2.40                     | 0.43              |
| 36:a:848:C:H2'    | 36:a:849:A:C8     | 2.49                     | 0.43              |
| 3:2:25:LYS:HB3    | 46:k:62:PRO:HG2   | 2.01                     | 0.43              |
| 8:7:38:ASP:O      | 8:7:44:ARG:NH2    | 2.50                     | 0.43              |
| 11:A:582:C:OP2    | 11:A:758:C:N4     | 2.46                     | 0.43              |
| 36:a:349:U:H2'    | 36:a:350:G:C8     | 2.54                     | 0.43              |
| 36:a:813:U:H2'    | 36:a:814:C:C6     | 2.53                     | 0.43              |
| 36:a:2567:G:H2'   | 36:a:2568:U:C6    | 2.54                     | 0.43              |
| 36:a:2898:U:H2'   | 36:a:2899:A:C8    | 2.53                     | 0.43              |
| 40:e:149:ILE:HG22 | 40:e:192:ALA:HB1  | 2.00                     | 0.43              |
| 44:i:1:MET:HE1    | 52:q:12:HIS:HB3   | 1.99                     | 0.43              |
| 1:0:6:ARG:NE      | 36:a:2285:C:OP2   | 2.51                     | 0.43              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 7:6:211:ARG:NH1    | 10:9:329:ASP:OD1  | 2.52                     | 0.43              |
| 15:E:165:LEU:HD12  | 15:E:165:LEU:HA   | 1.91                     | 0.43              |
| 19:I:88:MET:HE3    | 19:I:98:LEU:HD12  | 2.01                     | 0.43              |
| 22:L:81:LEU:HB2    | 22:L:102:LEU:HD12 | 2.00                     | 0.43              |
| 24:N:49:GLN:OE1    | 29:S:13:LEU:N     | 2.46                     | 0.43              |
| 29:S:28:LYS:NZ     | 29:S:46:GLY:O     | 2.52                     | 0.43              |
| 36:a:1197:G:H2'    | 36:a:1198:U:H6    | 1.84                     | 0.43              |
| 37:b:5:U:H2'       | 37:b:6:G:H8       | 1.84                     | 0.43              |
| 7:6:82:ILE:HD13    | 7:6:171:LEU:HD13  | 2.01                     | 0.42              |
| 10:9:472:GLY:HA2   | 10:9:475:MET:HE2  | 2.01                     | 0.42              |
| 11:A:438:U:H1'     | 14:D:120:HIS:CE1  | 2.54                     | 0.42              |
| 11:A:524:G:H2'     | 11:A:525:C:C6     | 2.54                     | 0.42              |
| 11:A:1115:U:OP1    | 20:J:68:ARG:NH1   | 2.45                     | 0.42              |
| 11:A:1130:A:O2'    | 19:I:5:GLN:OE1    | 2.29                     | 0.42              |
| 11:A:1266:G:N2     | 11:A:1269:A:OP2   | 2.38                     | 0.42              |
| 11:A:1522:U:OP1    | 21:K:128:ARG:NH2  | 2.51                     | 0.42              |
| 36:a:720:U:H2'     | 36:a:721:A:C8     | 2.54                     | 0.42              |
| 36:a:1394:U:H4'    | 36:a:1603:A:H4'   | 2.00                     | 0.42              |
| 36:a:2229:U:H2'    | 36:a:2230:G:C8    | 2.53                     | 0.42              |
| 36:a:2251:OMG:HM23 | 36:a:2251:OMG:H1' | 1.59                     | 0.42              |
| 41:f:119:ALA:HB1   | 41:f:167:ARG:HE   | 1.84                     | 0.42              |
| 36:a:247:G:OP2     | 36:a:249:C:N4     | 2.49                     | 0.42              |
| 36:a:272:A:H2'     | 36:a:273:G:H8     | 1.83                     | 0.42              |
| 36:a:820:A:H4'     | 36:a:836:G:H22    | 1.83                     | 0.42              |
| 36:a:1224:U:H2'    | 36:a:1225:G:C8    | 2.54                     | 0.42              |
| 36:a:1570:A:H2'    | 36:a:1571:A:C8    | 2.53                     | 0.42              |
| 36:a:2329:U:H2'    | 36:a:2330:G:C8    | 2.54                     | 0.42              |
| 36:a:2372:U:H2'    | 36:a:2373:G:C8    | 2.53                     | 0.42              |
| 41:f:106:ILE:HG21  | 41:f:139:PRO:HG3  | 2.01                     | 0.42              |
| 7:6:87:SER:O       | 7:6:91:ILE:HG12   | 2.18                     | 0.42              |
| 13:C:8:ASN:ND2     | 24:N:90:ARG:O     | 2.52                     | 0.42              |
| 21:K:112:ASP:HB3   | 31:U:2:PRO:HB2    | 2.01                     | 0.42              |
| 30:T:76:LYS:O      | 30:T:80:THR:OG1   | 2.28                     | 0.42              |
| 36:a:373:U:H2'     | 36:a:374:A:H8     | 1.84                     | 0.42              |
| 36:a:989:G:OP2     | 60:y:12:SER:OG    | 2.38                     | 0.42              |
| 36:a:1607:C:N4     | 36:a:1622:G:OP2   | 2.40                     | 0.42              |
| 36:a:1997:C:OP2    | 39:d:129:THR:OG1  | 2.28                     | 0.42              |
| 41:f:57:LEU:O      | 41:f:61:SER:OG    | 2.23                     | 0.42              |
| 50:o:87:LYS:HA     | 50:o:87:LYS:HD2   | 1.94                     | 0.42              |
| 7:6:241:GLN:HB2    | 8:7:83:ILE:HD11   | 2.01                     | 0.42              |
| 14:D:54:GLN:HB3    | 14:D:203:LEU:HB2  | 2.01                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:F:90:MET:HE3   | 16:F:90:MET:HB2   | 1.86                     | 0.42              |
| 30:T:27:MET:HB3   | 30:T:27:MET:HE3   | 1.80                     | 0.42              |
| 36:a:155:A:H2'    | 36:a:156:A:H8     | 1.85                     | 0.42              |
| 36:a:1447:C:H2'   | 36:a:1448:G:C8    | 2.54                     | 0.42              |
| 5:4:13:THR:O      | 5:4:13:THR:OG1    | 2.33                     | 0.42              |
| 28:R:65:LEU:HD23  | 28:R:65:LEU:HA    | 1.89                     | 0.42              |
| 29:S:51:VAL:HG21  | 29:S:71:LEU:HB3   | 2.01                     | 0.42              |
| 32:V:52:GLY:O     | 32:V:56:GLY:N     | 2.47                     | 0.42              |
| 36:a:569:U:O2'    | 36:a:983:A:N1     | 2.44                     | 0.42              |
| 36:a:739:A:H1'    | 36:a:740:C:H5     | 1.84                     | 0.42              |
| 36:a:1038:G:H2'   | 36:a:1039:A:C8    | 2.54                     | 0.42              |
| 10:9:62:SER:O     | 10:9:138:TYR:N    | 2.47                     | 0.42              |
| 10:9:407:GLU:OE1  | 10:9:407:GLU:N    | 2.51                     | 0.42              |
| 11:A:512:U:H2'    | 11:A:513:C:C6     | 2.54                     | 0.42              |
| 11:A:948:C:H2'    | 11:A:949:A:H8     | 1.85                     | 0.42              |
| 11:A:1524:C:H2'   | 11:A:1525:G:C8    | 2.55                     | 0.42              |
| 29:S:41:PHE:H     | 29:S:44:MET:HE3   | 1.85                     | 0.42              |
| 35:Z:6:A:H2'      | 35:Z:7:G:C8       | 2.55                     | 0.42              |
| 36:a:566:U:H5''   | 46:k:29:LYS:HE3   | 2.01                     | 0.42              |
| 36:a:2377:A:O2'   | 49:n:117:PHE:O    | 2.32                     | 0.42              |
| 36:a:2443:C:H2'   | 36:a:2444:G:H8    | 1.84                     | 0.42              |
| 38:c:145:GLU:HB2  | 38:c:188:CYS:HB3  | 2.01                     | 0.42              |
| 15:E:111:MET:HB3  | 15:E:111:MET:HE2  | 1.80                     | 0.42              |
| 31:U:60:LEU:O     | 31:U:64:ASN:ND2   | 2.44                     | 0.42              |
| 44:i:114:LEU:HG   | 44:i:118:MET:HE3  | 2.01                     | 0.42              |
| 55:t:14:LEU:HD11  | 55:t:71:ALA:HB2   | 2.00                     | 0.42              |
| 10:9:166:VAL:N    | 10:9:175:ASN:O    | 2.50                     | 0.42              |
| 10:9:262:THR:HG22 | 10:9:309:VAL:HG13 | 2.01                     | 0.42              |
| 11:A:977:A:N6     | 11:A:1224:U:O5'   | 2.53                     | 0.42              |
| 11:A:1175:G:H2'   | 11:A:1176:A:H8    | 1.85                     | 0.42              |
| 36:a:1689:A:H2'   | 36:a:1690:A:C8    | 2.54                     | 0.42              |
| 36:a:2615:U:C2    | 61:z:4:GLN:HA     | 2.54                     | 0.42              |
| 36:a:2646:C:OP2   | 36:a:2732:G:O2'   | 2.37                     | 0.42              |
| 10:9:120:PRO:HB2  | 10:9:129:PRO:HG3  | 2.01                     | 0.42              |
| 11:A:28:A:O2'     | 11:A:296:U:OP1    | 2.26                     | 0.42              |
| 18:H:111:MET:HB3  | 18:H:111:MET:HE2  | 1.75                     | 0.42              |
| 25:O:17:ARG:HH21  | 25:O:77:ARG:HH11  | 1.67                     | 0.42              |
| 36:a:172:A:H2'    | 36:a:173:A:C8     | 2.55                     | 0.42              |
| 36:a:2394:C:H5''  | 46:k:63:LYS:HE2   | 2.02                     | 0.42              |
| 10:9:227:ASP:OD1  | 10:9:227:ASP:N    | 2.53                     | 0.42              |
| 17:G:129:GLU:N    | 17:G:129:GLU:OE1  | 2.53                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 34:Y:5:G:H2'     | 34:Y:6:A:H8      | 1.85                     | 0.42              |
| 36:a:299:A:N3    | 36:a:319:G:O2'   | 2.44                     | 0.42              |
| 36:a:1754:A:O3'  | 50:o:103:ARG:NH2 | 2.52                     | 0.42              |
| 36:a:1889:A:H2'  | 36:a:1890:A:C8   | 2.55                     | 0.42              |
| 45:j:114:LYS:HE3 | 45:j:114:LYS:HB2 | 1.70                     | 0.42              |
| 11:A:493:A:H2'   | 11:A:494:G:C4    | 2.55                     | 0.41              |
| 11:A:1346:A:OP1  | 19:I:122:ARG:NH1 | 2.43                     | 0.41              |
| 37:b:36:C:N4     | 37:b:49:C:O2     | 2.52                     | 0.41              |
| 44:i:92:MET:HE3  | 44:i:92:MET:HB3  | 1.81                     | 0.41              |
| 11:A:182:A:N1    | 11:A:223:A:O2'   | 2.53                     | 0.41              |
| 11:A:254:G:N2    | 27:Q:18:GLU:OE2  | 2.51                     | 0.41              |
| 11:A:579:A:O2'   | 25:O:54:ARG:NH1  | 2.46                     | 0.41              |
| 11:A:579:A:H5'   | 11:A:728:A:H1'   | 2.02                     | 0.41              |
| 11:A:736:C:H2'   | 11:A:737:C:H6    | 1.85                     | 0.41              |
| 11:A:1363:A:O2'  | 11:A:1365:G:N7   | 2.44                     | 0.41              |
| 18:H:25:VAL:HG13 | 18:H:63:LEU:HD21 | 2.01                     | 0.41              |
| 36:a:742:A:H2'   | 36:a:743:A:H8    | 1.84                     | 0.41              |
| 36:a:927:A:H2'   | 36:a:928:A:C8    | 2.55                     | 0.41              |
| 36:a:1443:U:H2'  | 36:a:1444:G:H8   | 1.86                     | 0.41              |
| 36:a:2086:U:H2'  | 36:a:2087:G:C8   | 2.55                     | 0.41              |
| 11:A:944:G:N1    | 11:A:1338:G:OP2  | 2.48                     | 0.41              |
| 36:a:1683:U:H2'  | 36:a:1684:G:C8   | 2.55                     | 0.41              |
| 36:a:1716:U:H2'  | 36:a:1717:A:H8   | 1.85                     | 0.41              |
| 7:6:206:THR:HG21 | 7:6:401:PHE:HE2  | 1.85                     | 0.41              |
| 11:A:67:C:H2'    | 11:A:68:G:C8     | 2.55                     | 0.41              |
| 11:A:390:U:H2'   | 11:A:391:G:H8    | 1.85                     | 0.41              |
| 11:A:1006:G:H1   | 11:A:1023:U:H3   | 1.67                     | 0.41              |
| 16:F:88:MET:HE2  | 28:R:64:TYR:HD2  | 1.85                     | 0.41              |
| 21:K:35:THR:OG1  | 21:K:36:ASP:N    | 2.52                     | 0.41              |
| 7:6:279:PHE:O    | 7:6:283:ILE:HB   | 2.21                     | 0.41              |
| 11:A:579:A:H2'   | 11:A:580:C:C6    | 2.56                     | 0.41              |
| 11:A:619:U:H3    | 14:D:131:ASN:HB3 | 1.86                     | 0.41              |
| 11:A:696:A:H2'   | 11:A:697:U:H6    | 1.86                     | 0.41              |
| 11:A:1216:A:OP1  | 24:N:3:LYS:NZ    | 2.42                     | 0.41              |
| 19:I:41:ARG:NH2  | 19:I:43:THR:OG1  | 2.54                     | 0.41              |
| 23:M:78:LYS:HA   | 23:M:81:MET:HG3  | 2.03                     | 0.41              |
| 29:S:49:ILE:HD12 | 29:S:49:ILE:HA   | 1.84                     | 0.41              |
| 30:T:28:MET:HG3  | 30:T:58:VAL:HG12 | 2.02                     | 0.41              |
| 36:a:184:C:H2'   | 36:a:185:G:H8    | 1.84                     | 0.41              |
| 36:a:284:U:O2    | 36:a:356:G:N2    | 2.44                     | 0.41              |
| 36:a:1668:A:O2'  | 36:a:1674:G:N7   | 2.47                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 50:o:22:PRO:HD3  | 50:o:50:ILE:HD12  | 2.03                     | 0.41              |
| 7:6:130:PHE:HE2  | 7:6:290:ILE:HG12  | 1.85                     | 0.41              |
| 10:9:495:MET:HA  | 10:9:498:MET:HE3  | 2.02                     | 0.41              |
| 11:A:193:C:H2'   | 11:A:194:C:C6     | 2.55                     | 0.41              |
| 11:A:235:C:H2'   | 11:A:236:A:H8     | 1.83                     | 0.41              |
| 11:A:600:A:H2'   | 11:A:601:G:H8     | 1.86                     | 0.41              |
| 14:D:139:PRO:HB3 | 14:D:184:ARG:HA   | 2.02                     | 0.41              |
| 36:a:64:A:H2'    | 36:a:65:U:C6      | 2.56                     | 0.41              |
| 36:a:876:C:H2'   | 36:a:877:A:O4'    | 2.20                     | 0.41              |
| 36:a:1231:U:H2'  | 36:a:1232:G:H8    | 1.85                     | 0.41              |
| 36:a:1571:A:H2'  | 36:a:1572:A:H8    | 1.86                     | 0.41              |
| 36:a:1682:G:H2'  | 36:a:1683:U:C6    | 2.56                     | 0.41              |
| 38:c:5:LYS:HD2   | 38:c:17:VAL:HG22  | 2.02                     | 0.41              |
| 11:A:12:U:H4'    | 11:A:526:C:H4'    | 2.03                     | 0.41              |
| 11:A:35:G:N3     | 22:L:115:SER:OG   | 2.48                     | 0.41              |
| 11:A:908:A:H2'   | 11:A:909:A:H8     | 1.84                     | 0.41              |
| 19:I:33:ARG:HE   | 19:I:38:TYR:HD1   | 1.69                     | 0.41              |
| 36:a:160:A:N3    | 36:a:2208:C:O2'   | 2.44                     | 0.41              |
| 36:a:511:U:H4'   | 36:a:1235:G:H4'   | 2.03                     | 0.41              |
| 36:a:871:U:H2'   | 36:a:872:U:C6     | 2.56                     | 0.41              |
| 36:a:1292:G:H2'  | 36:a:1293:C:C6    | 2.56                     | 0.41              |
| 36:a:1564:C:H2'  | 36:a:1565:C:C6    | 2.56                     | 0.41              |
| 38:c:72:ASP:OD2  | 38:c:189:ARG:NH2  | 2.54                     | 0.41              |
| 40:e:149:ILE:HB  | 40:e:188:MET:HG2  | 2.03                     | 0.41              |
| 11:A:402:G:P     | 14:D:71:GLN:HE22  | 2.43                     | 0.41              |
| 11:A:427:U:O2'   | 11:A:541:G:OP1    | 2.35                     | 0.41              |
| 28:R:33:ILE:HD12 | 28:R:37:GLY:HA2   | 2.03                     | 0.41              |
| 36:a:554:U:H2'   | 36:a:555:G:O4'    | 2.21                     | 0.41              |
| 53:r:84:ARG:HB2  | 53:r:96:ILE:HB    | 2.03                     | 0.41              |
| 3:2:45:ARG:NH2   | 36:a:2349:G:OP1   | 2.53                     | 0.41              |
| 3:2:52:LYS:HB3   | 3:2:52:LYS:HE3    | 1.80                     | 0.41              |
| 7:6:405:SER:O    | 7:6:409:VAL:HG13  | 2.21                     | 0.41              |
| 7:6:416:PHE:O    | 7:6:420:VAL:HG13  | 2.20                     | 0.41              |
| 7:6:426:SER:O    | 7:6:430:GLU:N     | 2.53                     | 0.41              |
| 11:A:236:A:H2'   | 11:A:237:G:C8     | 2.55                     | 0.41              |
| 11:A:337:G:H2'   | 11:A:338:A:C8     | 2.55                     | 0.41              |
| 11:A:407:U:H2'   | 11:A:408:A:C8     | 2.55                     | 0.41              |
| 11:A:512:U:H2'   | 11:A:513:C:H6     | 1.85                     | 0.41              |
| 11:A:718:A:H5'   | 21:K:119:ASN:HD21 | 1.86                     | 0.41              |
| 11:A:859:G:H2'   | 11:A:860:A:C8     | 2.56                     | 0.41              |
| 11:A:881:G:OP2   | 22:L:9:ARG:NH2    | 2.52                     | 0.41              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 11:A:1217:C:OP1   | 24:N:9:ARG:NE    | 2.44                     | 0.41              |
| 24:N:49:GLN:NE2   | 29:S:11:ILE:O    | 2.47                     | 0.41              |
| 34:Y:64:U:H2'     | 34:Y:65:C:C6     | 2.56                     | 0.41              |
| 36:a:6:A:H2'      | 36:a:7:G:C8      | 2.56                     | 0.41              |
| 36:a:27:G:N2      | 36:a:512:G:H1'   | 2.36                     | 0.41              |
| 36:a:2081:U:H2'   | 36:a:2082:A:H8   | 1.86                     | 0.41              |
| 36:a:2443:C:H2'   | 36:a:2444:G:C8   | 2.56                     | 0.41              |
| 36:a:2705:A:O2'   | 36:a:2852:G:OP1  | 2.31                     | 0.41              |
| 39:d:181:ASP:OD2  | 39:d:184:ARG:NE  | 2.54                     | 0.41              |
| 45:j:106:GLU:OE1  | 45:j:106:GLU:N   | 2.53                     | 0.41              |
| 11:A:297:G:N2     | 11:A:300:A:OP2   | 2.36                     | 0.41              |
| 11:A:625:U:H2'    | 11:A:626:G:H8    | 1.86                     | 0.41              |
| 16:F:6:ILE:HG13   | 16:F:89:VAL:HG23 | 2.03                     | 0.41              |
| 36:a:1412:U:H2'   | 36:a:1413:A:C8   | 2.56                     | 0.41              |
| 38:c:165:VAL:HG21 | 38:c:181:MET:HE1 | 2.02                     | 0.41              |
| 57:v:72:LYS:HB2   | 57:v:72:LYS:HE2  | 1.91                     | 0.41              |
| 10:9:444:VAL:HG12 | 10:9:447:ARG:HA  | 2.02                     | 0.40              |
| 11:A:269:C:H2'    | 11:A:270:A:C8    | 2.55                     | 0.40              |
| 11:A:504:C:O2     | 11:A:511:C:N4    | 2.53                     | 0.40              |
| 11:A:553:A:H2'    | 11:A:554:A:C8    | 2.56                     | 0.40              |
| 11:A:918:A:H2'    | 11:A:919:A:C8    | 2.56                     | 0.40              |
| 30:T:29:ARG:O     | 30:T:33:LYS:HG3  | 2.21                     | 0.40              |
| 36:a:1880:U:H2'   | 36:a:1881:C:C6   | 2.57                     | 0.40              |
| 11:A:613:C:H2'    | 11:A:614:C:C6    | 2.56                     | 0.40              |
| 11:A:911:U:H2'    | 11:A:912:C:C6    | 2.56                     | 0.40              |
| 11:A:1238:A:OP1   | 11:A:1335:U:O2'  | 2.32                     | 0.40              |
| 36:a:30:G:O2'     | 36:a:1214:A:N3   | 2.50                     | 0.40              |
| 36:a:1794:A:H2'   | 36:a:1795:C:H6   | 1.86                     | 0.40              |
| 36:a:2314:A:H2'   | 36:a:2315:G:C8   | 2.56                     | 0.40              |
| 50:o:5:ILE:O      | 50:o:9:GLU:HG3   | 2.20                     | 0.40              |
| 7:6:48:VAL:HG23   | 7:6:148:LEU:HD23 | 2.03                     | 0.40              |
| 8:7:58:VAL:HG12   | 8:7:66:LYS:HE3   | 2.02                     | 0.40              |
| 10:9:142:GLU:O    | 10:9:169:ARG:NH2 | 2.54                     | 0.40              |
| 11:A:591:U:H2'    | 11:A:592:G:H8    | 1.86                     | 0.40              |
| 14:D:177:LYS:NZ   | 14:D:179:GLU:OE1 | 2.38                     | 0.40              |
| 21:K:79:ILE:HB    | 21:K:105:PHE:HE1 | 1.86                     | 0.40              |
| 36:a:2857:G:N2    | 36:a:2860:A:OP2  | 2.39                     | 0.40              |
| 37:b:52:A:N7      | 49:n:64:TYR:OH   | 2.48                     | 0.40              |
| 39:d:152:PRO:HG3  | 39:d:156:PHE:CZ  | 2.56                     | 0.40              |
| 40:e:168:ASP:OD2  | 40:e:170:ARG:NE  | 2.53                     | 0.40              |
| 57:v:37:ILE:HG21  | 57:v:80:ILE:HG21 | 2.02                     | 0.40              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 7:6:25:PHE:HZ    | 7:6:177:GLN:HG3   | 1.85                     | 0.40              |
| 10:9:475:MET:HA  | 10:9:478:ILE:HG22 | 2.04                     | 0.40              |
| 11:A:18:C:OP1    | 15:E:132:ASN:ND2  | 2.51                     | 0.40              |
| 11:A:131:A:H2'   | 11:A:132:C:C6     | 2.57                     | 0.40              |
| 13:C:9:GLY:HA3   | 24:N:89:MET:HE3   | 2.04                     | 0.40              |
| 20:J:92:LEU:HD23 | 20:J:92:LEU:HA    | 1.85                     | 0.40              |
| 36:a:419:U:H2'   | 36:a:420:C:C6     | 2.56                     | 0.40              |
| 36:a:858:G:H3'   | 36:a:859:G:C8     | 2.55                     | 0.40              |
| 10:9:426:LEU:O   | 10:9:430:MET:HG2  | 2.21                     | 0.40              |
| 11:A:486:U:H2'   | 11:A:487:A:C8     | 2.57                     | 0.40              |
| 11:A:513:C:H2'   | 11:A:514:C:H6     | 1.87                     | 0.40              |
| 11:A:601:G:H2'   | 11:A:602:A:H8     | 1.87                     | 0.40              |
| 11:A:601:G:H2'   | 11:A:602:A:C8     | 2.57                     | 0.40              |
| 11:A:1328:C:H2'  | 11:A:1329:A:H8    | 1.86                     | 0.40              |
| 36:a:171:U:H2'   | 36:a:172:A:C8     | 2.56                     | 0.40              |
| 36:a:1715:G:O2'  | 36:a:1743:G:O6    | 2.32                     | 0.40              |
| 42:g:107:LEU:O   | 42:g:152:ARG:NH2  | 2.51                     | 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     | 49/55 (89%)   | 48 (98%)  | 1 (2%)  | 0        | 100         | 100 |
| 2   | 1     | 44/46 (96%)   | 44 (100%) | 0       | 0        | 100         | 100 |
| 3   | 2     | 62/65 (95%)   | 61 (98%)  | 1 (2%)  | 0        | 100         | 100 |
| 4   | 3     | 36/38 (95%)   | 36 (100%) | 0       | 0        | 100         | 100 |
| 5   | 4     | 56/70 (80%)   | 52 (93%)  | 4 (7%)  | 0        | 100         | 100 |
| 7   | 6     | 419/443 (95%) | 404 (96%) | 15 (4%) | 0        | 100         | 100 |
| 8   | 7     | 112/127 (88%) | 107 (96%) | 5 (4%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured   | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|------------|---------|----------|-------------|-----|
| 9   | 8     | 52/110 (47%)  | 49 (94%)   | 3 (6%)  | 0        | 100         | 100 |
| 10  | 9     | 461/548 (84%) | 436 (95%)  | 25 (5%) | 0        | 100         | 100 |
| 12  | B     | 222/241 (92%) | 215 (97%)  | 7 (3%)  | 0        | 100         | 100 |
| 13  | C     | 204/233 (88%) | 199 (98%)  | 5 (2%)  | 0        | 100         | 100 |
| 14  | D     | 203/206 (98%) | 198 (98%)  | 5 (2%)  | 0        | 100         | 100 |
| 15  | E     | 154/167 (92%) | 151 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 16  | F     | 101/135 (75%) | 98 (97%)   | 3 (3%)  | 0        | 100         | 100 |
| 17  | G     | 151/179 (84%) | 146 (97%)  | 5 (3%)  | 0        | 100         | 100 |
| 18  | H     | 127/130 (98%) | 124 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 19  | I     | 125/130 (96%) | 120 (96%)  | 5 (4%)  | 0        | 100         | 100 |
| 20  | J     | 96/103 (93%)  | 91 (95%)   | 4 (4%)  | 1 (1%)   | 12          | 13  |
| 21  | K     | 115/129 (89%) | 111 (96%)  | 4 (4%)  | 0        | 100         | 100 |
| 22  | L     | 120/124 (97%) | 110 (92%)  | 10 (8%) | 0        | 100         | 100 |
| 23  | M     | 113/118 (96%) | 108 (96%)  | 5 (4%)  | 0        | 100         | 100 |
| 24  | N     | 98/101 (97%)  | 97 (99%)   | 1 (1%)  | 0        | 100         | 100 |
| 25  | O     | 86/89 (97%)   | 85 (99%)   | 1 (1%)  | 0        | 100         | 100 |
| 26  | P     | 79/82 (96%)   | 77 (98%)   | 2 (2%)  | 0        | 100         | 100 |
| 27  | Q     | 77/84 (92%)   | 71 (92%)   | 6 (8%)  | 0        | 100         | 100 |
| 28  | R     | 64/75 (85%)   | 62 (97%)   | 2 (3%)  | 0        | 100         | 100 |
| 29  | S     | 82/92 (89%)   | 79 (96%)   | 3 (4%)  | 0        | 100         | 100 |
| 30  | T     | 84/87 (97%)   | 83 (99%)   | 1 (1%)  | 0        | 100         | 100 |
| 31  | U     | 68/71 (96%)   | 66 (97%)   | 2 (3%)  | 0        | 100         | 100 |
| 32  | V     | 87/119 (73%)  | 82 (94%)   | 4 (5%)  | 1 (1%)   | 11          | 12  |
| 38  | c     | 269/273 (98%) | 263 (98%)  | 6 (2%)  | 0        | 100         | 100 |
| 39  | d     | 206/209 (99%) | 203 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 40  | e     | 199/201 (99%) | 198 (100%) | 1 (0%)  | 0        | 100         | 100 |
| 41  | f     | 175/179 (98%) | 166 (95%)  | 9 (5%)  | 0        | 100         | 100 |
| 42  | g     | 174/177 (98%) | 166 (95%)  | 8 (5%)  | 0        | 100         | 100 |
| 43  | h     | 39/149 (26%)  | 36 (92%)   | 3 (8%)  | 0        | 100         | 100 |
| 44  | i     | 140/142 (99%) | 138 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| 45  | j     | 121/123 (98%) | 120 (99%)  | 1 (1%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 46  | k     | 142/144 (99%)   | 138 (97%)  | 4 (3%)   | 0        | 100         | 100 |
| 47  | l     | 134/136 (98%)   | 133 (99%)  | 1 (1%)   | 0        | 100         | 100 |
| 48  | m     | 116/127 (91%)   | 113 (97%)  | 3 (3%)   | 0        | 100         | 100 |
| 49  | n     | 114/117 (97%)   | 111 (97%)  | 3 (3%)   | 0        | 100         | 100 |
| 50  | o     | 112/115 (97%)   | 111 (99%)  | 1 (1%)   | 0        | 100         | 100 |
| 51  | p     | 115/118 (98%)   | 114 (99%)  | 1 (1%)   | 0        | 100         | 100 |
| 52  | q     | 101/103 (98%)   | 95 (94%)   | 6 (6%)   | 0        | 100         | 100 |
| 53  | r     | 108/110 (98%)   | 108 (100%) | 0        | 0        | 100         | 100 |
| 54  | s     | 91/100 (91%)    | 91 (100%)  | 0        | 0        | 100         | 100 |
| 55  | t     | 100/104 (96%)   | 97 (97%)   | 3 (3%)   | 0        | 100         | 100 |
| 56  | u     | 92/94 (98%)     | 91 (99%)   | 1 (1%)   | 0        | 100         | 100 |
| 57  | v     | 76/85 (89%)     | 75 (99%)   | 1 (1%)   | 0        | 100         | 100 |
| 58  | w     | 75/78 (96%)     | 75 (100%)  | 0        | 0        | 100         | 100 |
| 59  | x     | 60/63 (95%)     | 60 (100%)  | 0        | 0        | 100         | 100 |
| 60  | y     | 56/59 (95%)     | 54 (96%)   | 2 (4%)   | 0        | 100         | 100 |
| 61  | z     | 54/57 (95%)     | 54 (100%)  | 0        | 0        | 100         | 100 |
| All | All   | 6616/7260 (91%) | 6420 (97%) | 194 (3%) | 2 (0%)   | 100         | 100 |

All (2) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 32  | V     | 88  | ARG  |
| 20  | J     | 57  | VAL  |

### 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     | 46/49 (94%)  | 46 (100%) | 0        | 100         | 100 |
| 2   | 1     | 38/38 (100%) | 38 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 3   | 2     | 51/52 (98%)    | 51 (100%)  | 0        | 100         | 100 |
| 4   | 3     | 34/34 (100%)   | 34 (100%)  | 0        | 100         | 100 |
| 5   | 4     | 55/62 (89%)    | 55 (100%)  | 0        | 100         | 100 |
| 7   | 6     | 344/359 (96%)  | 342 (99%)  | 2 (1%)   | 78          | 85  |
| 8   | 7     | 91/99 (92%)    | 91 (100%)  | 0        | 100         | 100 |
| 9   | 8     | 48/84 (57%)    | 47 (98%)   | 1 (2%)   | 47          | 60  |
| 10  | 9     | 400/469 (85%)  | 398 (100%) | 2 (0%)   | 81          | 87  |
| 12  | B     | 186/199 (94%)  | 184 (99%)  | 2 (1%)   | 65          | 75  |
| 13  | C     | 170/190 (90%)  | 170 (100%) | 0        | 100         | 100 |
| 14  | D     | 172/173 (99%)  | 171 (99%)  | 1 (1%)   | 78          | 85  |
| 15  | E     | 119/126 (94%)  | 119 (100%) | 0        | 100         | 100 |
| 16  | F     | 90/116 (78%)   | 90 (100%)  | 0        | 100         | 100 |
| 17  | G     | 126/147 (86%)  | 126 (100%) | 0        | 100         | 100 |
| 18  | H     | 104/105 (99%)  | 104 (100%) | 0        | 100         | 100 |
| 19  | I     | 105/107 (98%)  | 104 (99%)  | 1 (1%)   | 68          | 77  |
| 20  | J     | 86/90 (96%)    | 86 (100%)  | 0        | 100         | 100 |
| 21  | K     | 90/99 (91%)    | 89 (99%)   | 1 (1%)   | 65          | 75  |
| 22  | L     | 102/103 (99%)  | 102 (100%) | 0        | 100         | 100 |
| 23  | M     | 93/96 (97%)    | 92 (99%)   | 1 (1%)   | 65          | 75  |
| 24  | N     | 83/84 (99%)    | 83 (100%)  | 0        | 100         | 100 |
| 25  | O     | 76/77 (99%)    | 75 (99%)   | 1 (1%)   | 61          | 72  |
| 26  | P     | 65/65 (100%)   | 65 (100%)  | 0        | 100         | 100 |
| 27  | Q     | 73/78 (94%)    | 73 (100%)  | 0        | 100         | 100 |
| 28  | R     | 57/65 (88%)    | 57 (100%)  | 0        | 100         | 100 |
| 29  | S     | 72/79 (91%)    | 72 (100%)  | 0        | 100         | 100 |
| 30  | T     | 65/66 (98%)    | 65 (100%)  | 0        | 100         | 100 |
| 31  | U     | 60/61 (98%)    | 60 (100%)  | 0        | 100         | 100 |
| 32  | V     | 25/93 (27%)    | 25 (100%)  | 0        | 100         | 100 |
| 38  | c     | 216/218 (99%)  | 215 (100%) | 1 (0%)   | 81          | 87  |
| 39  | d     | 163/163 (100%) | 162 (99%)  | 1 (1%)   | 78          | 85  |
| 40  | e     | 165/165 (100%) | 165 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Rotameric   | Outliers | Percentiles |     |
|-----|-------|-----------------|-------------|----------|-------------|-----|
| 41  | f     | 148/150 (99%)   | 145 (98%)   | 3 (2%)   | 48          | 62  |
| 42  | g     | 137/138 (99%)   | 137 (100%)  | 0        | 100         | 100 |
| 43  | h     | 32/114 (28%)    | 32 (100%)   | 0        | 100         | 100 |
| 44  | i     | 116/116 (100%)  | 115 (99%)   | 1 (1%)   | 70          | 80  |
| 45  | j     | 104/104 (100%)  | 104 (100%)  | 0        | 100         | 100 |
| 46  | k     | 103/103 (100%)  | 103 (100%)  | 0        | 100         | 100 |
| 47  | l     | 109/109 (100%)  | 109 (100%)  | 0        | 100         | 100 |
| 48  | m     | 98/103 (95%)    | 98 (100%)   | 0        | 100         | 100 |
| 49  | n     | 86/87 (99%)     | 86 (100%)   | 0        | 100         | 100 |
| 50  | o     | 99/100 (99%)    | 99 (100%)   | 0        | 100         | 100 |
| 51  | p     | 89/90 (99%)     | 89 (100%)   | 0        | 100         | 100 |
| 52  | q     | 84/84 (100%)    | 84 (100%)   | 0        | 100         | 100 |
| 53  | r     | 93/93 (100%)    | 92 (99%)    | 1 (1%)   | 65          | 75  |
| 54  | s     | 80/84 (95%)     | 79 (99%)    | 1 (1%)   | 61          | 72  |
| 55  | t     | 83/85 (98%)     | 83 (100%)   | 0        | 100         | 100 |
| 56  | u     | 78/78 (100%)    | 76 (97%)    | 2 (3%)   | 40          | 53  |
| 57  | v     | 59/63 (94%)     | 59 (100%)   | 0        | 100         | 100 |
| 58  | w     | 67/68 (98%)     | 67 (100%)   | 0        | 100         | 100 |
| 59  | x     | 54/55 (98%)     | 54 (100%)   | 0        | 100         | 100 |
| 60  | y     | 48/49 (98%)     | 48 (100%)   | 0        | 100         | 100 |
| 61  | z     | 47/48 (98%)     | 47 (100%)   | 0        | 100         | 100 |
| All | All   | 5484/5932 (92%) | 5462 (100%) | 22 (0%)  | 81          | 89  |

All (22) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | 6     | 95  | LEU  |
| 7   | 6     | 414 | MET  |
| 9   | 8     | 11  | ILE  |
| 10  | 9     | 237 | THR  |
| 10  | 9     | 376 | GLN  |
| 12  | B     | 10  | LEU  |
| 12  | B     | 94  | HIS  |
| 14  | D     | 124 | MET  |
| 19  | I     | 89  | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 21  | K     | 74  | VAL  |
| 23  | M     | 42  | ASP  |
| 25  | O     | 24  | SER  |
| 38  | c     | 97  | LYS  |
| 39  | d     | 1   | MET  |
| 41  | f     | 49  | LEU  |
| 41  | f     | 50  | LEU  |
| 41  | f     | 85  | ILE  |
| 44  | i     | 1   | MET  |
| 53  | r     | 4   | ILE  |
| 54  | s     | 1   | MET  |
| 56  | u     | 61  | LEU  |
| 56  | u     | 65  | VAL  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | 1     | 26  | ASN  |
| 5   | 4     | 20  | ASN  |
| 7   | 6     | 252 | GLN  |
| 7   | 6     | 264 | HIS  |
| 9   | 8     | 72  | ASN  |
| 10  | 9     | 57  | GLN  |
| 10  | 9     | 323 | HIS  |
| 10  | 9     | 448 | GLN  |
| 10  | 9     | 527 | GLN  |
| 12  | B     | 109 | GLN  |
| 12  | B     | 177 | ASN  |
| 13  | C     | 100 | GLN  |
| 13  | C     | 102 | ASN  |
| 13  | C     | 123 | GLN  |
| 14  | D     | 74  | ASN  |
| 15  | E     | 122 | ASN  |
| 15  | E     | 146 | ASN  |
| 16  | F     | 55  | HIS  |
| 17  | G     | 28  | ASN  |
| 17  | G     | 122 | ASN  |
| 21  | K     | 24  | HIS  |
| 24  | N     | 43  | ASN  |
| 25  | O     | 35  | GLN  |
| 26  | P     | 40  | ASN  |
| 30  | T     | 48  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 30  | T     | 52  | ASN  |
| 38  | c     | 25  | HIS  |
| 40  | e     | 9   | GLN  |
| 40  | e     | 136 | GLN  |
| 45  | j     | 93  | GLN  |
| 47  | l     | 13  | HIS  |
| 48  | m     | 31  | HIS  |
| 50  | o     | 66  | ASN  |
| 51  | p     | 44  | GLN  |
| 53  | r     | 9   | HIS  |
| 54  | s     | 48  | GLN  |
| 58  | w     | 36  | HIS  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 11  | A     | 1516/1542 (98%) | 214 (14%)         | 2 (0%)          |
| 33  | X     | 8/9 (88%)       | 1 (12%)           | 0               |
| 34  | Y     | 76/77 (98%)     | 10 (13%)          | 2 (2%)          |
| 35  | Z     | 76/77 (98%)     | 11 (14%)          | 0               |
| 36  | a     | 2749/2904 (94%) | 309 (11%)         | 0               |
| 37  | b     | 118/120 (98%)   | 12 (10%)          | 0               |
| 6   | 5     | 1/2 (50%)       | 1 (100%)          | 0               |
| All | All   | 4544/4731 (96%) | 558 (12%)         | 4 (0%)          |

All (558) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | 5     | 76  | A    |
| 11  | A     | 4   | U    |
| 11  | A     | 5   | U    |
| 11  | A     | 6   | G    |
| 11  | A     | 7   | A    |
| 11  | A     | 8   | A    |
| 11  | A     | 9   | G    |
| 11  | A     | 13  | U    |
| 11  | A     | 22  | G    |
| 11  | A     | 32  | A    |
| 11  | A     | 39  | G    |
| 11  | A     | 47  | C    |
| 11  | A     | 48  | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11  | A     | 51  | A    |
| 11  | A     | 71  | A    |
| 11  | A     | 83  | C    |
| 11  | A     | 84  | U    |
| 11  | A     | 85  | U    |
| 11  | A     | 86  | G    |
| 11  | A     | 87  | C    |
| 11  | A     | 88  | U    |
| 11  | A     | 95  | C    |
| 11  | A     | 119 | A    |
| 11  | A     | 121 | U    |
| 11  | A     | 122 | G    |
| 11  | A     | 130 | A    |
| 11  | A     | 131 | A    |
| 11  | A     | 143 | A    |
| 11  | A     | 144 | G    |
| 11  | A     | 163 | C    |
| 11  | A     | 173 | U    |
| 11  | A     | 182 | A    |
| 11  | A     | 191 | G    |
| 11  | A     | 197 | A    |
| 11  | A     | 226 | G    |
| 11  | A     | 240 | G    |
| 11  | A     | 245 | U    |
| 11  | A     | 247 | G    |
| 11  | A     | 251 | G    |
| 11  | A     | 266 | G    |
| 11  | A     | 267 | C    |
| 11  | A     | 289 | G    |
| 11  | A     | 306 | A    |
| 11  | A     | 321 | A    |
| 11  | A     | 328 | C    |
| 11  | A     | 347 | G    |
| 11  | A     | 351 | G    |
| 11  | A     | 352 | C    |
| 11  | A     | 354 | G    |
| 11  | A     | 355 | C    |
| 11  | A     | 367 | U    |
| 11  | A     | 372 | C    |
| 11  | A     | 373 | A    |
| 11  | A     | 388 | G    |
| 11  | A     | 392 | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11  | A     | 398 | U    |
| 11  | A     | 406 | G    |
| 11  | A     | 412 | A    |
| 11  | A     | 413 | G    |
| 11  | A     | 414 | A    |
| 11  | A     | 418 | C    |
| 11  | A     | 421 | U    |
| 11  | A     | 422 | C    |
| 11  | A     | 423 | G    |
| 11  | A     | 424 | G    |
| 11  | A     | 429 | U    |
| 11  | A     | 431 | A    |
| 11  | A     | 438 | U    |
| 11  | A     | 448 | A    |
| 11  | A     | 453 | G    |
| 11  | A     | 456 | A    |
| 11  | A     | 457 | G    |
| 11  | A     | 458 | U    |
| 11  | A     | 463 | U    |
| 11  | A     | 465 | A    |
| 11  | A     | 467 | U    |
| 11  | A     | 468 | A    |
| 11  | A     | 469 | C    |
| 11  | A     | 475 | C    |
| 11  | A     | 478 | A    |
| 11  | A     | 479 | U    |
| 11  | A     | 481 | G    |
| 11  | A     | 484 | G    |
| 11  | A     | 486 | U    |
| 11  | A     | 492 | C    |
| 11  | A     | 495 | A    |
| 11  | A     | 496 | A    |
| 11  | A     | 497 | G    |
| 11  | A     | 504 | C    |
| 11  | A     | 505 | G    |
| 11  | A     | 509 | A    |
| 11  | A     | 510 | A    |
| 11  | A     | 511 | C    |
| 11  | A     | 518 | C    |
| 11  | A     | 521 | G    |
| 11  | A     | 527 | G7M  |
| 11  | A     | 532 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11  | A     | 547 | A    |
| 11  | A     | 559 | A    |
| 11  | A     | 564 | C    |
| 11  | A     | 572 | A    |
| 11  | A     | 573 | A    |
| 11  | A     | 576 | C    |
| 11  | A     | 577 | G    |
| 11  | A     | 633 | G    |
| 11  | A     | 642 | A    |
| 11  | A     | 650 | G    |
| 11  | A     | 653 | U    |
| 11  | A     | 665 | A    |
| 11  | A     | 687 | A    |
| 11  | A     | 702 | A    |
| 11  | A     | 718 | A    |
| 11  | A     | 723 | U    |
| 11  | A     | 724 | G    |
| 11  | A     | 734 | G    |
| 11  | A     | 747 | A    |
| 11  | A     | 755 | G    |
| 11  | A     | 777 | A    |
| 11  | A     | 793 | U    |
| 11  | A     | 794 | A    |
| 11  | A     | 815 | A    |
| 11  | A     | 817 | C    |
| 11  | A     | 821 | G    |
| 11  | A     | 851 | G    |
| 11  | A     | 890 | G    |
| 11  | A     | 902 | G    |
| 11  | A     | 914 | A    |
| 11  | A     | 934 | C    |
| 11  | A     | 935 | A    |
| 11  | A     | 960 | U    |
| 11  | A     | 966 | 2MG  |
| 11  | A     | 969 | A    |
| 11  | A     | 971 | G    |
| 11  | A     | 975 | A    |
| 11  | A     | 976 | G    |
| 11  | A     | 977 | A    |
| 11  | A     | 989 | U    |
| 11  | A     | 992 | U    |
| 11  | A     | 994 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 11  | A     | 996  | A    |
| 11  | A     | 1003 | G    |
| 11  | A     | 1004 | A    |
| 11  | A     | 1009 | U    |
| 11  | A     | 1028 | C    |
| 11  | A     | 1030 | U    |
| 11  | A     | 1031 | C    |
| 11  | A     | 1032 | G    |
| 11  | A     | 1033 | G    |
| 11  | A     | 1035 | A    |
| 11  | A     | 1036 | A    |
| 11  | A     | 1039 | G    |
| 11  | A     | 1042 | A    |
| 11  | A     | 1044 | A    |
| 11  | A     | 1065 | U    |
| 11  | A     | 1085 | U    |
| 11  | A     | 1094 | G    |
| 11  | A     | 1095 | U    |
| 11  | A     | 1101 | A    |
| 11  | A     | 1108 | G    |
| 11  | A     | 1125 | U    |
| 11  | A     | 1132 | C    |
| 11  | A     | 1133 | G    |
| 11  | A     | 1136 | C    |
| 11  | A     | 1137 | C    |
| 11  | A     | 1139 | G    |
| 11  | A     | 1151 | A    |
| 11  | A     | 1159 | U    |
| 11  | A     | 1196 | A    |
| 11  | A     | 1197 | A    |
| 11  | A     | 1213 | A    |
| 11  | A     | 1214 | C    |
| 11  | A     | 1215 | G    |
| 11  | A     | 1225 | A    |
| 11  | A     | 1227 | A    |
| 11  | A     | 1238 | A    |
| 11  | A     | 1241 | G    |
| 11  | A     | 1257 | A    |
| 11  | A     | 1258 | G    |
| 11  | A     | 1260 | G    |
| 11  | A     | 1275 | A    |
| 11  | A     | 1280 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 11  | A     | 1286 | U    |
| 11  | A     | 1287 | A    |
| 11  | A     | 1299 | A    |
| 11  | A     | 1300 | G    |
| 11  | A     | 1302 | C    |
| 11  | A     | 1305 | G    |
| 11  | A     | 1317 | C    |
| 11  | A     | 1320 | C    |
| 11  | A     | 1340 | A    |
| 11  | A     | 1346 | A    |
| 11  | A     | 1353 | G    |
| 11  | A     | 1363 | A    |
| 11  | A     | 1364 | U    |
| 11  | A     | 1370 | G    |
| 11  | A     | 1378 | C    |
| 11  | A     | 1379 | G    |
| 11  | A     | 1381 | U    |
| 11  | A     | 1398 | A    |
| 11  | A     | 1419 | G    |
| 11  | A     | 1429 | A    |
| 11  | A     | 1432 | G    |
| 11  | A     | 1441 | A    |
| 11  | A     | 1446 | A    |
| 11  | A     | 1487 | G    |
| 11  | A     | 1493 | A    |
| 11  | A     | 1494 | G    |
| 11  | A     | 1497 | G    |
| 11  | A     | 1499 | A    |
| 11  | A     | 1503 | A    |
| 11  | A     | 1506 | U    |
| 11  | A     | 1517 | G    |
| 11  | A     | 1529 | G    |
| 11  | A     | 1530 | G    |
| 11  | A     | 1534 | A    |
| 33  | X     | 7    | C    |
| 34  | Y     | 8    | U    |
| 34  | Y     | 9    | G    |
| 34  | Y     | 14   | A    |
| 34  | Y     | 20   | G    |
| 34  | Y     | 21   | U    |
| 34  | Y     | 22   | A    |
| 34  | Y     | 35   | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 34  | Y     | 46  | G    |
| 34  | Y     | 49  | C    |
| 34  | Y     | 75  | C    |
| 35  | Z     | 14  | A    |
| 35  | Z     | 16  | C    |
| 35  | Z     | 17  | U    |
| 35  | Z     | 19  | G    |
| 35  | Z     | 20  | G    |
| 35  | Z     | 21  | U    |
| 35  | Z     | 22  | A    |
| 35  | Z     | 46  | G    |
| 35  | Z     | 47  | G    |
| 35  | Z     | 48  | U    |
| 35  | Z     | 77  | A    |
| 36  | a     | 10  | A    |
| 36  | a     | 14  | A    |
| 36  | a     | 15  | G    |
| 36  | a     | 34  | U    |
| 36  | a     | 51  | G    |
| 36  | a     | 63  | A    |
| 36  | a     | 71  | A    |
| 36  | a     | 74  | A    |
| 36  | a     | 75  | G    |
| 36  | a     | 84  | A    |
| 36  | a     | 88  | G    |
| 36  | a     | 96  | C    |
| 36  | a     | 101 | A    |
| 36  | a     | 102 | U    |
| 36  | a     | 118 | A    |
| 36  | a     | 119 | A    |
| 36  | a     | 120 | U    |
| 36  | a     | 125 | A    |
| 36  | a     | 139 | U    |
| 36  | a     | 142 | A    |
| 36  | a     | 163 | C    |
| 36  | a     | 165 | A    |
| 36  | a     | 181 | A    |
| 36  | a     | 196 | A    |
| 36  | a     | 199 | A    |
| 36  | a     | 215 | G    |
| 36  | a     | 216 | A    |
| 36  | a     | 222 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 36  | a     | 248 | G    |
| 36  | a     | 272 | A    |
| 36  | a     | 276 | U    |
| 36  | a     | 278 | A    |
| 36  | a     | 281 | C    |
| 36  | a     | 282 | A    |
| 36  | a     | 285 | G    |
| 36  | a     | 288 | U    |
| 36  | a     | 311 | A    |
| 36  | a     | 329 | G    |
| 36  | a     | 330 | A    |
| 36  | a     | 331 | C    |
| 36  | a     | 345 | A    |
| 36  | a     | 362 | A    |
| 36  | a     | 386 | G    |
| 36  | a     | 396 | G    |
| 36  | a     | 405 | U    |
| 36  | a     | 411 | G    |
| 36  | a     | 412 | A    |
| 36  | a     | 481 | G    |
| 36  | a     | 491 | G    |
| 36  | a     | 504 | A    |
| 36  | a     | 505 | A    |
| 36  | a     | 508 | A    |
| 36  | a     | 509 | C    |
| 36  | a     | 529 | A    |
| 36  | a     | 532 | A    |
| 36  | a     | 544 | C    |
| 36  | a     | 545 | U    |
| 36  | a     | 546 | U    |
| 36  | a     | 547 | A    |
| 36  | a     | 549 | G    |
| 36  | a     | 563 | A    |
| 36  | a     | 573 | U    |
| 36  | a     | 575 | A    |
| 36  | a     | 603 | A    |
| 36  | a     | 615 | U    |
| 36  | a     | 627 | A    |
| 36  | a     | 637 | A    |
| 36  | a     | 645 | C    |
| 36  | a     | 646 | U    |
| 36  | a     | 647 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 36  | a     | 654 | A    |
| 36  | a     | 655 | A    |
| 36  | a     | 686 | U    |
| 36  | a     | 717 | C    |
| 36  | a     | 726 | G    |
| 36  | a     | 730 | A    |
| 36  | a     | 738 | G    |
| 36  | a     | 747 | U    |
| 36  | a     | 757 | G    |
| 36  | a     | 764 | A    |
| 36  | a     | 775 | G    |
| 36  | a     | 776 | G    |
| 36  | a     | 782 | A    |
| 36  | a     | 784 | G    |
| 36  | a     | 785 | G    |
| 36  | a     | 789 | A    |
| 36  | a     | 805 | G    |
| 36  | a     | 812 | C    |
| 36  | a     | 827 | U    |
| 36  | a     | 828 | U    |
| 36  | a     | 846 | U    |
| 36  | a     | 847 | U    |
| 36  | a     | 858 | G    |
| 36  | a     | 859 | G    |
| 36  | a     | 869 | G    |
| 36  | a     | 883 | G    |
| 36  | a     | 884 | U    |
| 36  | a     | 888 | C    |
| 36  | a     | 890 | C    |
| 36  | a     | 891 | G    |
| 36  | a     | 893 | C    |
| 36  | a     | 895 | U    |
| 36  | a     | 896 | A    |
| 36  | a     | 899 | A    |
| 36  | a     | 907 | G    |
| 36  | a     | 910 | A    |
| 36  | a     | 914 | G    |
| 36  | a     | 931 | U    |
| 36  | a     | 932 | U    |
| 36  | a     | 946 | C    |
| 36  | a     | 961 | C    |
| 36  | a     | 974 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 36  | a     | 983  | A    |
| 36  | a     | 996  | A    |
| 36  | a     | 1012 | U    |
| 36  | a     | 1013 | C    |
| 36  | a     | 1026 | G    |
| 36  | a     | 1027 | A    |
| 36  | a     | 1033 | U    |
| 36  | a     | 1045 | C    |
| 36  | a     | 1046 | A    |
| 36  | a     | 1047 | G    |
| 36  | a     | 1108 | U    |
| 36  | a     | 1110 | G    |
| 36  | a     | 1111 | A    |
| 36  | a     | 1112 | G    |
| 36  | a     | 1116 | G    |
| 36  | a     | 1122 | G    |
| 36  | a     | 1130 | U    |
| 36  | a     | 1132 | U    |
| 36  | a     | 1133 | A    |
| 36  | a     | 1135 | C    |
| 36  | a     | 1142 | A    |
| 36  | a     | 1206 | G    |
| 36  | a     | 1212 | G    |
| 36  | a     | 1236 | G    |
| 36  | a     | 1250 | G    |
| 36  | a     | 1253 | A    |
| 36  | a     | 1256 | G    |
| 36  | a     | 1271 | G    |
| 36  | a     | 1272 | A    |
| 36  | a     | 1273 | U    |
| 36  | a     | 1300 | G    |
| 36  | a     | 1301 | A    |
| 36  | a     | 1321 | A    |
| 36  | a     | 1322 | A    |
| 36  | a     | 1329 | U    |
| 36  | a     | 1352 | U    |
| 36  | a     | 1365 | A    |
| 36  | a     | 1378 | A    |
| 36  | a     | 1379 | U    |
| 36  | a     | 1383 | A    |
| 36  | a     | 1416 | G    |
| 36  | a     | 1428 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 36  | a     | 1437 | C    |
| 36  | a     | 1452 | G    |
| 36  | a     | 1453 | A    |
| 36  | a     | 1482 | G    |
| 36  | a     | 1493 | C    |
| 36  | a     | 1508 | A    |
| 36  | a     | 1509 | A    |
| 36  | a     | 1510 | G    |
| 36  | a     | 1515 | A    |
| 36  | a     | 1529 | G    |
| 36  | a     | 1535 | A    |
| 36  | a     | 1536 | C    |
| 36  | a     | 1537 | G    |
| 36  | a     | 1566 | A    |
| 36  | a     | 1569 | A    |
| 36  | a     | 1578 | U    |
| 36  | a     | 1583 | A    |
| 36  | a     | 1585 | C    |
| 36  | a     | 1607 | C    |
| 36  | a     | 1608 | A    |
| 36  | a     | 1647 | U    |
| 36  | a     | 1648 | U    |
| 36  | a     | 1649 | G    |
| 36  | a     | 1674 | G    |
| 36  | a     | 1715 | G    |
| 36  | a     | 1729 | U    |
| 36  | a     | 1730 | C    |
| 36  | a     | 1731 | G    |
| 36  | a     | 1732 | C    |
| 36  | a     | 1738 | G    |
| 36  | a     | 1764 | C    |
| 36  | a     | 1773 | A    |
| 36  | a     | 1782 | U    |
| 36  | a     | 1800 | C    |
| 36  | a     | 1801 | A    |
| 36  | a     | 1808 | A    |
| 36  | a     | 1816 | C    |
| 36  | a     | 1829 | A    |
| 36  | a     | 1847 | A    |
| 36  | a     | 1848 | A    |
| 36  | a     | 1858 | A    |
| 36  | a     | 1869 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 36  | a     | 1870 | C    |
| 36  | a     | 1871 | A    |
| 36  | a     | 1872 | A    |
| 36  | a     | 1906 | G    |
| 36  | a     | 1913 | A    |
| 36  | a     | 1914 | C    |
| 36  | a     | 1929 | G    |
| 36  | a     | 1930 | G    |
| 36  | a     | 1937 | A    |
| 36  | a     | 1939 | U    |
| 36  | a     | 1955 | U    |
| 36  | a     | 1964 | G    |
| 36  | a     | 1966 | A    |
| 36  | a     | 1967 | C    |
| 36  | a     | 1970 | A    |
| 36  | a     | 1971 | U    |
| 36  | a     | 1972 | G    |
| 36  | a     | 1991 | U    |
| 36  | a     | 1993 | U    |
| 36  | a     | 2020 | A    |
| 36  | a     | 2023 | C    |
| 36  | a     | 2030 | 6MZ  |
| 36  | a     | 2031 | A    |
| 36  | a     | 2033 | A    |
| 36  | a     | 2043 | C    |
| 36  | a     | 2055 | C    |
| 36  | a     | 2056 | G    |
| 36  | a     | 2060 | A    |
| 36  | a     | 2061 | G    |
| 36  | a     | 2062 | A    |
| 36  | a     | 2069 | G7M  |
| 36  | a     | 2093 | G    |
| 36  | a     | 2198 | A    |
| 36  | a     | 2204 | G    |
| 36  | a     | 2211 | A    |
| 36  | a     | 2225 | A    |
| 36  | a     | 2238 | G    |
| 36  | a     | 2239 | G    |
| 36  | a     | 2279 | G    |
| 36  | a     | 2283 | C    |
| 36  | a     | 2287 | A    |
| 36  | a     | 2288 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 36  | a     | 2305 | U    |
| 36  | a     | 2308 | G    |
| 36  | a     | 2309 | A    |
| 36  | a     | 2312 | U    |
| 36  | a     | 2322 | A    |
| 36  | a     | 2325 | G    |
| 36  | a     | 2333 | A    |
| 36  | a     | 2334 | U    |
| 36  | a     | 2345 | G    |
| 36  | a     | 2347 | C    |
| 36  | a     | 2350 | C    |
| 36  | a     | 2357 | G    |
| 36  | a     | 2361 | G    |
| 36  | a     | 2383 | G    |
| 36  | a     | 2385 | C    |
| 36  | a     | 2402 | U    |
| 36  | a     | 2403 | C    |
| 36  | a     | 2406 | A    |
| 36  | a     | 2425 | A    |
| 36  | a     | 2429 | G    |
| 36  | a     | 2435 | A    |
| 36  | a     | 2441 | U    |
| 36  | a     | 2448 | A    |
| 36  | a     | 2476 | A    |
| 36  | a     | 2478 | A    |
| 36  | a     | 2491 | U    |
| 36  | a     | 2498 | OMC  |
| 36  | a     | 2502 | G    |
| 36  | a     | 2505 | G    |
| 36  | a     | 2518 | A    |
| 36  | a     | 2520 | C    |
| 36  | a     | 2525 | G    |
| 36  | a     | 2529 | G    |
| 36  | a     | 2535 | G    |
| 36  | a     | 2547 | A    |
| 36  | a     | 2566 | A    |
| 36  | a     | 2567 | G    |
| 36  | a     | 2572 | A    |
| 36  | a     | 2602 | A    |
| 36  | a     | 2609 | U    |
| 36  | a     | 2613 | U    |
| 36  | a     | 2615 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 36  | a     | 2629 | U    |
| 36  | a     | 2630 | G    |
| 36  | a     | 2646 | C    |
| 36  | a     | 2663 | G    |
| 36  | a     | 2689 | U    |
| 36  | a     | 2690 | U    |
| 36  | a     | 2714 | G    |
| 36  | a     | 2716 | C    |
| 36  | a     | 2718 | G    |
| 36  | a     | 2726 | A    |
| 36  | a     | 2732 | G    |
| 36  | a     | 2733 | A    |
| 36  | a     | 2744 | G    |
| 36  | a     | 2748 | A    |
| 36  | a     | 2757 | A    |
| 36  | a     | 2765 | A    |
| 36  | a     | 2778 | A    |
| 36  | a     | 2798 | U    |
| 36  | a     | 2818 | U    |
| 36  | a     | 2820 | A    |
| 36  | a     | 2821 | A    |
| 36  | a     | 2835 | A    |
| 36  | a     | 2836 | U    |
| 36  | a     | 2861 | U    |
| 36  | a     | 2873 | A    |
| 36  | a     | 2880 | C    |
| 36  | a     | 2883 | A    |
| 36  | a     | 2884 | U    |
| 36  | a     | 2891 | U    |
| 37  | b     | 9    | G    |
| 37  | b     | 16   | G    |
| 37  | b     | 24   | G    |
| 37  | b     | 35   | C    |
| 37  | b     | 36   | C    |
| 37  | b     | 41   | G    |
| 37  | b     | 56   | G    |
| 37  | b     | 67   | G    |
| 37  | b     | 89   | U    |
| 37  | b     | 90   | C    |
| 37  | b     | 99   | A    |
| 37  | b     | 109  | A    |

All (4) RNA pucker outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 11  | A     | 428  | G    |
| 11  | A     | 1035 | A    |
| 34  | Y     | 13   | C    |
| 34  | Y     | 48   | U    |

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

34 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 | $\# Z  > 2$ |
| 36  | OMU  | a     | 2552 | 36    | 19,22,23     | 2.59 | 7 (36%)     | 26,31,34    | 1.87 | 5 (19%)     |
| 11  | 5MC  | A     | 1407 | 11    | 18,22,23     | 2.17 | 8 (44%)     | 26,32,35    | 1.17 | 2 (7%)      |
| 36  | PSU  | a     | 2605 | 36    | 18,21,22     | 2.11 | 8 (44%)     | 22,30,33    | 1.76 | 4 (18%)     |
| 11  | UR3  | A     | 1498 | 11    | 19,22,23     | 2.38 | 6 (31%)     | 26,32,35    | 1.14 | 1 (3%)      |
| 36  | PSU  | a     | 2580 | 36    | 18,21,22     | 2.16 | 9 (50%)     | 22,30,33    | 1.76 | 4 (18%)     |
| 36  | OMC  | a     | 2498 | 36,63 | 19,22,23     | 1.85 | 5 (26%)     | 26,31,34    | 0.97 | 1 (3%)      |
| 36  | PSU  | a     | 2457 | 36    | 18,21,22     | 2.15 | 8 (44%)     | 22,30,33    | 1.78 | 5 (22%)     |
| 11  | 5MC  | A     | 967  | 11    | 18,22,23     | 2.16 | 7 (38%)     | 26,32,35    | 1.21 | 1 (3%)      |
| 11  | PSU  | A     | 516  | 11    | 18,21,22     | 2.01 | 8 (44%)     | 22,30,33    | 1.75 | 4 (18%)     |
| 36  | OMG  | a     | 2251 | 36,35 | 23,26,27     | 2.70 | 5 (21%)     | 33,38,41    | 1.96 | 10 (30%)    |
| 36  | G7M  | a     | 2069 | 36    | 23,26,27     | 2.42 | 5 (21%)     | 35,39,42    | 1.64 | 6 (17%)     |
| 36  | 6MZ  | a     | 2030 | 36    | 22,25,26     | 2.28 | 3 (13%)     | 30,36,39    | 2.59 | 11 (36%)    |
| 36  | H2U  | a     | 2449 | 36    | 18,21,22     | 4.21 | 5 (27%)     | 21,30,33    | 4.65 | 6 (28%)     |
| 22  | D2T  | L     | 89   | 22    | 7,9,10       | 1.36 | 1 (14%)     | 6,11,13     | 1.43 | 1 (16%)     |
| 36  | 6MZ  | a     | 1618 | 36    | 22,25,26     | 2.31 | 3 (13%)     | 30,36,39    | 2.41 | 11 (36%)    |
| 11  | 4OC  | A     | 1402 | 11    | 20,23,24     | 2.53 | 5 (25%)     | 26,32,35    | 1.05 | 2 (7%)      |
| 11  | 2MG  | A     | 1516 | 11    | 23,26,27     | 2.65 | 6 (26%)     | 32,38,41    | 2.08 | 11 (34%)    |
| 36  | PSU  | a     | 1917 | 36    | 18,21,22     | 2.08 | 8 (44%)     | 22,30,33    | 1.61 | 3 (13%)     |
| 36  | 5MC  | a     | 1962 | 36    | 18,22,23     | 2.17 | 7 (38%)     | 26,32,35    | 1.24 | 2 (7%)      |
| 36  | 2MG  | a     | 2445 | 36    | 23,26,27     | 2.67 | 6 (26%)     | 32,38,41    | 2.05 | 11 (34%)    |

| Mol | Type | Chain | Res  | Link  | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|-------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 11  | 2MG  | A     | 1207 | 11    | 23,26,27     | 2.65 | 6 (26%)  | 32,38,41    | 2.06 | 10 (31%) |
| 36  | 1MG  | a     | 745  | 36    | 22,26,27     | 2.44 | 6 (27%)  | 33,39,42    | 1.91 | 10 (30%) |
| 36  | PSU  | a     | 746  | 36,63 | 18,21,22     | 2.08 | 9 (50%)  | 22,30,33    | 1.66 | 4 (18%)  |
| 36  | 2MG  | a     | 1835 | 36    | 23,26,27     | 2.64 | 5 (21%)  | 32,38,41    | 2.22 | 11 (34%) |
| 11  | MA6  | A     | 1519 | 11    | 23,26,27     | 1.16 | 3 (13%)  | 34,38,41    | 2.25 | 10 (29%) |
| 11  | MA6  | A     | 1518 | 11    | 23,26,27     | 1.18 | 3 (13%)  | 34,38,41    | 2.25 | 9 (26%)  |
| 36  | 2MA  | a     | 2503 | 36,63 | 22,25,26     | 1.37 | 2 (9%)   | 33,37,40    | 2.10 | 7 (21%)  |
| 36  | PSU  | a     | 2604 | 36    | 18,21,22     | 2.09 | 8 (44%)  | 22,30,33    | 1.74 | 4 (18%)  |
| 11  | 2MG  | A     | 966  | 11    | 23,26,27     | 2.66 | 5 (21%)  | 32,38,41    | 2.19 | 10 (31%) |
| 11  | G7M  | A     | 527  | 11    | 23,26,27     | 2.39 | 5 (21%)  | 35,39,42    | 1.65 | 7 (20%)  |
| 36  | PSU  | a     | 2504 | 36    | 18,21,22     | 2.14 | 8 (44%)  | 22,30,33    | 1.70 | 3 (13%)  |
| 39  | MEQ  | d     | 150  | 39    | 8,9,10       | 0.88 | 0        | 5,10,12     | 0.49 | 0        |
| 36  | PSU  | a     | 1911 | 36    | 18,21,22     | 2.05 | 8 (44%)  | 22,30,33    | 1.77 | 4 (18%)  |
| 36  | PSU  | a     | 955  | 36    | 18,21,22     | 2.13 | 8 (44%)  | 22,30,33    | 1.77 | 4 (18%)  |

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   |
|-----|------|-------|------|-------|---------|-----------|---------|
| 36  | OMU  | a     | 2552 | 36    | -       | 0/9/27/28 | 0/2/2/2 |
| 11  | 5MC  | A     | 1407 | 11    | -       | 0/7/25/26 | 0/2/2/2 |
| 36  | PSU  | a     | 2605 | 36    | -       | 0/7/25/26 | 0/2/2/2 |
| 11  | UR3  | A     | 1498 | 11    | -       | 0/7/25/26 | 0/2/2/2 |
| 36  | PSU  | a     | 2580 | 36    | -       | 0/7/25/26 | 0/2/2/2 |
| 36  | OMC  | a     | 2498 | 36,63 | -       | 0/9/27/28 | 0/2/2/2 |
| 36  | PSU  | a     | 2457 | 36    | -       | 0/7/25/26 | 0/2/2/2 |
| 11  | 5MC  | A     | 967  | 11    | -       | 0/7/25/26 | 0/2/2/2 |
| 11  | PSU  | A     | 516  | 11    | -       | 0/7/25/26 | 0/2/2/2 |
| 36  | OMG  | a     | 2251 | 36,35 | -       | 1/9/27/28 | 0/3/3/3 |
| 36  | G7M  | a     | 2069 | 36    | -       | 1/7/25/26 | 0/3/3/3 |
| 36  | 6MZ  | a     | 2030 | 36    | -       | 2/9/27/28 | 0/3/3/3 |
| 36  | H2U  | a     | 2449 | 36    | -       | 0/7/38/39 | 0/2/2/2 |
| 22  | D2T  | L     | 89   | 22    | -       | 1/7/12/14 | -       |
| 36  | 6MZ  | a     | 1618 | 36    | -       | 0/9/27/28 | 0/3/3/3 |
| 11  | 4OC  | A     | 1402 | 11    | -       | 2/9/29/30 | 0/2/2/2 |
| 11  | 2MG  | A     | 1516 | 11    | -       | 0/9/27/28 | 0/3/3/3 |
| 36  | PSU  | a     | 1917 | 36    | -       | 0/7/25/26 | 0/2/2/2 |

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| Mol | Type | Chain | Res  | Link  | Chirals | Torsions   | Rings   |
|-----|------|-------|------|-------|---------|------------|---------|
| 36  | 5MC  | a     | 1962 | 36    | -       | 0/7/25/26  | 0/2/2/2 |
| 36  | 2MG  | a     | 2445 | 36    | -       | 2/9/27/28  | 0/3/3/3 |
| 11  | 2MG  | A     | 1207 | 11    | -       | 2/9/27/28  | 0/3/3/3 |
| 36  | 1MG  | a     | 745  | 36    | -       | 0/7/25/26  | 0/3/3/3 |
| 36  | PSU  | a     | 746  | 36,63 | -       | 1/7/25/26  | 0/2/2/2 |
| 36  | 2MG  | a     | 1835 | 36    | -       | 2/9/27/28  | 0/3/3/3 |
| 11  | MA6  | A     | 1519 | 11    | -       | 5/11/29/30 | 0/3/3/3 |
| 11  | MA6  | A     | 1518 | 11    | -       | 2/11/29/30 | 0/3/3/3 |
| 36  | 2MA  | a     | 2503 | 36,63 | -       | 2/7/25/26  | 0/3/3/3 |
| 36  | PSU  | a     | 2604 | 36    | -       | 0/7/25/26  | 0/2/2/2 |
| 11  | 2MG  | A     | 966  | 11    | -       | 2/9/27/28  | 0/3/3/3 |
| 11  | G7M  | A     | 527  | 11    | -       | 3/7/25/26  | 0/3/3/3 |
| 36  | PSU  | a     | 2504 | 36    | -       | 2/7/25/26  | 0/2/2/2 |
| 39  | MEQ  | d     | 150  | 39    | -       | 6/8/9/11   | -       |
| 36  | PSU  | a     | 1911 | 36    | -       | 0/7/25/26  | 0/2/2/2 |
| 36  | PSU  | a     | 955  | 36    | -       | 0/7/25/26  | 0/2/2/2 |

All (196) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 11  | A     | 966  | 2MG  | O6-C6 | 9.91 | 1.42        | 1.23     |
| 11  | A     | 1207 | 2MG  | O6-C6 | 9.89 | 1.42        | 1.23     |
| 11  | A     | 1516 | 2MG  | O6-C6 | 9.86 | 1.42        | 1.23     |
| 36  | a     | 2449 | H2U  | O4-C4 | 9.85 | 1.43        | 1.23     |
| 36  | a     | 1835 | 2MG  | O6-C6 | 9.76 | 1.42        | 1.23     |
| 36  | a     | 2445 | 2MG  | O6-C6 | 9.73 | 1.42        | 1.23     |
| 36  | a     | 1618 | 6MZ  | C6-N6 | 9.69 | 1.44        | 1.34     |
| 36  | a     | 2251 | OMG  | O6-C6 | 9.67 | 1.42        | 1.23     |
| 36  | a     | 2030 | 6MZ  | C6-N6 | 9.32 | 1.44        | 1.34     |
| 11  | A     | 1402 | 4OC  | O2-C2 | 8.91 | 1.40        | 1.23     |
| 11  | A     | 527  | G7M  | O6-C6 | 8.74 | 1.40        | 1.23     |
| 36  | a     | 2449 | H2U  | O2-C2 | 8.70 | 1.39        | 1.23     |
| 36  | a     | 2069 | G7M  | O6-C6 | 8.66 | 1.40        | 1.23     |
| 36  | a     | 2449 | H2U  | C2-N1 | 8.32 | 1.47        | 1.35     |
| 36  | a     | 2552 | OMU  | O4-C4 | 8.08 | 1.40        | 1.24     |
| 11  | A     | 1498 | UR3  | O4-C4 | 7.85 | 1.40        | 1.23     |
| 36  | a     | 745  | 1MG  | O6-C6 | 7.41 | 1.38        | 1.23     |
| 36  | a     | 2449 | H2U  | C2-N3 | 7.06 | 1.50        | 1.38     |
| 36  | a     | 2251 | OMG  | C2-N2 | 7.05 | 1.50        | 1.34     |
| 36  | a     | 745  | 1MG  | C2-N2 | 6.79 | 1.46        | 1.34     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 11  | A     | 966  | 2MG  | C2-N2 | 5.25  | 1.45        | 1.33     |
| 11  | A     | 1207 | 2MG  | C2-N2 | 5.23  | 1.45        | 1.33     |
| 11  | A     | 967  | 5MC  | C4-N4 | 5.16  | 1.47        | 1.34     |
| 11  | A     | 1516 | 2MG  | C2-N2 | 5.16  | 1.44        | 1.33     |
| 11  | A     | 1407 | 5MC  | C4-N4 | 5.13  | 1.47        | 1.34     |
| 36  | a     | 1962 | 5MC  | C4-N4 | 5.09  | 1.47        | 1.34     |
| 36  | a     | 2445 | 2MG  | C2-N2 | 5.04  | 1.44        | 1.33     |
| 36  | a     | 1835 | 2MG  | C2-N2 | 5.04  | 1.44        | 1.33     |
| 36  | a     | 2449 | H2U  | C4-N3 | 4.89  | 1.45        | 1.37     |
| 36  | a     | 2498 | OMC  | C4-N4 | 4.78  | 1.45        | 1.33     |
| 11  | A     | 527  | G7M  | C2-N2 | 4.77  | 1.45        | 1.34     |
| 36  | a     | 2069 | G7M  | C2-N2 | 4.64  | 1.45        | 1.34     |
| 11  | A     | 1402 | 4OC  | C4-N4 | 4.47  | 1.45        | 1.35     |
| 36  | a     | 2503 | 2MA  | C6-N6 | 4.31  | 1.44        | 1.34     |
| 36  | a     | 1962 | 5MC  | O2-C2 | -4.25 | 1.15        | 1.23     |
| 11  | A     | 1407 | 5MC  | O2-C2 | -4.20 | 1.15        | 1.23     |
| 11  | A     | 967  | 5MC  | O2-C2 | -4.13 | 1.16        | 1.23     |
| 11  | A     | 1498 | UR3  | C4-N3 | -4.05 | 1.31        | 1.40     |
| 36  | a     | 2552 | OMU  | C2-N1 | -4.02 | 1.32        | 1.38     |
| 36  | a     | 2580 | PSU  | C2-N1 | -3.85 | 1.31        | 1.36     |
| 36  | a     | 2457 | PSU  | C4-N3 | -3.84 | 1.31        | 1.38     |
| 36  | a     | 2504 | PSU  | C2-N1 | -3.83 | 1.31        | 1.36     |
| 36  | a     | 2580 | PSU  | C4-N3 | -3.78 | 1.31        | 1.38     |
| 36  | a     | 955  | PSU  | C4-N3 | -3.76 | 1.31        | 1.38     |
| 36  | a     | 955  | PSU  | C2-N1 | -3.74 | 1.31        | 1.36     |
| 36  | a     | 2457 | PSU  | C2-N1 | -3.72 | 1.31        | 1.36     |
| 36  | a     | 2605 | PSU  | C4-N3 | -3.69 | 1.32        | 1.38     |
| 36  | a     | 1917 | PSU  | C2-N1 | -3.68 | 1.31        | 1.36     |
| 36  | a     | 2604 | PSU  | C2-N1 | -3.66 | 1.31        | 1.36     |
| 36  | a     | 2504 | PSU  | C4-N3 | -3.66 | 1.32        | 1.38     |
| 36  | a     | 2604 | PSU  | C4-N3 | -3.66 | 1.32        | 1.38     |
| 36  | a     | 746  | PSU  | C4-N3 | -3.66 | 1.32        | 1.38     |
| 36  | a     | 2605 | PSU  | C2-N1 | -3.63 | 1.31        | 1.36     |
| 11  | A     | 1402 | 4OC  | C2-N1 | -3.61 | 1.32        | 1.40     |
| 36  | a     | 2498 | OMC  | C2-N1 | -3.60 | 1.32        | 1.40     |
| 36  | a     | 2552 | OMU  | C4-N3 | -3.59 | 1.32        | 1.38     |
| 36  | a     | 2069 | G7M  | C5-N7 | -3.57 | 1.35        | 1.39     |
| 36  | a     | 1917 | PSU  | C4-N3 | -3.56 | 1.32        | 1.38     |
| 36  | a     | 2457 | PSU  | C2-N3 | -3.54 | 1.31        | 1.37     |
| 36  | a     | 1911 | PSU  | C4-N3 | -3.54 | 1.32        | 1.38     |
| 36  | a     | 746  | PSU  | C2-N1 | -3.51 | 1.32        | 1.36     |
| 36  | a     | 2069 | G7M  | C6-N1 | -3.50 | 1.32        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 36  | a     | 1911 | PSU  | C2-N1  | -3.48 | 1.32        | 1.36     |
| 36  | a     | 2605 | PSU  | C2-N3  | -3.48 | 1.31        | 1.37     |
| 36  | a     | 955  | PSU  | C2-N3  | -3.44 | 1.31        | 1.37     |
| 36  | a     | 2580 | PSU  | C2-N3  | -3.42 | 1.31        | 1.37     |
| 36  | a     | 2604 | PSU  | C2-N3  | -3.42 | 1.31        | 1.37     |
| 11  | A     | 516  | PSU  | C2-N1  | -3.42 | 1.32        | 1.36     |
| 36  | a     | 2504 | PSU  | C2-N3  | -3.41 | 1.31        | 1.37     |
| 11  | A     | 1207 | 2MG  | CM2-N2 | 3.40  | 1.51        | 1.45     |
| 11  | A     | 966  | 2MG  | CM2-N2 | 3.40  | 1.51        | 1.45     |
| 36  | a     | 2552 | OMU  | C2-N3  | -3.39 | 1.31        | 1.38     |
| 36  | a     | 1917 | PSU  | C2-N3  | -3.38 | 1.31        | 1.37     |
| 11  | A     | 516  | PSU  | C4-N3  | -3.37 | 1.32        | 1.38     |
| 36  | a     | 746  | PSU  | C2-N3  | -3.35 | 1.31        | 1.37     |
| 11  | A     | 1516 | 2MG  | CM2-N2 | 3.35  | 1.51        | 1.45     |
| 11  | A     | 527  | G7M  | C5-N7  | -3.34 | 1.35        | 1.39     |
| 36  | a     | 1962 | 5MC  | C6-N1  | -3.31 | 1.32        | 1.38     |
| 11  | A     | 527  | G7M  | C6-N1  | -3.29 | 1.32        | 1.38     |
| 36  | a     | 2030 | 6MZ  | C8-N9  | -3.29 | 1.31        | 1.37     |
| 36  | a     | 1911 | PSU  | C2-N3  | -3.27 | 1.31        | 1.37     |
| 36  | a     | 1835 | 2MG  | CM2-N2 | 3.22  | 1.51        | 1.45     |
| 36  | a     | 2445 | 2MG  | C2-N1  | -3.22 | 1.31        | 1.36     |
| 36  | a     | 1911 | PSU  | C6-C5  | 3.20  | 1.39        | 1.35     |
| 11  | A     | 1518 | MA6  | C6-N6  | 3.17  | 1.46        | 1.36     |
| 36  | a     | 1618 | 6MZ  | C8-N9  | -3.14 | 1.31        | 1.37     |
| 11  | A     | 516  | PSU  | C6-C5  | 3.13  | 1.39        | 1.35     |
| 11  | A     | 516  | PSU  | C2-N3  | -3.12 | 1.32        | 1.37     |
| 11  | A     | 967  | 5MC  | C6-N1  | -3.12 | 1.32        | 1.38     |
| 36  | a     | 2445 | 2MG  | CM2-N2 | 3.12  | 1.51        | 1.45     |
| 11  | A     | 1407 | 5MC  | C6-N1  | -3.11 | 1.32        | 1.38     |
| 11  | A     | 1519 | MA6  | C6-N6  | 3.08  | 1.46        | 1.36     |
| 36  | a     | 1917 | PSU  | C6-C5  | 3.08  | 1.38        | 1.35     |
| 36  | a     | 2605 | PSU  | C6-C5  | 3.06  | 1.38        | 1.35     |
| 11  | A     | 1498 | UR3  | C2-N1  | -3.04 | 1.34        | 1.38     |
| 36  | a     | 1962 | 5MC  | C2-N1  | -3.04 | 1.33        | 1.40     |
| 36  | a     | 2604 | PSU  | C6-C5  | 3.03  | 1.38        | 1.35     |
| 36  | a     | 2504 | PSU  | C6-C5  | 3.03  | 1.38        | 1.35     |
| 11  | A     | 1518 | MA6  | C8-N9  | -3.02 | 1.32        | 1.37     |
| 36  | a     | 1835 | 2MG  | C2-N1  | -3.02 | 1.31        | 1.36     |
| 11  | A     | 967  | 5MC  | C2-N1  | -2.98 | 1.33        | 1.40     |
| 36  | a     | 955  | PSU  | C6-C5  | 2.97  | 1.38        | 1.35     |
| 11  | A     | 1407 | 5MC  | C2-N1  | -2.95 | 1.33        | 1.40     |
| 36  | a     | 746  | PSU  | C6-C5  | 2.95  | 1.38        | 1.35     |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 11  | A     | 1519 | MA6  | C8-N9  | -2.95 | 1.32        | 1.37     |
| 36  | a     | 2503 | 2MA  | C8-N9  | -2.91 | 1.32        | 1.37     |
| 36  | a     | 2457 | PSU  | C6-C5  | 2.89  | 1.38        | 1.35     |
| 36  | a     | 2580 | PSU  | C6-C5  | 2.83  | 1.38        | 1.35     |
| 11  | A     | 966  | 2MG  | C2-N1  | -2.83 | 1.32        | 1.36     |
| 36  | a     | 2445 | 2MG  | C6-N1  | -2.80 | 1.33        | 1.38     |
| 36  | a     | 2498 | OMC  | O2-C2  | -2.79 | 1.18        | 1.23     |
| 11  | A     | 967  | 5MC  | CM5-C5 | 2.77  | 1.57        | 1.50     |
| 36  | a     | 1962 | 5MC  | CM5-C5 | 2.71  | 1.57        | 1.50     |
| 11  | A     | 1407 | 5MC  | CM5-C5 | 2.70  | 1.57        | 1.50     |
| 36  | a     | 2457 | PSU  | O4-C4  | -2.70 | 1.18        | 1.23     |
| 11  | A     | 1516 | 2MG  | C2-N1  | -2.69 | 1.32        | 1.36     |
| 36  | a     | 745  | 1MG  | C5-N7  | -2.68 | 1.33        | 1.39     |
| 11  | A     | 1207 | 2MG  | C2-N1  | -2.68 | 1.32        | 1.36     |
| 36  | a     | 745  | 1MG  | C6-N1  | -2.67 | 1.34        | 1.40     |
| 36  | a     | 2580 | PSU  | O4-C4  | -2.67 | 1.18        | 1.23     |
| 36  | a     | 746  | PSU  | O4-C4  | -2.67 | 1.18        | 1.23     |
| 36  | a     | 955  | PSU  | O4-C4  | -2.66 | 1.18        | 1.23     |
| 36  | a     | 2605 | PSU  | O4-C4  | -2.66 | 1.18        | 1.23     |
| 36  | a     | 1917 | PSU  | C1'-C5 | 2.63  | 1.56        | 1.50     |
| 36  | a     | 2504 | PSU  | C6-N1  | -2.62 | 1.31        | 1.36     |
| 36  | a     | 2504 | PSU  | O4-C4  | -2.59 | 1.18        | 1.23     |
| 36  | a     | 2604 | PSU  | O4-C4  | -2.59 | 1.18        | 1.23     |
| 36  | a     | 2457 | PSU  | C6-N1  | -2.59 | 1.31        | 1.36     |
| 36  | a     | 955  | PSU  | C6-N1  | -2.58 | 1.31        | 1.36     |
| 36  | a     | 2580 | PSU  | C6-N1  | -2.57 | 1.32        | 1.36     |
| 36  | a     | 2504 | PSU  | C1'-C5 | 2.54  | 1.56        | 1.50     |
| 36  | a     | 1835 | 2MG  | C6-N1  | -2.53 | 1.34        | 1.38     |
| 36  | a     | 1917 | PSU  | O4-C4  | -2.51 | 1.18        | 1.23     |
| 36  | a     | 2604 | PSU  | C6-N1  | -2.51 | 1.32        | 1.36     |
| 36  | a     | 1911 | PSU  | O4-C4  | -2.51 | 1.18        | 1.23     |
| 36  | a     | 2552 | OMU  | O2-C2  | -2.48 | 1.18        | 1.23     |
| 11  | A     | 516  | PSU  | O4-C4  | -2.47 | 1.18        | 1.23     |
| 11  | A     | 516  | PSU  | C1'-C5 | 2.47  | 1.55        | 1.50     |
| 11  | A     | 1498 | UR3  | C6-C5  | 2.47  | 1.40        | 1.35     |
| 36  | a     | 2605 | PSU  | C6-N1  | -2.46 | 1.32        | 1.36     |
| 36  | a     | 2030 | 6MZ  | C5-N7  | -2.46 | 1.34        | 1.39     |
| 11  | A     | 516  | PSU  | C6-N1  | -2.45 | 1.32        | 1.36     |
| 36  | a     | 955  | PSU  | O2-C2  | -2.44 | 1.18        | 1.23     |
| 11  | A     | 966  | 2MG  | C6-N1  | -2.44 | 1.34        | 1.38     |
| 11  | A     | 1516 | 2MG  | C6-N1  | -2.44 | 1.34        | 1.38     |
| 36  | a     | 1618 | 6MZ  | C5-N7  | -2.42 | 1.34        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 36  | a     | 1917 | PSU  | C6-N1   | -2.42 | 1.32        | 1.36     |
| 36  | a     | 2251 | OMG  | C6-N1   | -2.41 | 1.34        | 1.38     |
| 36  | a     | 1911 | PSU  | C6-N1   | -2.40 | 1.32        | 1.36     |
| 36  | a     | 955  | PSU  | C1'-C5  | 2.38  | 1.55        | 1.50     |
| 11  | A     | 1207 | 2MG  | C6-N1   | -2.38 | 1.34        | 1.38     |
| 36  | a     | 2504 | PSU  | O2-C2   | -2.37 | 1.18        | 1.23     |
| 36  | a     | 1911 | PSU  | C1'-C5  | 2.37  | 1.55        | 1.50     |
| 11  | A     | 1519 | MA6  | C5-N7   | -2.37 | 1.34        | 1.39     |
| 36  | a     | 2580 | PSU  | O2-C2   | -2.36 | 1.18        | 1.23     |
| 36  | a     | 746  | PSU  | C6-N1   | -2.36 | 1.32        | 1.36     |
| 36  | a     | 2498 | OMC  | C6-N1   | -2.35 | 1.32        | 1.38     |
| 36  | a     | 2457 | PSU  | C1'-C5  | 2.34  | 1.55        | 1.50     |
| 36  | a     | 2604 | PSU  | C1'-C5  | 2.34  | 1.55        | 1.50     |
| 36  | a     | 2457 | PSU  | O2-C2   | -2.34 | 1.18        | 1.23     |
| 36  | a     | 2605 | PSU  | C1'-C5  | 2.33  | 1.55        | 1.50     |
| 36  | a     | 2605 | PSU  | O2-C2   | -2.31 | 1.18        | 1.23     |
| 11  | A     | 1498 | UR3  | C6-N1   | -2.30 | 1.32        | 1.38     |
| 36  | a     | 2604 | PSU  | O2-C2   | -2.30 | 1.18        | 1.23     |
| 36  | a     | 2552 | OMU  | C5-C4   | -2.29 | 1.38        | 1.43     |
| 36  | a     | 2580 | PSU  | O4'-C1' | -2.28 | 1.40        | 1.43     |
| 36  | a     | 2069 | G7M  | C2-N1   | -2.27 | 1.32        | 1.37     |
| 36  | a     | 2251 | OMG  | C5-N7   | -2.27 | 1.34        | 1.39     |
| 11  | A     | 1402 | 4OC  | C6-N1   | -2.26 | 1.32        | 1.38     |
| 36  | a     | 2552 | OMU  | C6-N1   | -2.25 | 1.32        | 1.38     |
| 36  | a     | 745  | 1MG  | C4-N9   | -2.24 | 1.32        | 1.38     |
| 36  | a     | 1911 | PSU  | O2-C2   | -2.23 | 1.18        | 1.23     |
| 36  | a     | 746  | PSU  | C1'-C5  | 2.22  | 1.55        | 1.50     |
| 36  | a     | 2580 | PSU  | C1'-C5  | 2.22  | 1.55        | 1.50     |
| 36  | a     | 2445 | 2MG  | C4-N9   | -2.22 | 1.32        | 1.38     |
| 11  | A     | 1516 | 2MG  | C4-N9   | -2.21 | 1.32        | 1.38     |
| 36  | a     | 2498 | OMC  | C2-N3   | -2.21 | 1.31        | 1.36     |
| 11  | A     | 1402 | 4OC  | C2-N3   | -2.21 | 1.31        | 1.36     |
| 36  | a     | 746  | PSU  | O2-C2   | -2.20 | 1.18        | 1.23     |
| 11  | A     | 1518 | MA6  | C5-N7   | -2.19 | 1.34        | 1.39     |
| 11  | A     | 1498 | UR3  | C2-N3   | -2.17 | 1.34        | 1.39     |
| 11  | A     | 516  | PSU  | O2-C2   | -2.17 | 1.18        | 1.23     |
| 36  | a     | 1917 | PSU  | O2-C2   | -2.16 | 1.18        | 1.23     |
| 11  | A     | 967  | 5MC  | C6-C5   | 2.16  | 1.38        | 1.34     |
| 11  | A     | 1407 | 5MC  | C6-C5   | 2.15  | 1.38        | 1.34     |
| 36  | a     | 745  | 1MG  | C5-C6   | -2.14 | 1.40        | 1.45     |
| 36  | a     | 2251 | OMG  | C8-N9   | -2.14 | 1.32        | 1.37     |
| 11  | A     | 1407 | 5MC  | C4-N3   | -2.14 | 1.30        | 1.34     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 11  | A     | 527  | G7M  | C2-N1   | -2.08 | 1.32        | 1.37     |
| 36  | a     | 1962 | 5MC  | C4-N3   | -2.07 | 1.30        | 1.34     |
| 11  | A     | 1207 | 2MG  | C4-N9   | -2.07 | 1.32        | 1.38     |
| 36  | a     | 746  | PSU  | O4'-C1' | -2.06 | 1.41        | 1.43     |
| 36  | a     | 1962 | 5MC  | C2-N3   | -2.05 | 1.32        | 1.36     |
| 11  | A     | 967  | 5MC  | C4-N3   | -2.03 | 1.30        | 1.34     |
| 11  | A     | 1407 | 5MC  | C2-N3   | -2.02 | 1.32        | 1.36     |
| 22  | L     | 89   | D2T  | CB1-SB  | -2.01 | 1.75        | 1.79     |

All (194) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms    | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 36  | a     | 2449 | H2U  | C4-N3-C2 | -13.69 | 114.44      | 125.79   |
| 36  | a     | 2449 | H2U  | O2-C2-N1 | -10.63 | 109.77      | 123.11   |
| 36  | a     | 2449 | H2U  | O4-C4-N3 | -7.52  | 108.36      | 120.28   |
| 36  | a     | 2503 | 2MA  | C5-C4-N3 | -6.91  | 119.42      | 127.19   |
| 36  | a     | 1835 | 2MG  | C2-N3-C4 | 6.86   | 120.54      | 112.04   |
| 11  | A     | 966  | 2MG  | C2-N3-C4 | 6.67   | 120.31      | 112.04   |
| 36  | a     | 2030 | 6MZ  | C9-N6-C6 | -6.61  | 117.18      | 122.87   |
| 11  | A     | 1207 | 2MG  | C2-N3-C4 | 6.36   | 119.92      | 112.04   |
| 36  | a     | 2449 | H2U  | O4-C4-C5 | -6.32  | 108.66      | 122.17   |
| 36  | a     | 2445 | 2MG  | C2-N3-C4 | 6.32   | 119.88      | 112.04   |
| 11  | A     | 1516 | 2MG  | C2-N3-C4 | 6.32   | 119.87      | 112.04   |
| 36  | a     | 2552 | OMU  | N3-C2-N1 | 5.99   | 122.84      | 114.89   |
| 36  | a     | 2251 | OMG  | C5-C4-N3 | -5.94  | 118.83      | 128.46   |
| 36  | a     | 2449 | H2U  | O2-C2-N3 | -5.83  | 110.64      | 121.50   |
| 11  | A     | 1519 | MA6  | C5-C4-N3 | -5.81  | 119.17      | 126.75   |
| 36  | a     | 745  | 1MG  | C5-C4-N3 | -5.76  | 119.11      | 128.46   |
| 11  | A     | 966  | 2MG  | C5-C4-N3 | -5.59  | 119.39      | 128.46   |
| 36  | a     | 1835 | 2MG  | C5-C4-N3 | -5.54  | 119.47      | 128.46   |
| 36  | a     | 1618 | 6MZ  | C5-C4-N3 | -5.52  | 119.55      | 126.75   |
| 36  | a     | 1618 | 6MZ  | N1-C2-N3 | -5.50  | 120.00      | 128.60   |
| 36  | a     | 2457 | PSU  | N1-C2-N3 | 5.47   | 121.33      | 115.13   |
| 36  | a     | 2030 | 6MZ  | N1-C2-N3 | -5.47  | 120.05      | 128.60   |
| 36  | a     | 955  | PSU  | N1-C2-N3 | 5.45   | 121.31      | 115.13   |
| 36  | a     | 1911 | PSU  | N1-C2-N3 | 5.42   | 121.27      | 115.13   |
| 11  | A     | 1518 | MA6  | C5-C4-N3 | -5.41  | 119.69      | 126.75   |
| 11  | A     | 516  | PSU  | N1-C2-N3 | 5.38   | 121.22      | 115.13   |
| 36  | a     | 2580 | PSU  | N1-C2-N3 | 5.34   | 121.18      | 115.13   |
| 36  | a     | 2604 | PSU  | N1-C2-N3 | 5.32   | 121.15      | 115.13   |
| 36  | a     | 2605 | PSU  | N1-C2-N3 | 5.31   | 121.15      | 115.13   |
| 36  | a     | 2504 | PSU  | N1-C2-N3 | 5.23   | 121.06      | 115.13   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 36  | a     | 746  | PSU  | N1-C2-N3 | 5.13  | 120.94      | 115.13   |
| 11  | A     | 1207 | 2MG  | C5-C4-N3 | -5.05 | 120.26      | 128.46   |
| 36  | a     | 1917 | PSU  | N1-C2-N3 | 5.03  | 120.83      | 115.13   |
| 36  | a     | 2445 | 2MG  | C5-C4-N3 | -5.01 | 120.34      | 128.46   |
| 36  | a     | 2030 | 6MZ  | C5-C4-N3 | -5.00 | 120.23      | 126.75   |
| 11  | A     | 1516 | 2MG  | C5-C4-N3 | -4.94 | 120.44      | 128.46   |
| 36  | a     | 2251 | OMG  | C2-N3-C4 | 4.94  | 121.09      | 112.30   |
| 36  | a     | 2503 | 2MA  | N3-C4-N9 | 4.83  | 133.69      | 126.99   |
| 11  | A     | 967  | 5MC  | C5-C6-N1 | -4.73 | 118.47      | 123.34   |
| 11  | A     | 527  | G7M  | C2-N3-C4 | 4.64  | 120.56      | 112.30   |
| 36  | a     | 1962 | 5MC  | C5-C6-N1 | -4.62 | 118.59      | 123.34   |
| 36  | a     | 2552 | OMU  | C4-N3-C2 | -4.55 | 120.57      | 126.58   |
| 36  | a     | 2069 | G7M  | C2-N3-C4 | 4.49  | 120.30      | 112.30   |
| 11  | A     | 1518 | MA6  | N1-C2-N3 | -4.46 | 121.62      | 128.60   |
| 11  | A     | 1407 | 5MC  | C5-C6-N1 | -4.44 | 118.77      | 123.34   |
| 11  | A     | 1518 | MA6  | C5-N7-C8 | 4.34  | 109.68      | 103.51   |
| 11  | A     | 1519 | MA6  | C5-N7-C8 | 4.28  | 109.59      | 103.51   |
| 11  | A     | 966  | 2MG  | N9-C4-N3 | 4.22  | 134.41      | 125.94   |
| 36  | a     | 745  | 1MG  | N9-C4-N3 | 4.21  | 134.40      | 125.94   |
| 11  | A     | 1519 | MA6  | N1-C2-N3 | -4.20 | 122.03      | 128.60   |
| 36  | a     | 1618 | 6MZ  | N3-C4-N9 | 4.19  | 133.99      | 127.08   |
| 11  | A     | 527  | G7M  | C5-C4-N3 | -4.18 | 120.13      | 128.15   |
| 11  | A     | 1518 | MA6  | C2-N1-C6 | 4.15  | 121.56      | 111.75   |
| 36  | a     | 1618 | 6MZ  | C2-N3-C4 | 4.15  | 121.55      | 111.75   |
| 11  | A     | 1518 | MA6  | N9-C8-N7 | -4.10 | 108.30      | 113.91   |
| 11  | A     | 1518 | MA6  | C4-C5-N7 | -4.09 | 105.64      | 110.62   |
| 11  | A     | 1519 | MA6  | N3-C4-N9 | 4.08  | 133.81      | 127.08   |
| 36  | a     | 1618 | 6MZ  | C9-N6-C6 | -4.05 | 119.39      | 122.87   |
| 36  | a     | 2449 | H2U  | N3-C2-N1 | -4.03 | 112.39      | 116.65   |
| 36  | a     | 2030 | 6MZ  | N9-C8-N7 | -4.03 | 108.40      | 113.91   |
| 36  | a     | 1835 | 2MG  | N9-C4-N3 | 4.02  | 134.00      | 125.94   |
| 36  | a     | 2030 | 6MZ  | C2-N3-C4 | 3.97  | 121.12      | 111.75   |
| 36  | a     | 2251 | OMG  | N9-C4-N3 | 3.96  | 133.90      | 125.94   |
| 36  | a     | 2069 | G7M  | C5-C4-N3 | -3.94 | 120.60      | 128.15   |
| 11  | A     | 1519 | MA6  | C2-N1-C6 | 3.90  | 120.95      | 111.75   |
| 11  | A     | 1519 | MA6  | C4-C5-N7 | -3.88 | 105.89      | 110.62   |
| 36  | a     | 745  | 1MG  | C2-N3-C4 | 3.88  | 120.69      | 111.98   |
| 11  | A     | 1519 | MA6  | N9-C8-N7 | -3.88 | 108.61      | 113.91   |
| 11  | A     | 1519 | MA6  | C2-N3-C4 | 3.86  | 120.88      | 111.75   |
| 36  | a     | 2030 | 6MZ  | C5-N7-C8 | 3.85  | 108.98      | 103.51   |
| 11  | A     | 1518 | MA6  | C2-N3-C4 | 3.84  | 120.82      | 111.75   |
| 36  | a     | 2503 | 2MA  | N9-C8-N7 | -3.84 | 108.67      | 113.91   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 36  | a     | 2069 | G7M  | C6-C5-N7 | 3.82  | 136.86      | 132.25   |
| 36  | a     | 2503 | 2MA  | C5-N7-C8 | 3.77  | 108.86      | 103.51   |
| 36  | a     | 2445 | 2MG  | N9-C4-N3 | 3.74  | 133.46      | 125.94   |
| 36  | a     | 1618 | 6MZ  | N9-C8-N7 | -3.68 | 108.88      | 113.91   |
| 11  | A     | 1518 | MA6  | N3-C4-N9 | 3.67  | 133.12      | 127.08   |
| 36  | a     | 1835 | 2MG  | C2-N1-C6 | -3.65 | 120.28      | 124.48   |
| 11  | A     | 527  | G7M  | C6-C5-N7 | 3.64  | 136.65      | 132.25   |
| 36  | a     | 1618 | 6MZ  | C5-N7-C8 | 3.63  | 108.67      | 103.51   |
| 36  | a     | 2605 | PSU  | C4-N3-C2 | -3.62 | 121.13      | 126.34   |
| 11  | A     | 1207 | 2MG  | N9-C4-N3 | 3.60  | 133.16      | 125.94   |
| 11  | A     | 1498 | UR3  | C4-N3-C2 | -3.60 | 121.18      | 124.56   |
| 36  | a     | 2030 | 6MZ  | N3-C4-N9 | 3.60  | 133.01      | 127.08   |
| 11  | A     | 966  | 2MG  | C2-N1-C6 | -3.56 | 120.39      | 124.48   |
| 11  | A     | 527  | G7M  | C5-C6-N1 | 3.53  | 119.17      | 111.79   |
| 36  | a     | 2069 | G7M  | C5-C6-N1 | 3.51  | 119.13      | 111.79   |
| 36  | a     | 1911 | PSU  | C4-N3-C2 | -3.50 | 121.29      | 126.34   |
| 36  | a     | 955  | PSU  | C4-N3-C2 | -3.49 | 121.31      | 126.34   |
| 36  | a     | 746  | PSU  | C4-N3-C2 | -3.47 | 121.33      | 126.34   |
| 36  | a     | 2604 | PSU  | C4-N3-C2 | -3.43 | 121.39      | 126.34   |
| 36  | a     | 2457 | PSU  | C4-N3-C2 | -3.41 | 121.42      | 126.34   |
| 36  | a     | 2030 | 6MZ  | C6-C5-N7 | 3.40  | 136.07      | 132.39   |
| 11  | A     | 516  | PSU  | C4-N3-C2 | -3.35 | 121.50      | 126.34   |
| 11  | A     | 1516 | 2MG  | C2-N1-C6 | -3.35 | 120.63      | 124.48   |
| 11  | A     | 1516 | 2MG  | N9-C4-N3 | 3.30  | 132.57      | 125.94   |
| 36  | a     | 2503 | 2MA  | C4-C5-N7 | -3.29 | 106.61      | 110.62   |
| 36  | a     | 2504 | PSU  | C4-N3-C2 | -3.28 | 121.61      | 126.34   |
| 11  | A     | 527  | G7M  | N9-C4-N3 | 3.24  | 132.44      | 125.94   |
| 36  | a     | 955  | PSU  | O2-C2-N1 | -3.24 | 119.23      | 122.79   |
| 11  | A     | 516  | PSU  | O2-C2-N1 | -3.23 | 119.24      | 122.79   |
| 36  | a     | 2030 | 6MZ  | C4-C5-N7 | -3.20 | 106.72      | 110.62   |
| 11  | A     | 1518 | MA6  | C4-N9-C8 | 3.20  | 109.19      | 105.73   |
| 11  | A     | 1207 | 2MG  | C2-N1-C6 | -3.18 | 120.82      | 124.48   |
| 36  | a     | 2504 | PSU  | O2-C2-N1 | -3.18 | 119.29      | 122.79   |
| 36  | a     | 2457 | PSU  | O2-C2-N1 | -3.16 | 119.31      | 122.79   |
| 36  | a     | 745  | 1MG  | C5-C6-N1 | 3.15  | 120.99      | 114.91   |
| 36  | a     | 2030 | 6MZ  | C4-N9-C8 | 3.14  | 109.13      | 105.73   |
| 36  | a     | 2604 | PSU  | O2-C2-N1 | -3.14 | 119.33      | 122.79   |
| 36  | a     | 2580 | PSU  | O2-C2-N1 | -3.13 | 119.35      | 122.79   |
| 36  | a     | 2580 | PSU  | C4-N3-C2 | -3.12 | 121.84      | 126.34   |
| 36  | a     | 1911 | PSU  | O2-C2-N1 | -3.10 | 119.38      | 122.79   |
| 36  | a     | 2069 | G7M  | N9-C4-N3 | 3.05  | 132.07      | 125.94   |
| 11  | A     | 1516 | 2MG  | C6-C5-N7 | 3.05  | 135.93      | 130.25   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 36  | a     | 2503 | 2MA  | C4-N9-C8    | 2.99  | 108.97      | 105.73   |
| 36  | a     | 1917 | PSU  | O2-C2-N1    | -2.94 | 119.56      | 122.79   |
| 36  | a     | 2605 | PSU  | O2-C2-N1    | -2.93 | 119.57      | 122.79   |
| 36  | a     | 1917 | PSU  | C4-N3-C2    | -2.92 | 122.13      | 126.34   |
| 36  | a     | 2552 | OMU  | O2-C2-N1    | -2.92 | 118.91      | 122.79   |
| 11  | A     | 1519 | MA6  | C4-N9-C8    | 2.91  | 108.89      | 105.73   |
| 36  | a     | 1618 | 6MZ  | C4-N9-C8    | 2.90  | 108.87      | 105.73   |
| 36  | a     | 1618 | 6MZ  | C4-C5-N7    | -2.87 | 107.12      | 110.62   |
| 11  | A     | 1207 | 2MG  | C6-C5-N7    | 2.86  | 135.57      | 130.25   |
| 36  | a     | 2445 | 2MG  | C6-C5-N7    | 2.80  | 135.46      | 130.25   |
| 36  | a     | 2251 | OMG  | C4-C5-N7    | -2.79 | 106.31      | 110.72   |
| 36  | a     | 1835 | 2MG  | C6-C5-N7    | 2.75  | 135.36      | 130.25   |
| 11  | A     | 1402 | 4OC  | C5-C4-N3    | -2.74 | 118.18      | 122.59   |
| 36  | a     | 746  | PSU  | O2-C2-N1    | -2.73 | 119.78      | 122.79   |
| 36  | a     | 1835 | 2MG  | C5-C6-N1    | 2.71  | 120.08      | 113.19   |
| 36  | a     | 2251 | OMG  | C8-N7-C5    | 2.70  | 109.13      | 104.24   |
| 36  | a     | 2445 | 2MG  | C2-N1-C6    | -2.69 | 121.39      | 124.48   |
| 11  | A     | 966  | 2MG  | C5-C6-N1    | 2.68  | 120.00      | 113.19   |
| 36  | a     | 2552 | OMU  | C5-C4-N3    | 2.67  | 118.83      | 114.84   |
| 36  | a     | 2251 | OMG  | C6-C5-N7    | 2.65  | 135.17      | 130.25   |
| 36  | a     | 2069 | G7M  | O6-C6-C5    | -2.60 | 122.19      | 128.06   |
| 36  | a     | 745  | 1MG  | C6-C5-N7    | 2.60  | 135.23      | 129.35   |
| 11  | A     | 1516 | 2MG  | C5-C6-N1    | 2.60  | 119.78      | 113.19   |
| 36  | a     | 2498 | OMC  | O2-C2-N3    | -2.59 | 118.11      | 122.33   |
| 11  | A     | 527  | G7M  | O6-C6-C5    | -2.57 | 122.25      | 128.06   |
| 11  | A     | 1207 | 2MG  | C5-C6-N1    | 2.56  | 119.69      | 113.19   |
| 36  | a     | 1618 | 6MZ  | C6-C5-N7    | 2.54  | 135.13      | 132.39   |
| 36  | a     | 745  | 1MG  | C2-N1-C6    | -2.53 | 118.89      | 120.95   |
| 36  | a     | 2552 | OMU  | O4-C4-C5    | -2.53 | 120.72      | 125.16   |
| 36  | a     | 2251 | OMG  | C2-N1-C6    | -2.52 | 120.51      | 125.10   |
| 11  | A     | 966  | 2MG  | O6-C6-C5    | -2.50 | 119.97      | 126.60   |
| 36  | a     | 2445 | 2MG  | C5-C6-N1    | 2.50  | 119.53      | 113.19   |
| 11  | A     | 966  | 2MG  | C6-C5-N7    | 2.50  | 134.89      | 130.25   |
| 36  | a     | 1835 | 2MG  | C8-N7-C5    | 2.46  | 108.69      | 104.24   |
| 11  | A     | 1516 | 2MG  | C4-C5-N7    | -2.45 | 106.85      | 110.72   |
| 11  | A     | 1516 | 2MG  | O6-C6-C5    | -2.44 | 120.12      | 126.60   |
| 36  | a     | 1835 | 2MG  | O6-C6-C5    | -2.44 | 120.14      | 126.60   |
| 36  | a     | 2445 | 2MG  | N9-C8-N7    | -2.39 | 108.88      | 113.39   |
| 11  | A     | 966  | 2MG  | C8-N7-C5    | 2.39  | 108.57      | 104.24   |
| 36  | a     | 2445 | 2MG  | C8-N7-C5    | 2.38  | 108.55      | 104.24   |
| 36  | a     | 2580 | PSU  | O4'-C1'-C2' | 2.38  | 108.50      | 105.14   |
| 36  | a     | 2251 | OMG  | C5-C6-N1    | 2.37  | 119.20      | 113.19   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 11  | A     | 1207 | 2MG  | O6-C6-C5    | -2.35 | 120.36      | 126.60   |
| 11  | A     | 1207 | 2MG  | C8-N7-C5    | 2.35  | 108.50      | 104.24   |
| 11  | A     | 1516 | 2MG  | C8-N7-C5    | 2.35  | 108.49      | 104.24   |
| 36  | a     | 2445 | 2MG  | O6-C6-C5    | -2.32 | 120.44      | 126.60   |
| 36  | a     | 746  | PSU  | C5-C6-N1    | -2.32 | 118.64      | 122.11   |
| 36  | a     | 1835 | 2MG  | C4-C5-N7    | -2.31 | 107.06      | 110.72   |
| 36  | a     | 2251 | OMG  | N9-C8-N7    | -2.31 | 109.05      | 113.39   |
| 11  | A     | 1207 | 2MG  | C4-C5-N7    | -2.30 | 107.08      | 110.72   |
| 36  | a     | 1835 | 2MG  | CM2-N2-C2   | -2.30 | 118.79      | 123.86   |
| 11  | A     | 1207 | 2MG  | N9-C8-N7    | -2.28 | 109.11      | 113.39   |
| 36  | a     | 745  | 1MG  | C6-C5-C4    | -2.26 | 117.47      | 119.97   |
| 36  | a     | 1835 | 2MG  | N9-C8-N7    | -2.26 | 109.14      | 113.39   |
| 11  | A     | 1516 | 2MG  | N9-C8-N7    | -2.25 | 109.15      | 113.39   |
| 36  | a     | 2605 | PSU  | C5-C6-N1    | -2.23 | 118.76      | 122.11   |
| 36  | a     | 1911 | PSU  | C5-C6-N1    | -2.22 | 118.78      | 122.11   |
| 36  | a     | 2251 | OMG  | O6-C6-C5    | -2.21 | 120.73      | 126.60   |
| 36  | a     | 2457 | PSU  | C5-C6-N1    | -2.21 | 118.80      | 122.11   |
| 36  | a     | 745  | 1MG  | C8-N7-C5    | 2.20  | 108.22      | 104.24   |
| 11  | A     | 966  | 2MG  | N9-C8-N7    | -2.19 | 109.26      | 113.39   |
| 36  | a     | 745  | 1MG  | N9-C8-N7    | -2.19 | 109.27      | 113.39   |
| 22  | L     | 89   | D2T  | O-C-CA      | -2.18 | 119.05      | 124.78   |
| 36  | a     | 2445 | 2MG  | C4-C5-N7    | -2.17 | 107.28      | 110.72   |
| 36  | a     | 745  | 1MG  | C4-C5-N7    | -2.16 | 107.31      | 110.72   |
| 11  | A     | 966  | 2MG  | C4-C5-N7    | -2.15 | 107.31      | 110.72   |
| 36  | a     | 2604 | PSU  | C5-C6-N1    | -2.15 | 118.89      | 122.11   |
| 36  | a     | 2030 | 6MZ  | C2-N1-C6    | 2.14  | 122.44      | 115.25   |
| 36  | a     | 2503 | 2MA  | N3-C2-N1    | -2.12 | 121.82      | 125.72   |
| 36  | a     | 1618 | 6MZ  | C2-N1-C6    | 2.11  | 122.33      | 115.25   |
| 11  | A     | 1407 | 5MC  | O2-C2-N3    | -2.10 | 118.91      | 122.33   |
| 36  | a     | 955  | PSU  | C5-C6-N1    | -2.08 | 118.99      | 122.11   |
| 36  | a     | 2445 | 2MG  | CM2-N2-C2   | -2.08 | 119.27      | 123.86   |
| 11  | A     | 516  | PSU  | O4'-C1'-C2' | 2.07  | 108.07      | 105.14   |
| 11  | A     | 527  | G7M  | C2-N1-C6    | -2.06 | 121.35      | 125.10   |
| 11  | A     | 1519 | MA6  | C4-C5-C6    | 2.05  | 118.18      | 115.88   |
| 36  | a     | 1962 | 5MC  | O2-C2-N3    | -2.05 | 119.00      | 122.33   |
| 11  | A     | 1516 | 2MG  | CM2-N2-C2   | -2.03 | 119.39      | 123.86   |
| 36  | a     | 2457 | PSU  | O4'-C1'-C2' | 2.00  | 107.97      | 105.14   |
| 11  | A     | 1402 | 4OC  | C4-N3-C2    | 2.00  | 122.84      | 120.12   |

There are no chirality outliers.

All (36) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 11  | A     | 527  | G7M  | C3'-C4'-C5'-O5' |
| 11  | A     | 1207 | 2MG  | N1-C2-N2-CM2    |
| 11  | A     | 1207 | 2MG  | N3-C2-N2-CM2    |
| 11  | A     | 1519 | MA6  | C5-C6-N6-C9     |
| 11  | A     | 1519 | MA6  | C5-C6-N6-C10    |
| 22  | L     | 89   | D2T  | O-C-CA-CB       |
| 39  | d     | 150  | MEQ  | N-CA-CB-CG      |
| 39  | d     | 150  | MEQ  | O-C-CA-CB       |
| 36  | a     | 2251 | OMG  | C1'-C2'-O2'-CM2 |
| 36  | a     | 2030 | 6MZ  | O4'-C4'-C5'-O5' |
| 36  | a     | 2030 | 6MZ  | C3'-C4'-C5'-O5' |
| 36  | a     | 2504 | PSU  | O4'-C4'-C5'-O5' |
| 11  | A     | 1402 | 4OC  | O4'-C4'-C5'-O5' |
| 36  | a     | 2504 | PSU  | C3'-C4'-C5'-O5' |
| 11  | A     | 1519 | MA6  | N1-C6-N6-C10    |
| 39  | d     | 150  | MEQ  | OE1-CD-CG-CB    |
| 39  | d     | 150  | MEQ  | NE2-CD-CG-CB    |
| 11  | A     | 527  | G7M  | O4'-C4'-C5'-O5' |
| 11  | A     | 966  | 2MG  | C3'-C4'-C5'-O5' |
| 11  | A     | 1402 | 4OC  | C3'-C4'-C5'-O5' |
| 39  | d     | 150  | MEQ  | C-CA-CB-CG      |
| 11  | A     | 1518 | MA6  | C5-C6-N6-C10    |
| 36  | a     | 2445 | 2MG  | C3'-C4'-C5'-O5' |
| 11  | A     | 1519 | MA6  | O4'-C4'-C5'-O5' |
| 11  | A     | 966  | 2MG  | O4'-C4'-C5'-O5' |
| 11  | A     | 1518 | MA6  | C5-C6-N6-C9     |
| 11  | A     | 527  | G7M  | C4'-C5'-O5'-P   |
| 39  | d     | 150  | MEQ  | CA-CB-CG-CD     |
| 11  | A     | 1519 | MA6  | C3'-C4'-C5'-O5' |
| 36  | a     | 1835 | 2MG  | C3'-C4'-C5'-O5' |
| 36  | a     | 2503 | 2MA  | O4'-C4'-C5'-O5' |
| 36  | a     | 1835 | 2MG  | O4'-C4'-C5'-O5' |
| 36  | a     | 2069 | G7M  | O4'-C4'-C5'-O5' |
| 36  | a     | 2445 | 2MG  | O4'-C4'-C5'-O5' |
| 36  | a     | 746  | PSU  | O4'-C1'-C5-C6   |
| 36  | a     | 2503 | 2MA  | C4'-C5'-O5'-P   |

There are no ring outliers.

5 monomers are involved in 4 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 36  | a     | 2251 | OMG  | 1       | 0            |
| 36  | a     | 2030 | 6MZ  | 1       | 0            |

*Continued on next page...*

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| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 11  | A     | 1402 | 4OC  | 1       | 0            |
| 11  | A     | 1516 | 2MG  | 1       | 0            |
| 11  | A     | 1519 | MA6  | 1       | 0            |

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 313 ligands modelled in this entry, 311 are monoatomic - leaving 2 for Mogul analysis.

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

| Mol | Type | Chain | Res  | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |      |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 65  | SPM  | a     | 6209 | -    | 13,13,13     | 0.35 | 0           | 12,12,12    | 0.82 | 0           |
| 64  | PRO  | Y     | 101  | 34   | 5,7,8        | 0.57 | 0           | 7,8,10      | 1.27 | 1 (14%)     |

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   |
|-----|------|-------|------|------|---------|------------|---------|
| 65  | SPM  | a     | 6209 | -    | -       | 7/11/11/11 | -       |
| 64  | PRO  | Y     | 101  | 34   | -       | 0/0/9/11   | 0/1/1/1 |

There are no bond length outliers.

All (1) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 64  | Y     | 101 | PRO  | O-C-CA | -2.27 | 118.84      | 124.78   |

There are no chirality outliers.

All (7) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 65  | a     | 6209 | SPM  | C7-C8-C9-N10    |
| 65  | a     | 6209 | SPM  | C2-C3-C4-N5     |
| 65  | a     | 6209 | SPM  | C7-C6-N5-C4     |
| 65  | a     | 6209 | SPM  | C11-C12-C13-N14 |
| 65  | a     | 6209 | SPM  | C6-C7-C8-C9     |
| 65  | a     | 6209 | SPM  | C8-C9-N10-C11   |
| 65  | a     | 6209 | SPM  | N10-C11-C12-C13 |

There are no ring outliers.

1 monomer is involved in 1 short contact:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 65  | a     | 6209 | SPM  | 1       | 0            |

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

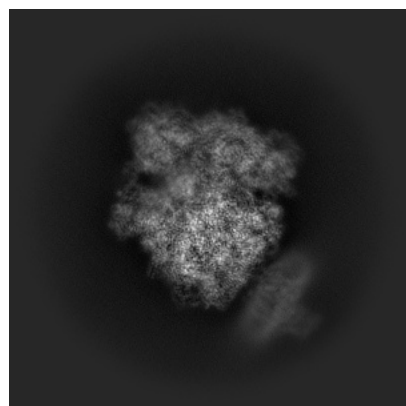
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-53892. These allow visual inspection of the internal detail of the map and identification of artifacts.

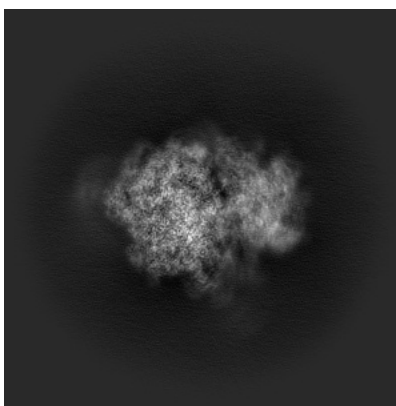
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

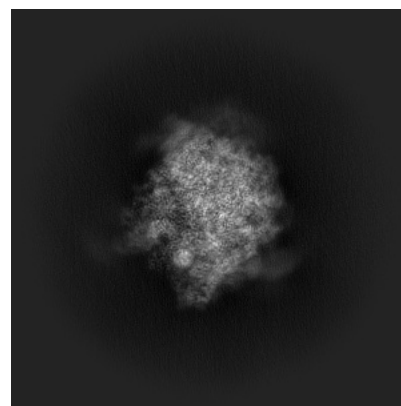
#### 6.1.1 Primary map



X

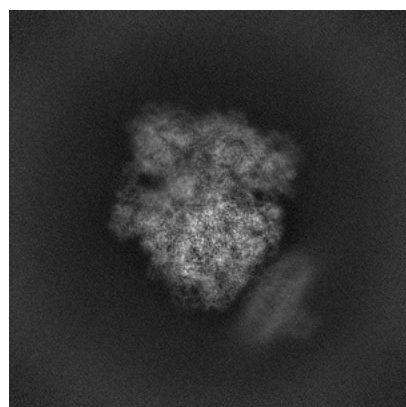


Y

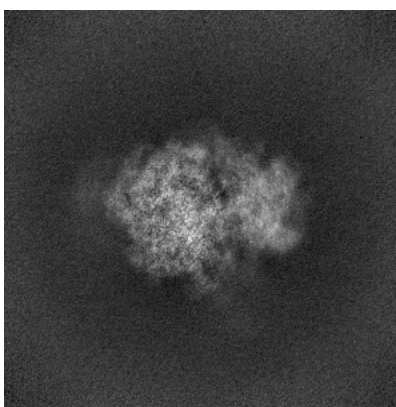


Z

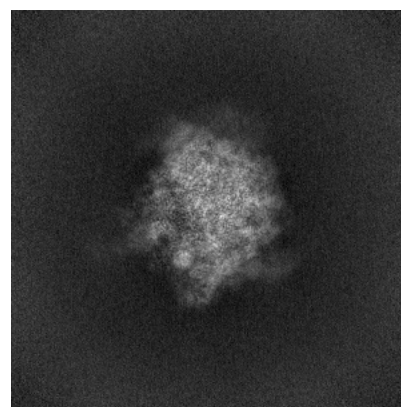
#### 6.1.2 Raw map



X



Y

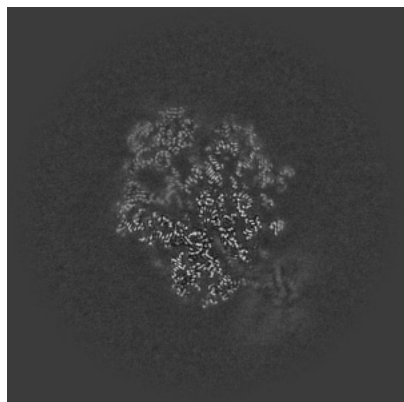


Z

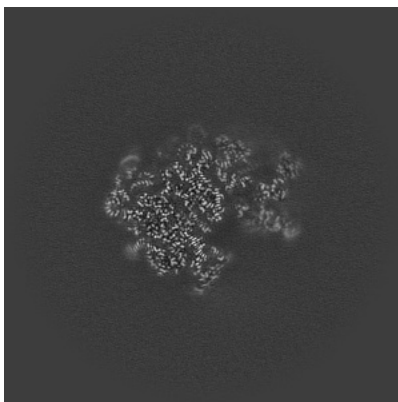
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

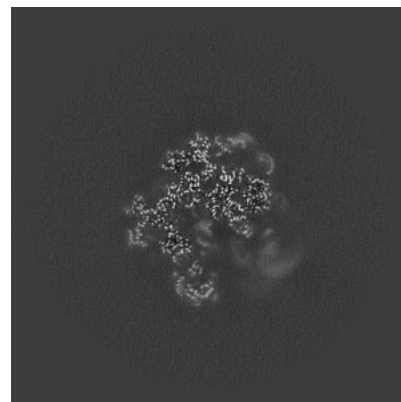
### 6.2.1 Primary map



X Index: 340

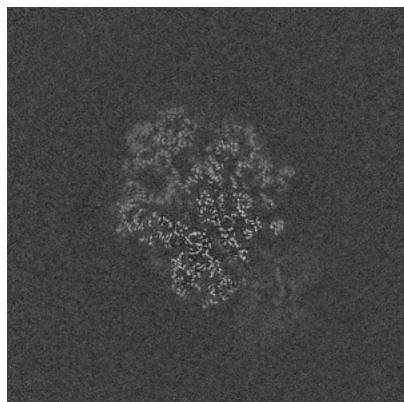


Y Index: 340

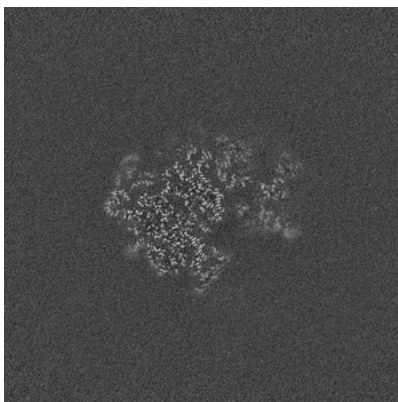


Z Index: 340

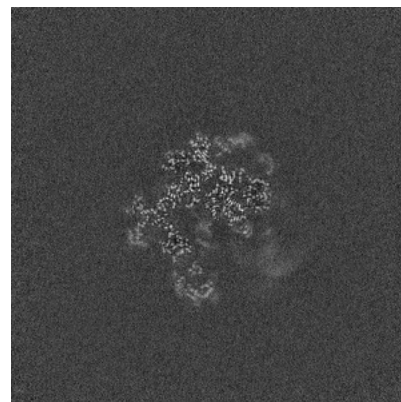
### 6.2.2 Raw map



X Index: 340



Y Index: 340

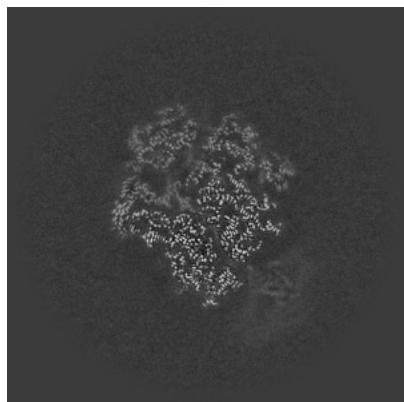


Z Index: 340

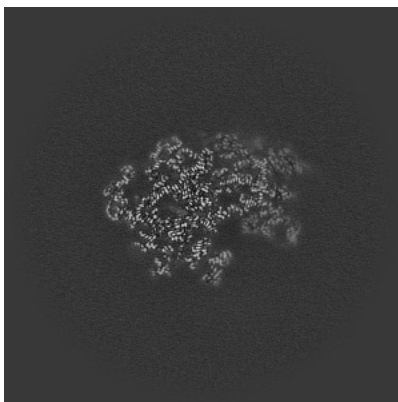
The images above show central slices of the map in three orthogonal directions.

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

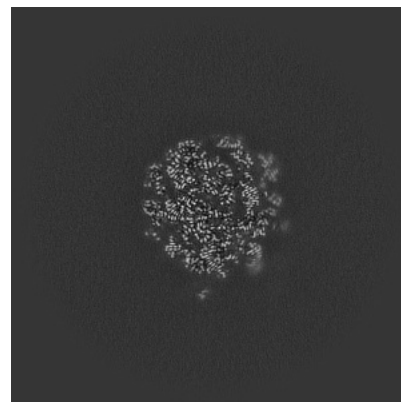
### 6.3.1 Primary map



X Index: 334

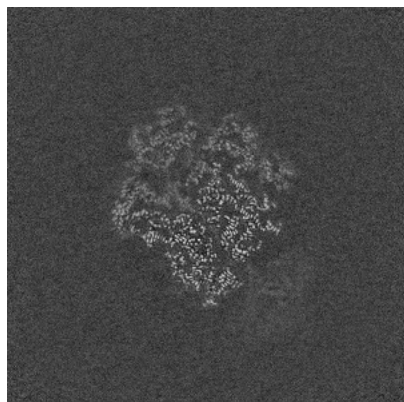


Y Index: 354

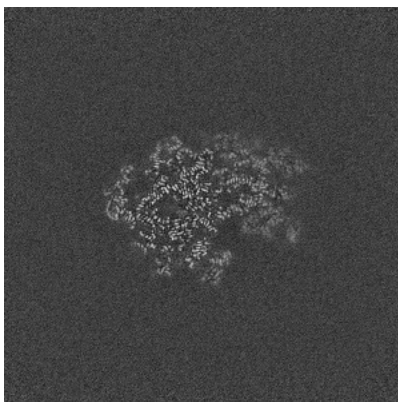


Z Index: 288

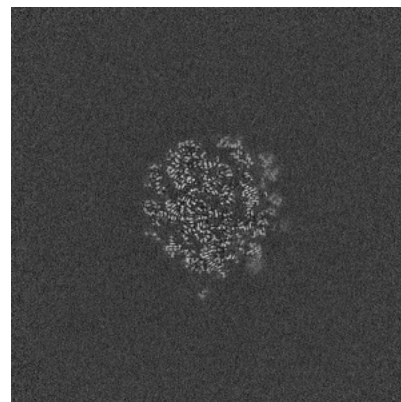
### 6.3.2 Raw map



X Index: 334



Y Index: 353

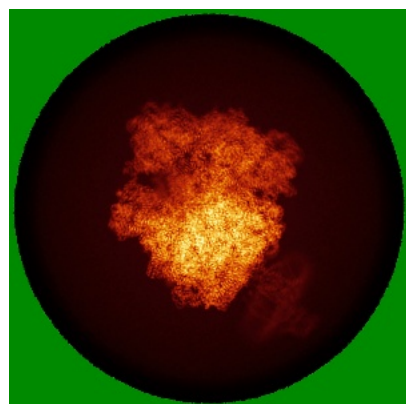


Z Index: 288

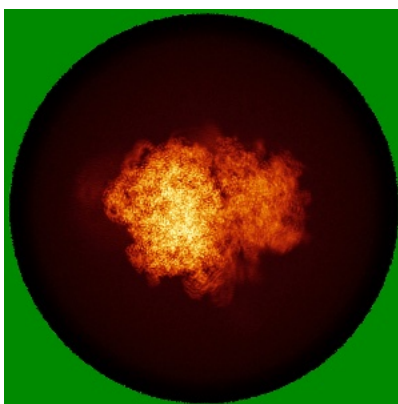
The images above show the largest variance slices of the map in three orthogonal directions.

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

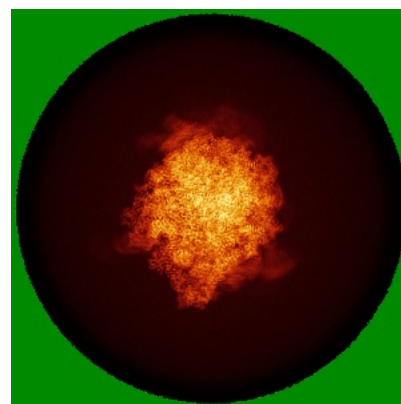
### 6.4.1 Primary map



X

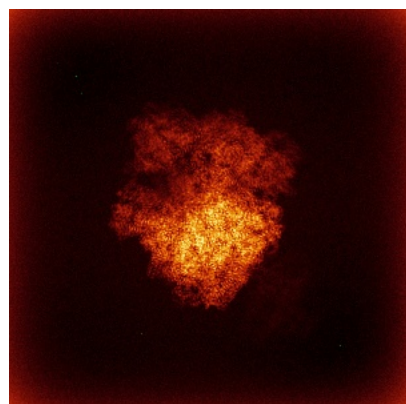


Y

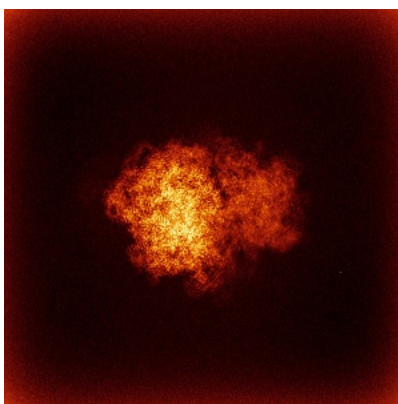


Z

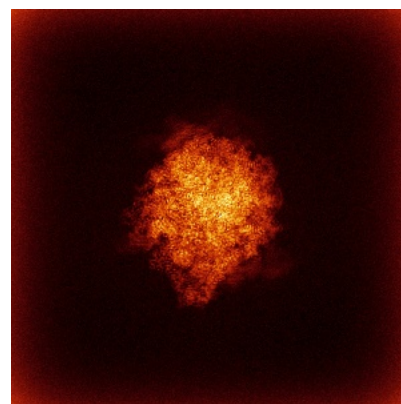
### 6.4.2 Raw map



X



Y



Z

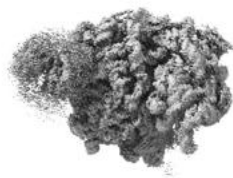
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

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

### 6.5.1 Primary map



X



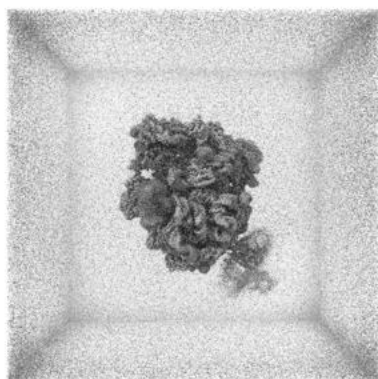
Y



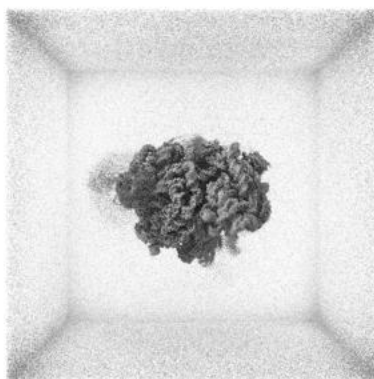
Z

The images above show the 3D surface view of the map at the recommended contour level 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

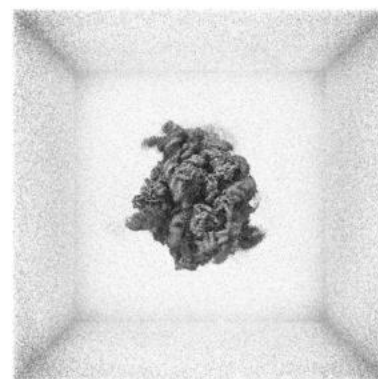
### 6.5.2 Raw map



X



Y



Z

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

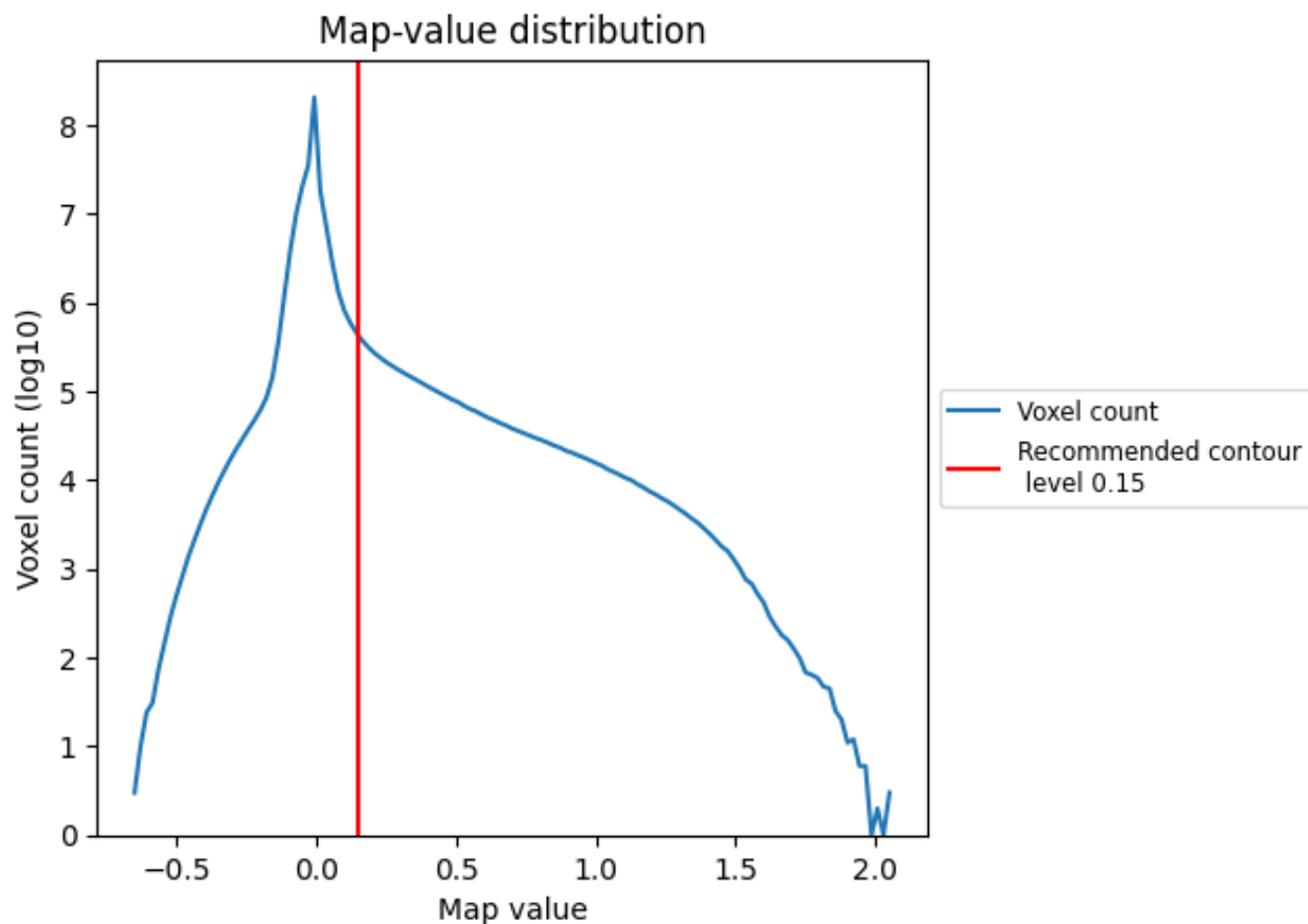
## 6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

## 7 Map analysis [i](#)

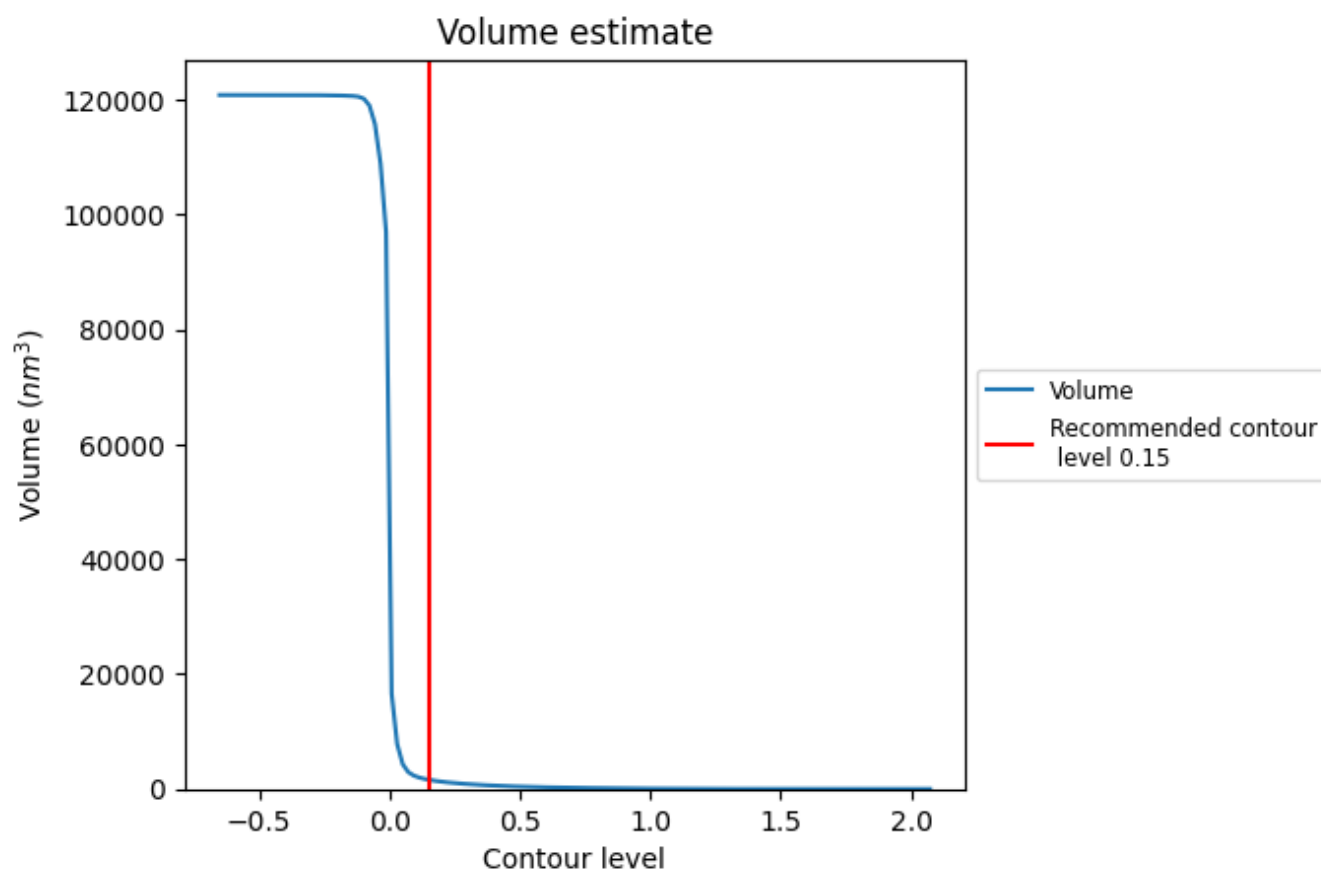
This section contains the results of statistical analysis of the map.

### 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.

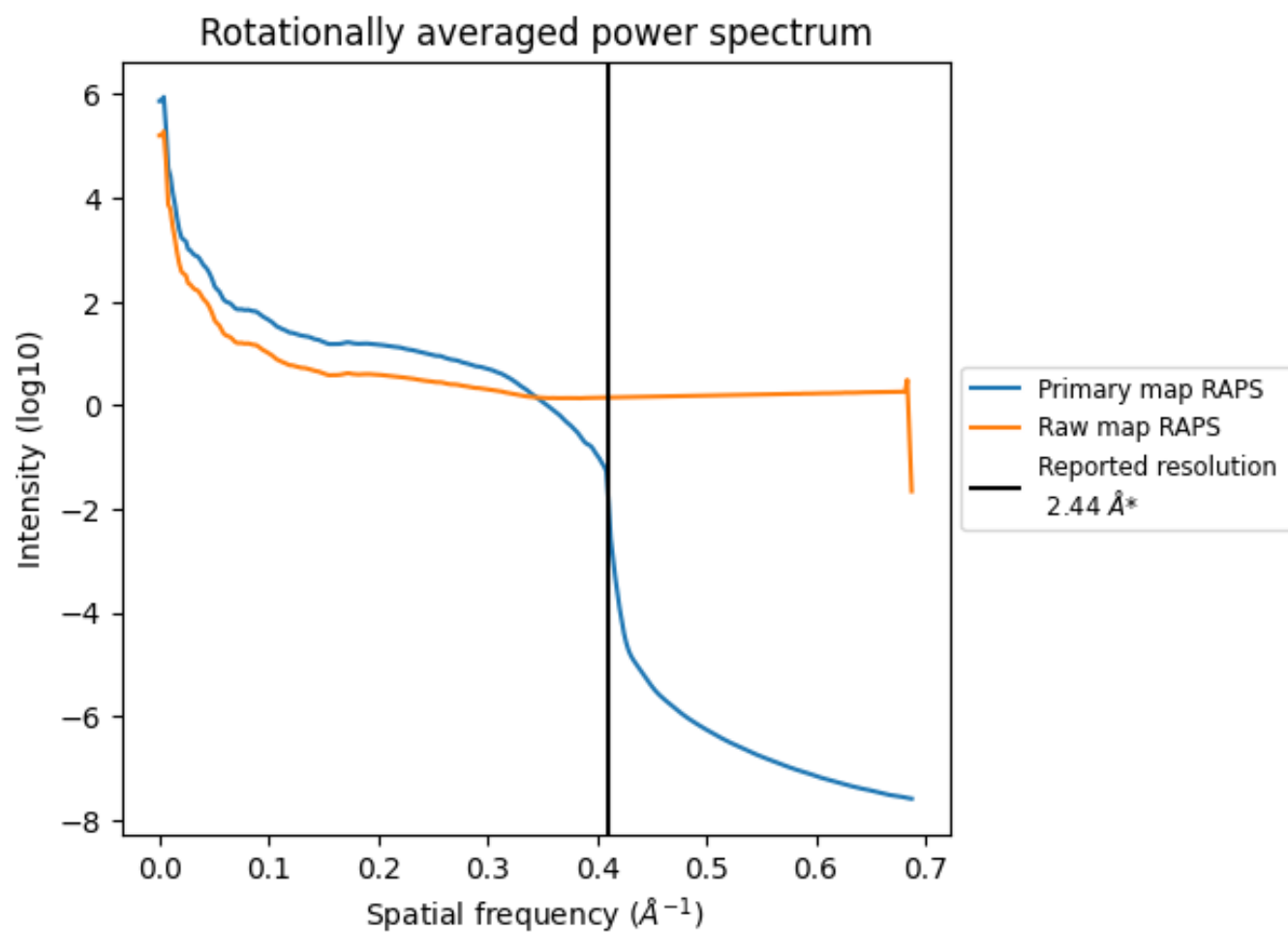
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1607  $\text{nm}^3$ ; this corresponds to an approximate mass of 1452 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 ⓘ

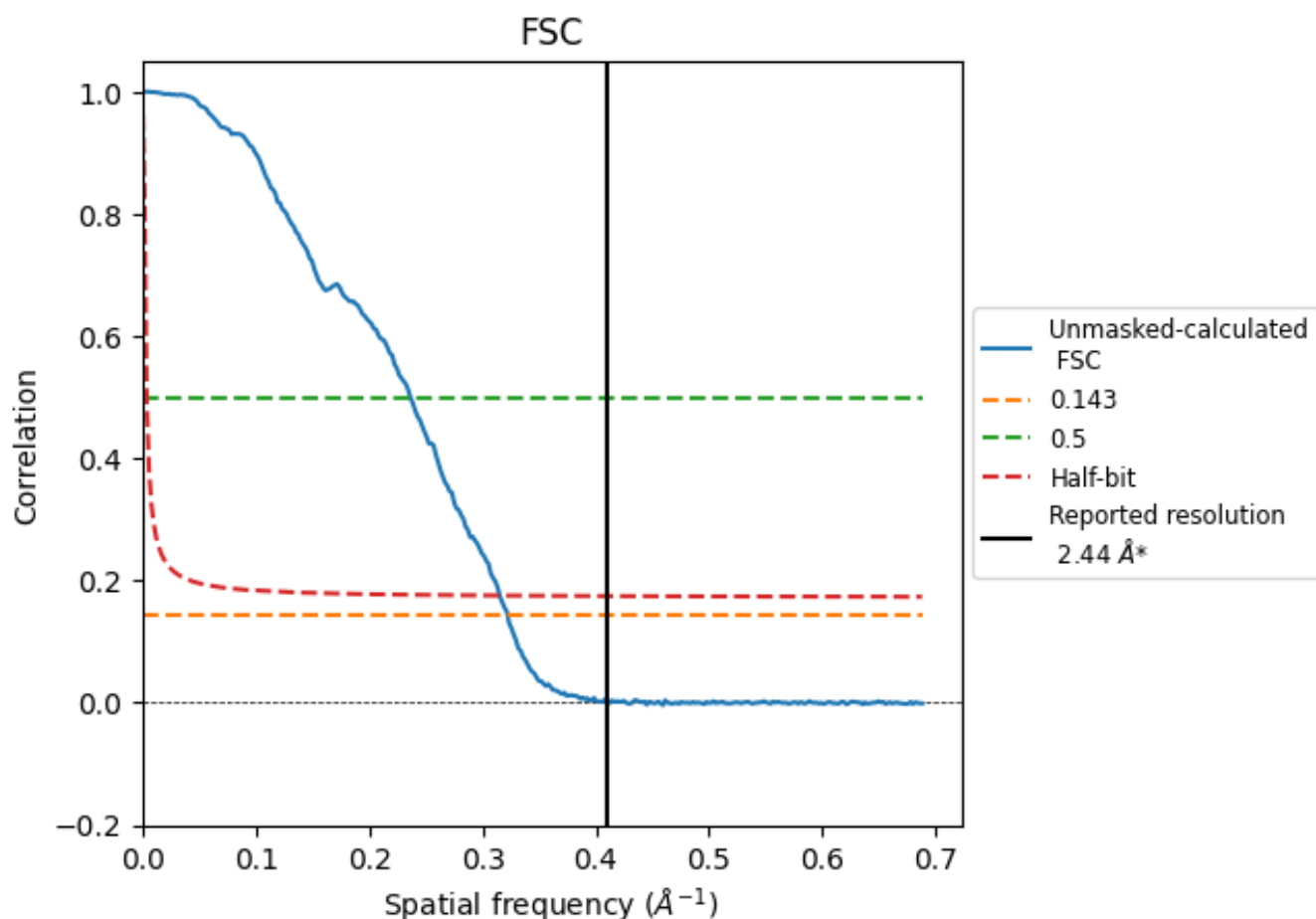


\*Reported resolution corresponds to spatial frequency of 0.410  $\text{\AA}^{-1}$

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.410  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

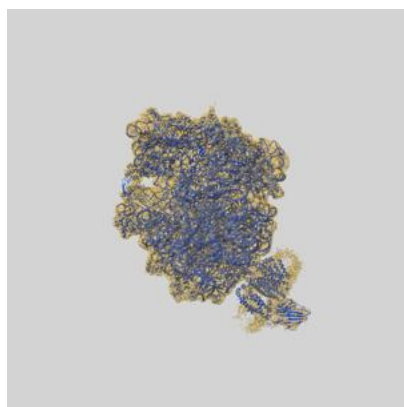
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 2.44                               | -    | -        |
| Author-provided FSC curve | -                                  | -    | -        |
| Unmasked-calculated*      | 3.10                               | 4.23 | 3.17     |

\*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 3.10 differs from the reported value 2.44 by more than 10 %

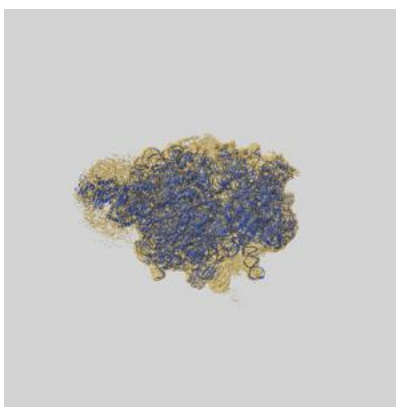
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-53892 and PDB model 9RBF. Per-residue inclusion information can be found in section 3 on page 17.

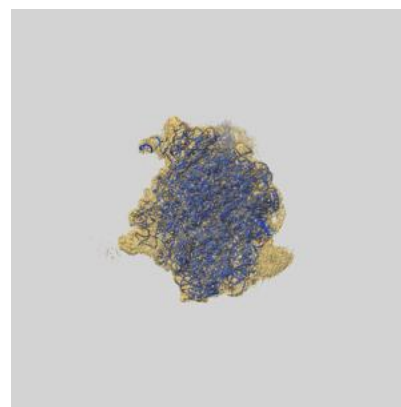
### 9.1 Map-model overlay [i](#)



X



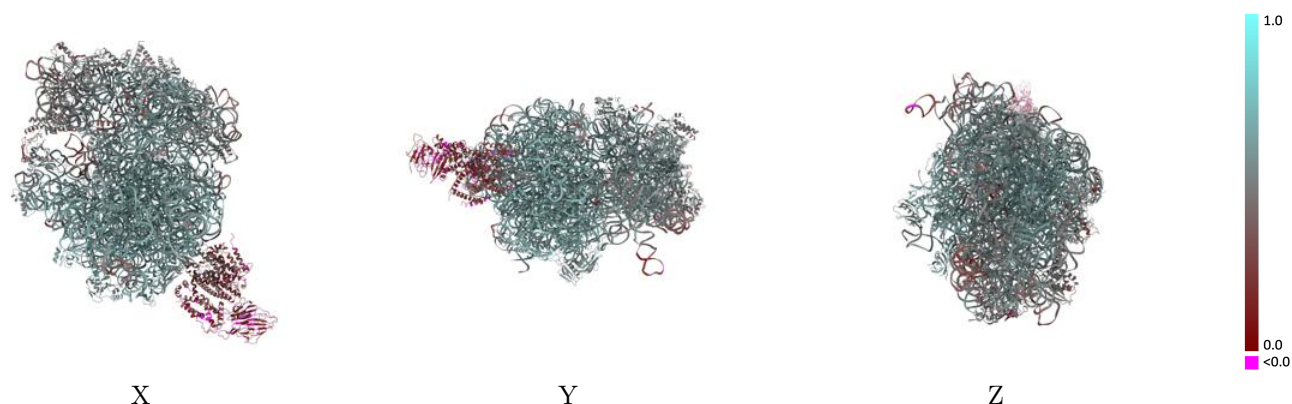
Y



Z

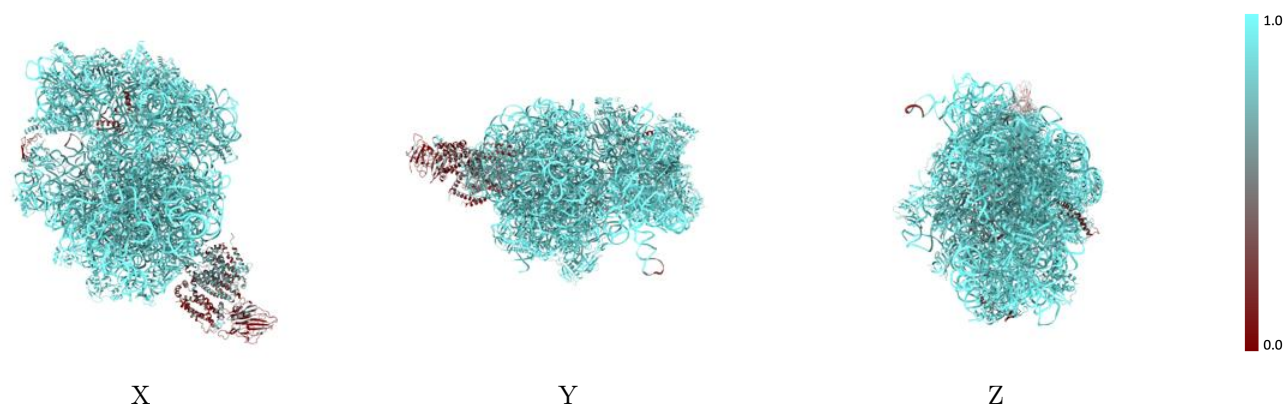
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



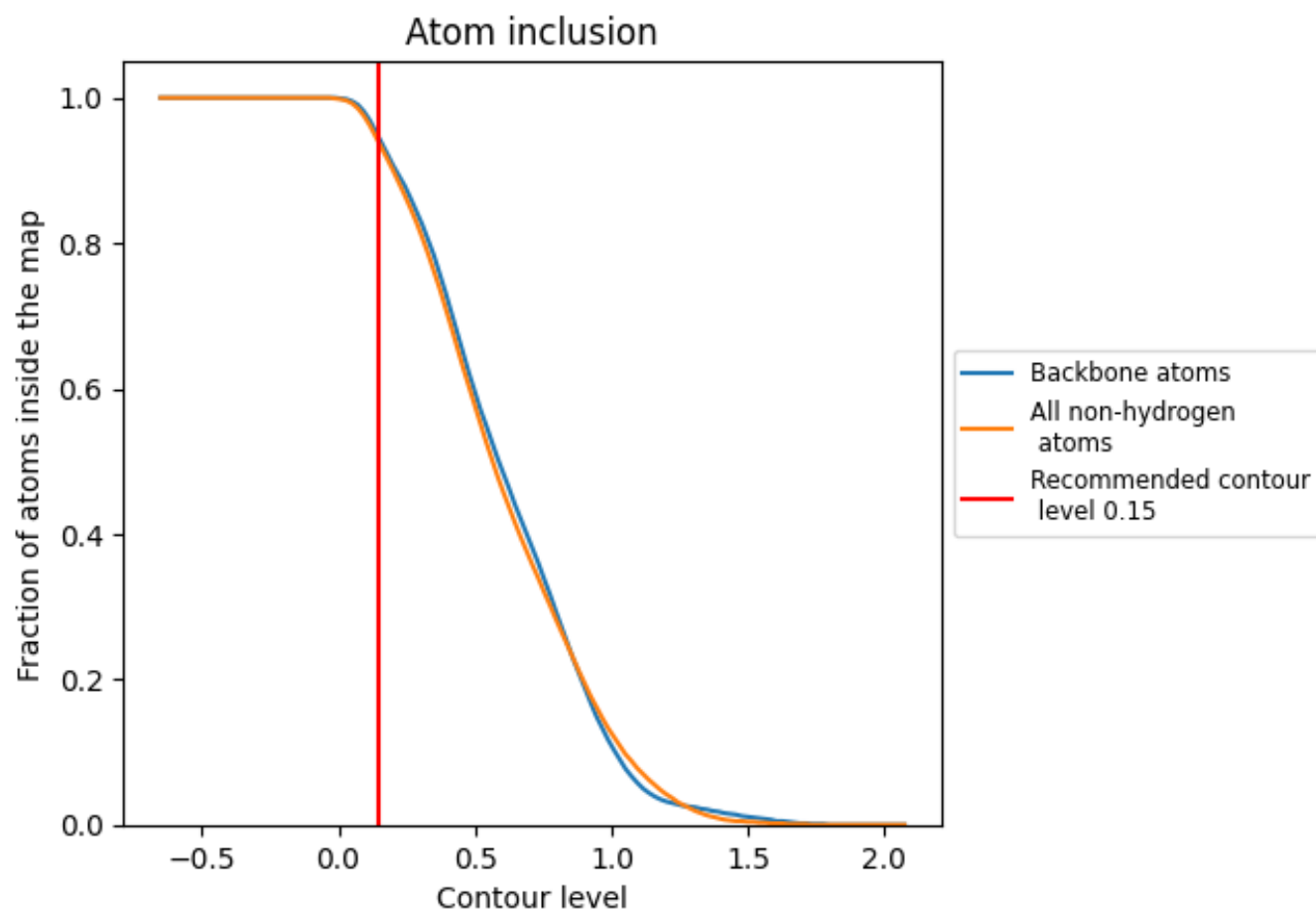
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.15).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 94% 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 (0.15) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.9370   |  0.5550   |
| 0     |  0.9120   |  0.6000   |
| 1     |  0.9780   |  0.6350   |
| 2     |  0.9780   |  0.6360   |
| 3     |  0.9830   |  0.6280   |
| 4     |  0.0640   |  0.2500   |
| 5     |  0.8570   |  0.5940   |
| 6     |  0.5600   |  0.2810   |
| 7     |  0.5080   |  0.2350   |
| 8     |  0.2800   |  0.1990   |
| 9     |  0.2210   |  0.1610   |
| A     |  0.9870   |  0.5320   |
| B     |  0.9070   |  0.4980   |
| C     |  0.9310   |  0.5320   |
| D     |  0.8620  |  0.4940  |
| E     |  0.9590 |  0.5730 |
| F     |  0.9390 |  0.5270 |
| G     |  0.8880 |  0.4460 |
| H     |  0.9560 |  0.5750 |
| I     |  0.9410 |  0.4650 |
| J     |  0.9360 |  0.4800 |
| K     |  0.9250 |  0.5160 |
| L     |  0.8930 |  0.5210 |
| M     |  0.9060 |  0.4700 |
| N     |  0.9510 |  0.4990 |
| O     |  0.9570 |  0.5360 |
| P     |  0.9360 |  0.5290 |
| Q     |  0.9380 |  0.5240 |
| R     |  0.8740 |  0.5010 |
| S     |  0.9030 |  0.4760 |
| T     |  0.9300 |  0.5210 |
| U     |  0.3090 |  0.4000 |
| V     |  0.6160 |  0.3750 |
| X     |  0.8730 |  0.5140 |
| Y     |  0.7360 |  0.5090 |



*Continued on next page...*

*Continued from previous page...*

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| Z     |  0.9640   |  0.4950   |
| a     |  0.9950   |  0.6140   |
| b     |  0.9980   |  0.5780   |
| c     |  0.9890   |  0.6390   |
| d     |  0.9740   |  0.6320   |
| e     |  0.9740   |  0.6070   |
| f     |  0.9200   |  0.4980   |
| g     |  0.9520   |  0.5510   |
| h     |  0.9570   |  0.5490   |
| i     |  0.9790   |  0.6260   |
| j     |  0.9810   |  0.6300   |
| k     |  0.9840   |  0.6240   |
| l     |  0.9780   |  0.6240   |
| m     |  0.9950   |  0.6450   |
| n     |  0.9720   |  0.5720   |
| o     |  0.9720   |  0.6290   |
| p     |  0.9910   |  0.6380   |
| q     |  0.9670  |  0.6170  |
| r     |  0.9710 |  0.6300 |
| s     |  0.9600 |  0.6160 |
| t     |  0.9530 |  0.5900 |
| u     |  0.9610 |  0.5980 |
| v     |  0.9670 |  0.6270 |
| w     |  0.9680 |  0.6130 |
| x     |  0.9320 |  0.5610 |
| y     |  0.9700 |  0.6160 |
| z     |  0.9770 |  0.6270 |