



## Full wwPDB EM Validation Report ⓘ

Mar 3, 2024 – 12:57 PM EST

PDB ID : 5WFS  
EMDB ID : EMD-8829  
Title : 70S ribosome-EF-Tu H84A complex with GTP and near-cognate tRNA (Complex C4)  
Authors : Fislage, M.; Frank, J.  
Deposited on : 2017-07-12  
Resolution : 3.00 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.dev70  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

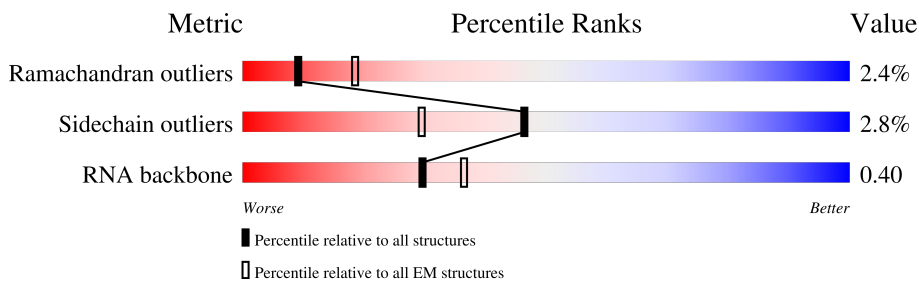
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.00 Å.

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



| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) |
|-----------------------|-----------------------------|-----------------------------|
| Ramachandran outliers | 154571                      | 4023                        |
| Sidechain outliers    | 154315                      | 3826                        |
| RNA backbone          | 4643                        | 859                         |

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   | A     | 2903   |                  |
| 2   | B     | 120    |                  |
| 3   | C     | 271    |                  |
| 4   | D     | 208    |                  |
| 5   | E     | 200    |                  |
| 6   | F     | 177    |                  |
| 7   | G     | 174    |                  |
| 8   | H     | 149    |                  |


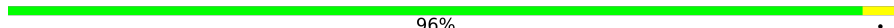
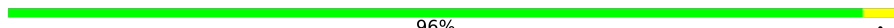
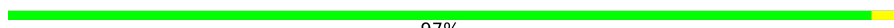
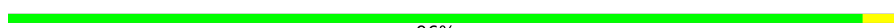








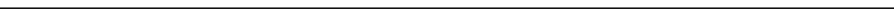

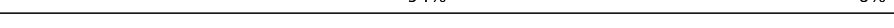
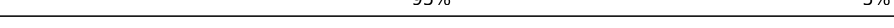
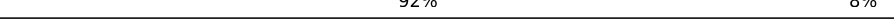

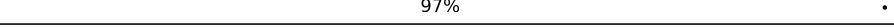
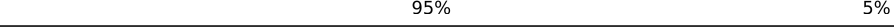




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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 9   | I     | 141    | 24%<br>92%<br>7% |
| 10  | J     | 141    | 98%              |
| 11  | K     | 122    | 94%<br>6%        |
| 12  | L     | 143    | 90%<br>9%        |
| 13  | M     | 136    | 97%              |
| 14  | N     | 119    | 96%<br>..        |
| 15  | O     | 116    | 99%<br>.         |
| 16  | P     | 114    | 98%<br>.         |
| 17  | Q     | 115    | 97%<br>.         |
| 18  | R     | 102    | 95%<br>5%        |
| 19  | S     | 109    | 98%<br>.         |
| 20  | T     | 92     | 95%<br>5%        |
| 21  | U     | 102    | 94%<br>6%        |
| 22  | V     | 92     | 98%<br>.         |
| 23  | W     | 75     | 97%<br>.         |
| 24  | X     | 77     | 99%<br>.         |
| 25  | Y     | 60     | 97%<br>.         |
| 26  | Z     | 56     | 100%             |
| 27  | 0     | 55     | 96%<br>.         |
| 28  | 1     | 51     | 100%             |
| 29  | 2     | 45     | 96%<br>.         |
| 30  | 3     | 64     | 97%<br>.         |
| 31  | 4     | 38     | 100%             |
| 32  | 5     | 131    | 89%<br>92%<br>8% |
| 33  | 6     | 66     | 95%<br>5%        |

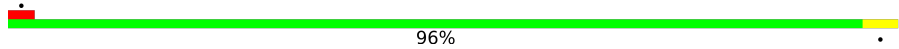
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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 34  | a     | 1540   |  67% 32%         |
| 35  | b     | 218    |  96% .           |
| 36  | c     | 206    |  96% .           |
| 37  | d     | 205    |  97% .           |
| 38  | e     | 157    |  96% .           |
| 39  | f     | 100    |  93% 7%          |
| 40  | g     | 151    |  92% 8%          |
| 41  | h     | 129    |  98% .           |
| 42  | i     | 127    |  94% 5% .        |
| 43  | j     | 98     |  94% 6%          |
| 44  | k     | 116    |  93% 7%          |
| 45  | l     | 121    |  93% 7% .        |
| 46  | m     | 115    |  97% .         |
| 47  | n     | 101    |  94% 6%        |
| 48  | o     | 88     |  94% 6%        |
| 49  | p     | 82     |  95% 5%        |
| 50  | q     | 80     |  92% 8%        |
| 51  | r     | 65     |  86% 14%       |
| 52  | s     | 79     |  97% .         |
| 53  | t     | 85     |  95% 5%        |
| 54  | u     | 65     |  82% 18%       |
| 55  | v     | 77     |  66% 31% .     |
| 55  | w     | 77     |  8% 53% 42% 5% |
| 56  | x     | 12     |  67% 33%       |
| 57  | y     | 76     |  53% 42% 5%    |

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| Mol | Chain | Length | Quality of chain  |
|-----|-------|--------|---|
| 58  | z     | 393    | <br>96% |

## 2 Entry composition [i](#)

There are 64 unique types of molecules in this entry. The entry contains 155100 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 23S rRNA.

| Mol | Chain | Residues | Atoms |       |       |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|-------|
|     |       |          | Total | C     | N     | O     | P    |         |       |
| 1   | A     | 2900     | 62277 | 27788 | 11459 | 20130 | 2900 | 0       | 0     |

There are 3 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference |
|-------|---------|----------|--------|----------|-----------|
| A     | 747     | 5MC      | U      | conflict | GB 216643 |
| A     | 1723    | G        | A      | conflict | GB 216643 |
| A     | 1847    | G        | A      | conflict | GB 216643 |

- Molecule 2 is a RNA chain called 5S rRNA.

| Mol | Chain | Residues | Atoms |      |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|-------|
|     |       |          | Total | C    | N   | O   | P   |         |       |
| 2   | B     | 120      | 2572  | 1145 | 471 | 836 | 120 | 0       | 0     |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference     |
|-------|---------|----------|--------|----------|---------------|
| B     | 120     | A        | U      | conflict | GB 1199817771 |

- Molecule 3 is a protein called 50S ribosomal protein L2.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
|     |       |          | Total | C    | N   | O   | S |         |       |
| 3   | C     | 271      | 2082  | 1288 | 423 | 364 | 7 | 0       | 0     |

- Molecule 4 is a protein called 50S ribosomal protein L3.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 4   | D     | 208      | 1557  | 974 | 287 | 293 | 3 | 0       | 0     |

- Molecule 5 is a protein called 50S ribosomal protein L4.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 5   | E     | 200      | 1544  | 969 | 282 | 289 | 4 | 0       | 0     |

- Molecule 6 is a protein called 50S ribosomal protein L5.

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

- Molecule 7 is a protein called 50S ribosomal protein L6.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 7   | G     | 174      | 1304  | 820 | 239 | 243 | 2 | 0       | 0     |

- Molecule 8 is a protein called 50S ribosomal protein L9.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 8   | H     | 149      | 1111  | 699 | 197 | 214 | 1 | 0       | 0     |

- Molecule 9 is a protein called 50S ribosomal protein L11.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 9   | I     | 141      | 1032  | 651 | 179 | 196 | 6 | 0       | 0     |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 10  | J     | 141      | 1120  | 708 | 211 | 197 | 4 | 0       | 0     |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 11  | K     | 122      | 938   | 587 | 180 | 165 | 6 | 0       | 0     |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 12  | L     | 143      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1043  | 649 | 206 | 186 | 2 |         |       |

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

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

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

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

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

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

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

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

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

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 17  | Q     | 115      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 933   | 595 | 190 | 148 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 18  | R     | 102      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 810   | 513 | 152 | 143 | 2 |         |       |

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



| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 19  | S     | 109      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 845   | 526 | 162 | 154 | 3 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 20  | T     | 92       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 730   | 461 | 138 | 130 | 1 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 21  | U     | 102      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 779   | 492 | 146 | 141 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 22  | V     | 92       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 739   | 471 | 135 | 131 | 2 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 23  | W     | 75       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 572   | 355 | 116 | 100 | 1 |         |       |

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

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

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

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 25  | Y     | 60       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 494   | 305 | 96 | 91 | 2 |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 26  | Z     | 56       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 434   | 273 | 85 | 74 | 2 |         |       |

- Molecule 27 is a protein called 50S ribosomal protein L32.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 27  | 0     | 55       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 434   | 263 | 92 | 78 | 1 |         |       |

- Molecule 28 is a protein called 50S ribosomal protein L33.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 28  | 1     | 51       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 417   | 269 | 76 | 72 |         |       |

- Molecule 29 is a protein called 50S ribosomal protein L34.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 29  | 2     | 45       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 367   | 222 | 88 | 55 | 2 |         |       |

- Molecule 30 is a protein called 50S ribosomal protein L35.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 30  | 3     | 64       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 504   | 323 | 105 | 74 | 2 |         |       |

- Molecule 31 is a protein called 50S ribosomal protein L36 1.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 31  | 4     | 38       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 302   | 185 | 65 | 48 | 4 |         |       |

- Molecule 32 is a protein called 50S ribosomal protein L10.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 32  | 5     | 131      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 988   | 625 | 175 | 183 | 5 |         |       |

- Molecule 33 is a protein called 50S ribosomal protein L31.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 33  | 6     | 66       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 522   | 323 | 99 | 94 | 6 |         |       |

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

| Mol | Chain | Residues | Atoms |       |      |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|-------|
| 34  | a     | 1540     | Total | C     | N    | O     | P    | 0       | 0     |
|     |       |          | 33050 | 14748 | 6057 | 10705 | 1540 |         |       |

- Molecule 35 is a protein called 30S ribosomal protein S2.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 35  | b     | 218      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1704  | 1081 | 305 | 311 | 7 |         |       |

- Molecule 36 is a protein called 30S ribosomal protein S3.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 36  | c     | 206      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1624  | 1028 | 305 | 288 | 3 |         |       |

- Molecule 37 is a protein called 30S ribosomal protein S4.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 37  | d     | 205      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1643  | 1026 | 315 | 298 | 4 |         |       |

- Molecule 38 is a protein called 30S ribosomal protein S5.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 38  | e     | 157      | Total | C   | N   | O   | S | 1       | 0     |
|     |       |          | 1164  | 724 | 221 | 213 | 6 |         |       |

- Molecule 39 is a protein called 30S ribosomal protein S6.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 39  | f     | 100      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 817   | 515 | 148 | 148 | 6 |         |       |

- Molecule 40 is a protein called 30S ribosomal protein S7.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 40  | g     | 151      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1181  | 735 | 227 | 215 | 4 |         |       |

- Molecule 41 is a protein called 30S ribosomal protein S8.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 41  | h     | 129      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 979   | 616 | 173 | 184 | 6 |         |       |

- Molecule 42 is a protein called 30S ribosomal protein S9.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 42  | i     | 127      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1022  | 634 | 206 | 179 | 3 |         |       |

- Molecule 43 is a protein called 30S ribosomal protein S10.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 43  | j     | 98       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 786   | 493 | 150 | 142 | 1 |         |       |

- Molecule 44 is a protein called 30S ribosomal protein S11.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 44  | k     | 116      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 869   | 535 | 173 | 158 | 3 |         |       |

- Molecule 45 is a protein called 30S ribosomal protein S12.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 45  | l     | 121      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 940   | 581 | 193 | 162 | 4 |         |       |

- Molecule 46 is a protein called 30S ribosomal protein S13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 46  | m     | 115      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 891   | 552 | 179 | 157 | 3 |         |       |

- Molecule 47 is a protein called 30S ribosomal protein S14.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 47  | n     | 101      | 810   | 502 | 165 | 140 | 3 | 0       | 0     |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment   | Reference  |
|-------|---------|----------|--------|-----------|------------|
| n     | 35      | ALA      | -      | insertion | UNP B7MCS2 |

- Molecule 48 is a protein called 30S ribosomal protein S15.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 48  | o     | 88       | 714   | 439 | 144 | 130 | 1 | 0       | 0     |

- Molecule 49 is a protein called 30S ribosomal protein S16.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 49  | p     | 82       | 649   | 406 | 128 | 114 | 1 | 0       | 0     |

- Molecule 50 is a protein called 30S ribosomal protein S17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 50  | q     | 80       | 648   | 411 | 121 | 113 | 3 | 0       | 0     |

- Molecule 51 is a protein called 30S ribosomal protein S18.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
|     |       |          | Total | C   | N   | O  | S |         |       |
| 51  | r     | 65       | 535   | 339 | 100 | 95 | 1 | 0       | 0     |

- Molecule 52 is a protein called 30S ribosomal protein S19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 52  | s     | 79       | 637   | 408 | 120 | 107 | 2 | 0       | 0     |

- Molecule 53 is a protein called 30S ribosomal protein S20.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 53  | t     | 85       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 665   | 411 | 137 | 114 | 3 |         |       |

- Molecule 54 is a protein called 30S ribosomal protein S21.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 54  | u     | 65       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 544   | 335 | 117 | 91 | 1 |         |       |

- Molecule 55 is a RNA chain called tRNA-fMet.

| Mol | Chain | Residues | Atoms |     |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---|---------|-------|
| 55  | v     | 77       | Total | C   | N   | O   | P  | S | 0       | 0     |
|     |       |          | 1644  | 733 | 297 | 536 | 77 | 1 |         |       |
| 55  | w     | 77       | Total | C   | N   | O   | P  | S | 0       | 0     |
|     |       |          | 1644  | 733 | 297 | 536 | 77 | 1 |         |       |

- Molecule 56 is a RNA chain called mRNA.

| Mol | Chain | Residues | Atoms |     |    |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|----|---------|-------|
| 56  | x     | 12       | Total | C   | N  | O  | P  | 0       | 0     |
|     |       |          | 252   | 113 | 43 | 84 | 12 |         |       |

- Molecule 57 is a RNA chain called Phe-tRNA-Phe.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |   |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|---|
| 57  | y     | 76       | Total | C   | N   | O   | P  | S       | 0     | 0 |
|     |       |          | 1632  | 731 | 290 | 533 | 76 | 2       |       |   |

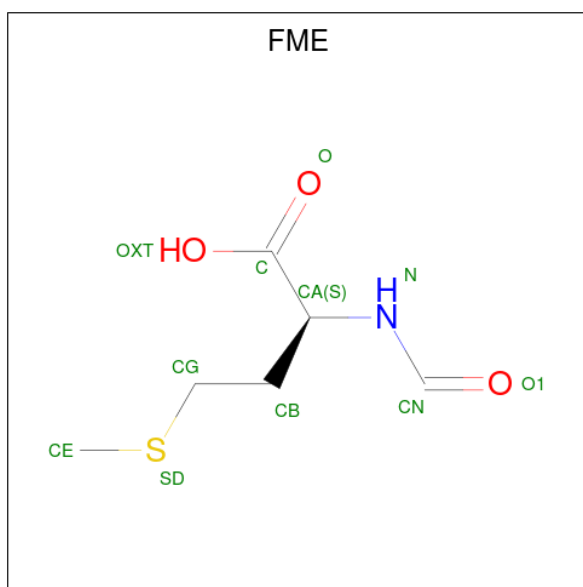
- Molecule 58 is a protein called Elongation factor Tu 2.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 58  | z     | 393      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3031  | 1915 | 522 | 581 | 13 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| z     | 84      | ALA      | HIS    | engineered mutation | UNP A7ZUJ2 |

- Molecule 59 is N-FORMYLMETHIONINE (three-letter code: FME) (formula: C<sub>6</sub>H<sub>11</sub>NO<sub>3</sub>S).



| Mol | Chain | Residues | Atoms |   |   |   |   | AltConf |
|-----|-------|----------|-------|---|---|---|---|---------|
|     |       |          | Total | C | N | O | S |         |
| 59  | A     | 1        | 10    | 6 | 1 | 2 | 1 | 0       |

- Molecule 60 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |      | AltConf |
|-----|-------|----------|-------|------|---------|
|     |       |          | Total | Mg   |         |
| 60  | A     | 1011     | 1011  | 1011 | 0       |
| 60  | B     | 37       | 37    | 37   | 0       |
| 60  | C     | 1        | 1     | 1    | 0       |
| 60  | D     | 2        | 2     | 2    | 0       |
| 60  | E     | 1        | 1     | 1    | 0       |
| 60  | M     | 2        | 2     | 2    | 0       |
| 60  | N     | 1        | 1     | 1    | 0       |
| 60  | Q     | 1        | 1     | 1    | 0       |
| 60  | T     | 1        | 1     | 1    | 0       |
| 60  | W     | 1        | 1     | 1    | 0       |
| 60  | 0     | 3        | 3     | 3    | 0       |

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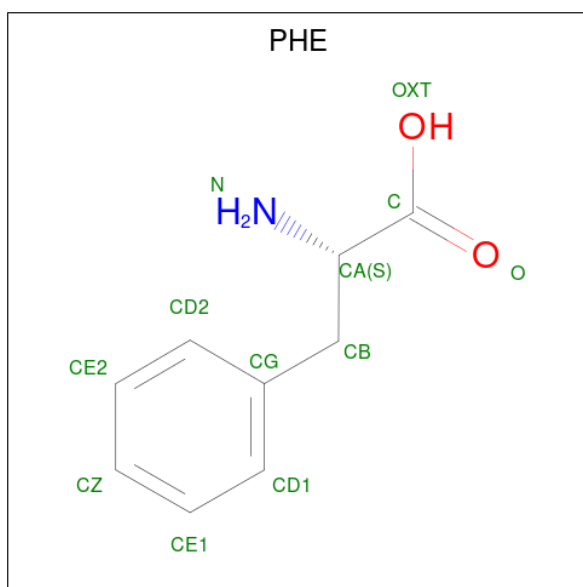
| Mol | Chain | Residues | Atoms        |           | AltConf |
|-----|-------|----------|--------------|-----------|---------|
| 60  | 2     | 1        | Total<br>1   | Mg<br>1   | 0       |
| 60  | a     | 392      | Total<br>392 | Mg<br>392 | 0       |
| 60  | d     | 1        | Total<br>1   | Mg<br>1   | 0       |
| 60  | e     | 1        | Total<br>1   | Mg<br>1   | 0       |
| 60  | i     | 1        | Total<br>1   | Mg<br>1   | 0       |
| 60  | u     | 1        | Total<br>1   | Mg<br>1   | 0       |
| 60  | v     | 6        | Total<br>6   | Mg<br>6   | 0       |
| 60  | w     | 2        | Total<br>2   | Mg<br>2   | 0       |
| 60  | x     | 1        | Total<br>1   | Mg<br>1   | 0       |
| 60  | y     | 2        | Total<br>2   | Mg<br>2   | 0       |
| 60  | z     | 2        | Total<br>2   | Mg<br>2   | 0       |

- Molecule 61 is POTASSIUM ION (three-letter code: K) (formula: K).

| Mol | Chain | Residues | Atoms      |        | AltConf |
|-----|-------|----------|------------|--------|---------|
| 61  | A     | 6        | Total<br>6 | K<br>6 | 0       |
| 61  | a     | 1        | Total<br>1 | K<br>1 | 0       |

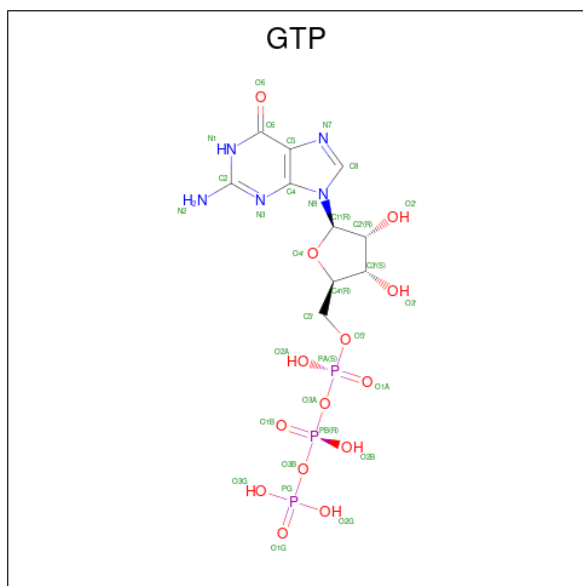
- Molecule 62 is PHENYLALANINE (three-letter code: PHE) (formula: C<sub>9</sub>H<sub>11</sub>NO<sub>2</sub>).





| Mol | Chain | Residues | Atoms |   |   |   | AltConf |
|-----|-------|----------|-------|---|---|---|---------|
|     |       |          | Total | C | N | O |         |
| 62  | z     | 1        | 11    | 9 | 1 | 1 | 0       |

- Molecule 63 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula:  $C_{10}H_{16}N_5O_{14}P_3$ ).



| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
|     |       |          | Total | C  | N | O  | P |         |
| 63  | z     | 1        | 32    | 10 | 5 | 14 | 3 | 0       |

- Molecule 64 is water.

| Mol | Chain | Residues | Atoms        |          | AltConf |
|-----|-------|----------|--------------|----------|---------|
| 64  | A     | 828      | Total<br>828 | O<br>828 | 0       |
| 64  | B     | 29       | Total<br>29  | O<br>29  | 0       |
| 64  | C     | 5        | Total<br>5   | O<br>5   | 0       |
| 64  | D     | 6        | Total<br>6   | O<br>6   | 0       |
| 64  | E     | 5        | Total<br>5   | O<br>5   | 0       |
| 64  | J     | 4        | Total<br>4   | O<br>4   | 0       |
| 64  | L     | 5        | Total<br>5   | O<br>5   | 0       |
| 64  | N     | 1        | Total<br>1   | O<br>1   | 0       |
| 64  | O     | 1        | Total<br>1   | O<br>1   | 0       |
| 64  | Q     | 3        | Total<br>3   | O<br>3   | 0       |
| 64  | R     | 1        | Total<br>1   | O<br>1   | 0       |
| 64  | S     | 3        | Total<br>3   | O<br>3   | 0       |
| 64  | W     | 2        | Total<br>2   | O<br>2   | 0       |
| 64  | X     | 3        | Total<br>3   | O<br>3   | 0       |
| 64  | Y     | 1        | Total<br>1   | O<br>1   | 0       |
| 64  | 0     | 2        | Total<br>2   | O<br>2   | 0       |
| 64  | 1     | 1        | Total<br>1   | O<br>1   | 0       |
| 64  | 2     | 2        | Total<br>2   | O<br>2   | 0       |
| 64  | 3     | 1        | Total<br>1   | O<br>1   | 0       |
| 64  | a     | 253      | Total<br>253 | O<br>253 | 0       |
| 64  | c     | 1        | Total<br>1   | O<br>1   | 0       |
| 64  | i     | 1        | Total<br>1   | O<br>1   | 0       |

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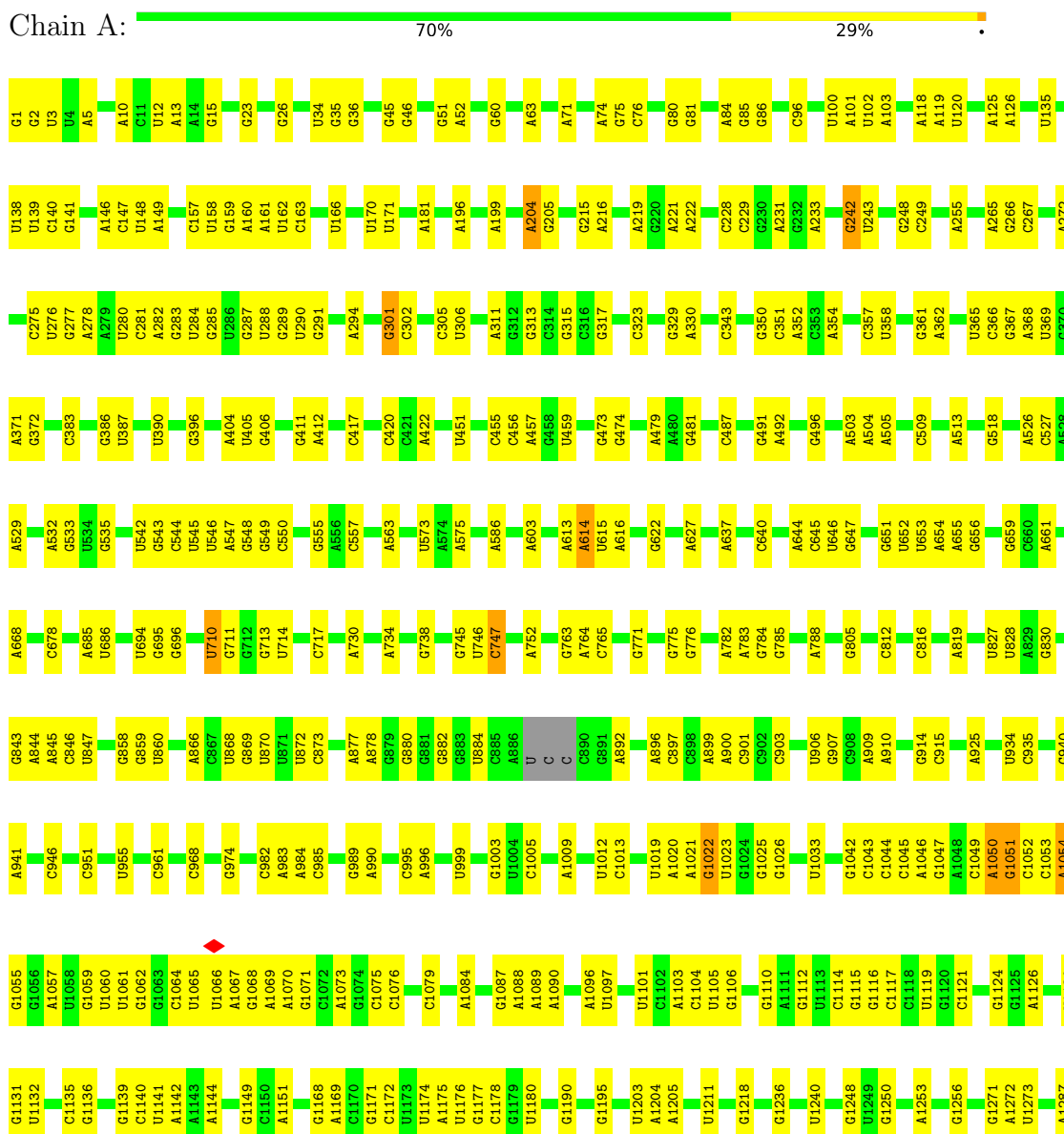
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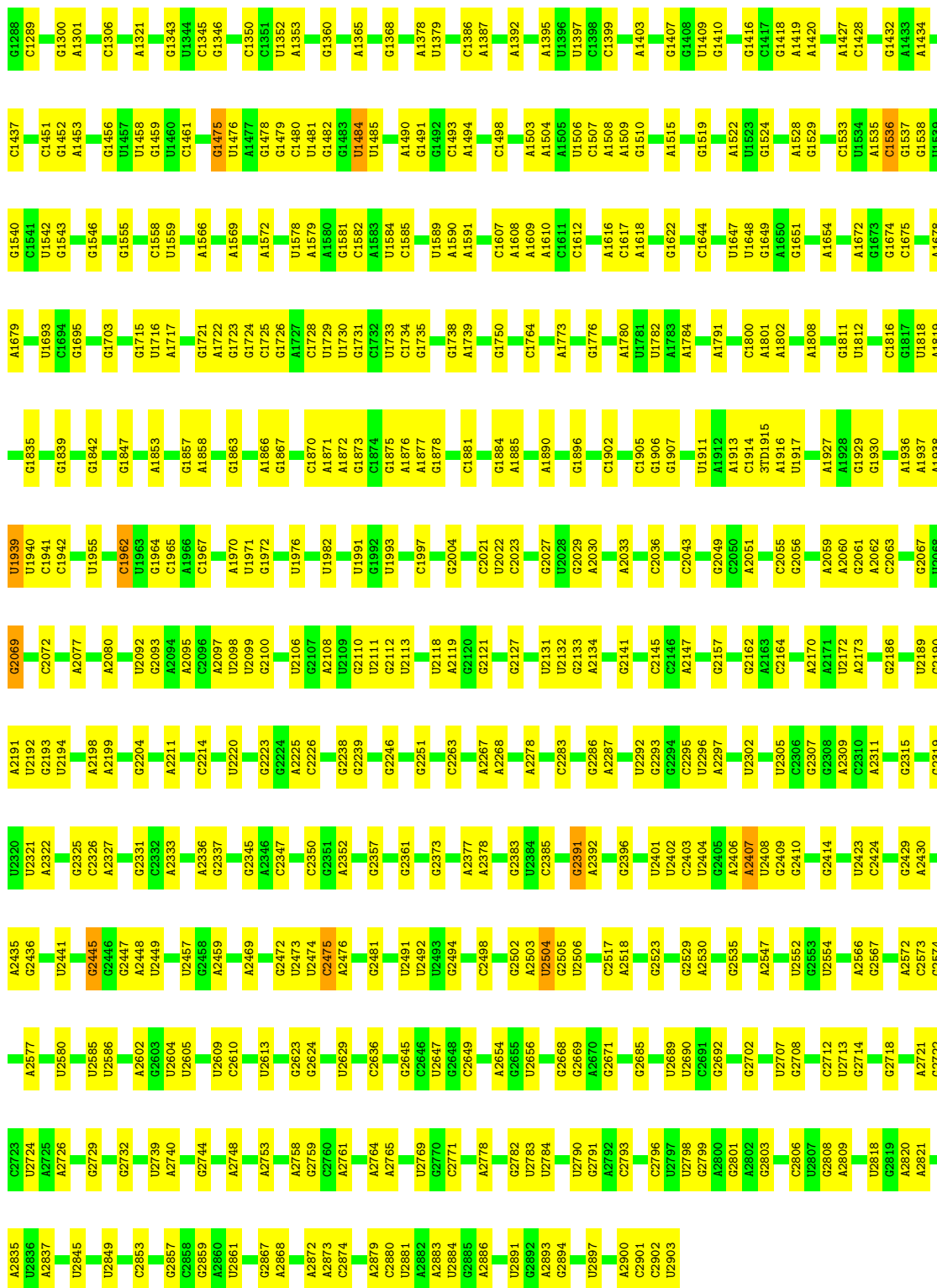
| Mol | Chain | Residues | Atoms      |        | AltConf |
|-----|-------|----------|------------|--------|---------|
| 64  | j     | 1        | Total<br>1 | O<br>1 | 0       |
| 64  | l     | 2        | Total<br>2 | O<br>2 | 0       |
| 64  | m     | 1        | Total<br>1 | O<br>1 | 0       |
| 64  | o     | 1        | Total<br>1 | O<br>1 | 0       |
| 64  | q     | 1        | Total<br>1 | O<br>1 | 0       |
| 64  | s     | 3        | Total<br>3 | O<br>3 | 0       |
| 64  | u     | 1        | Total<br>1 | O<br>1 | 0       |
| 64  | v     | 3        | Total<br>3 | O<br>3 | 0       |
| 64  | w     | 1        | Total<br>1 | O<br>1 | 0       |
| 64  | x     | 1        | Total<br>1 | O<br>1 | 0       |
| 64  | y     | 2        | Total<br>2 | O<br>2 | 0       |

### 3 Residue-property plots

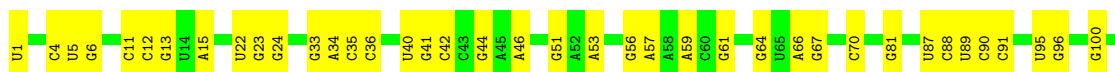
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: 23S rRNA





• Molecule 2: 5S rRNA





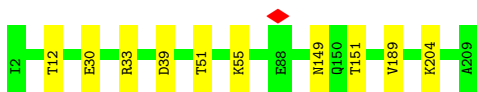
- Molecule 3: 50S ribosomal protein L2

Chain C: 96%



- Molecule 4: 50S ribosomal protein L3

Chain D: 95%



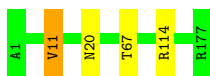
- Molecule 5: 50S ribosomal protein L4

Chain E: 94%



- Molecule 6: 50S ribosomal protein L5

Chain F: 98%



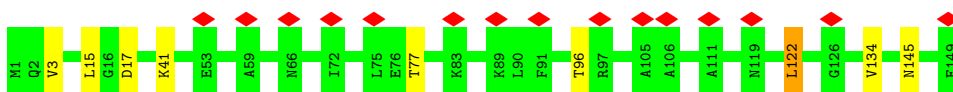
- Molecule 7: 50S ribosomal protein L6

Chain G: 99%



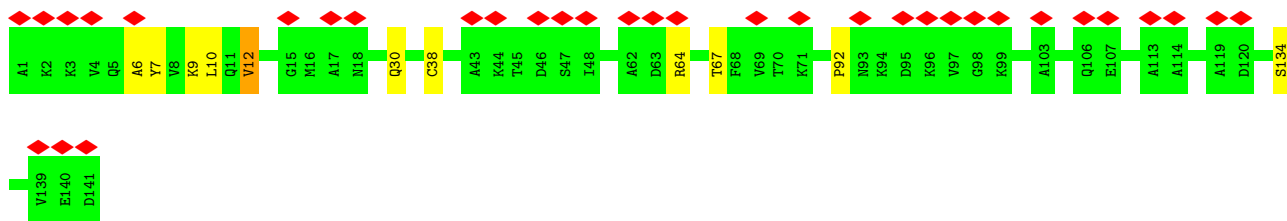
- Molecule 8: 50S ribosomal protein L9

Chain H: 10% 94% 5%



- Molecule 9: 50S ribosomal protein L11

Chain I: 24% 92% 7%



- Molecule 10: 50S ribosomal protein L13

Chain J: 98%



- Molecule 11: 50S ribosomal protein L14

Chain K: 94% 6%



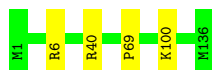
- Molecule 12: 50S ribosomal protein L15

Chain L: 90% 9%



- Molecule 13: 50S ribosomal protein L16

Chain M: 97%



- Molecule 14: 50S ribosomal protein L17

Chain N: 96%



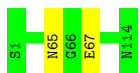
- Molecule 15: 50S ribosomal protein L18

Chain O: 99%



- Molecule 16: 50S ribosomal protein L19

Chain P:  98%



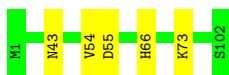
• Molecule 17: 50S ribosomal protein L20

Chain Q:  97%



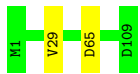
• Molecule 18: 50S ribosomal protein L21

Chain R:  95% 5%



• Molecule 19: 50S ribosomal protein L22

Chain S:  98%



• Molecule 20: 50S ribosomal protein L23

Chain T:  95% 5%



• Molecule 21: 50S ribosomal protein L24

Chain U:  94% 6%



• Molecule 22: 50S ribosomal protein L25

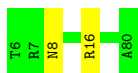
Chain V:  98%



• Molecule 23: 50S ribosomal protein L27



Chain W:  97%



- Molecule 24: 50S ribosomal protein L28

Chain X:  99%



- Molecule 25: 50S ribosomal protein L29

Chain Y:  97%



- Molecule 26: 50S ribosomal protein L30

Chain Z:  100%

There are no outlier residues recorded for this chain.

- Molecule 27: 50S ribosomal protein L32

Chain 0:  96%



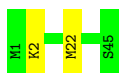
- Molecule 28: 50S ribosomal protein L33

Chain 1:  100%

There are no outlier residues recorded for this chain.

- Molecule 29: 50S ribosomal protein L34

Chain 2:  96%



- Molecule 30: 50S ribosomal protein L35

Chain 3:  97%



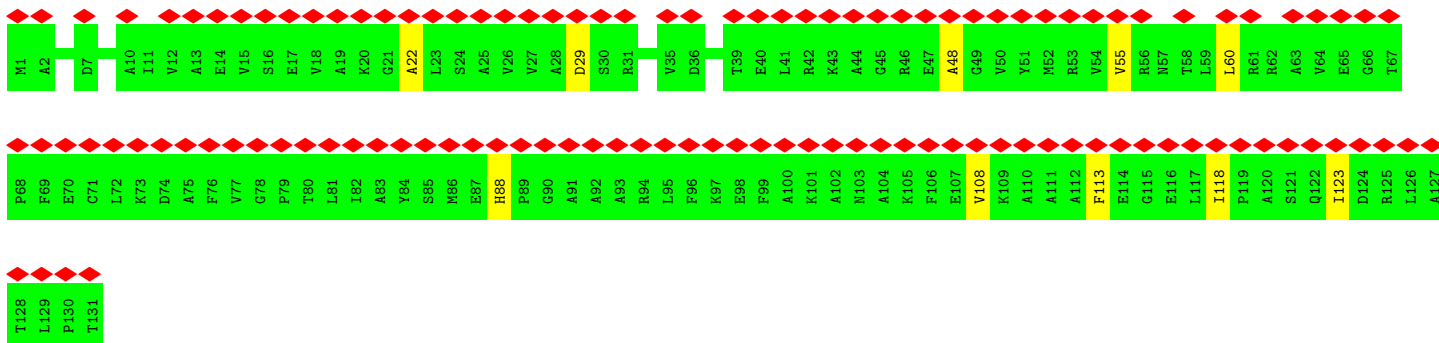
- Molecule 31: 50S ribosomal protein L36 1

Chain 4: 100%

There are no outlier residues recorded for this chain.

- Molecule 32: 50S ribosomal protein L10

Chain 5: 89%  
92% 8%



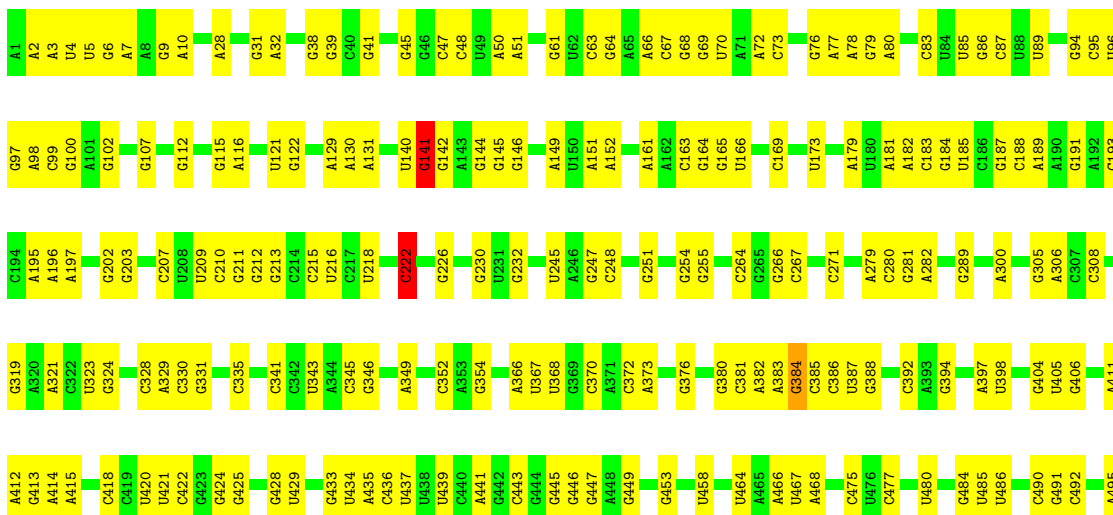
- Molecule 33: 50S ribosomal protein L31

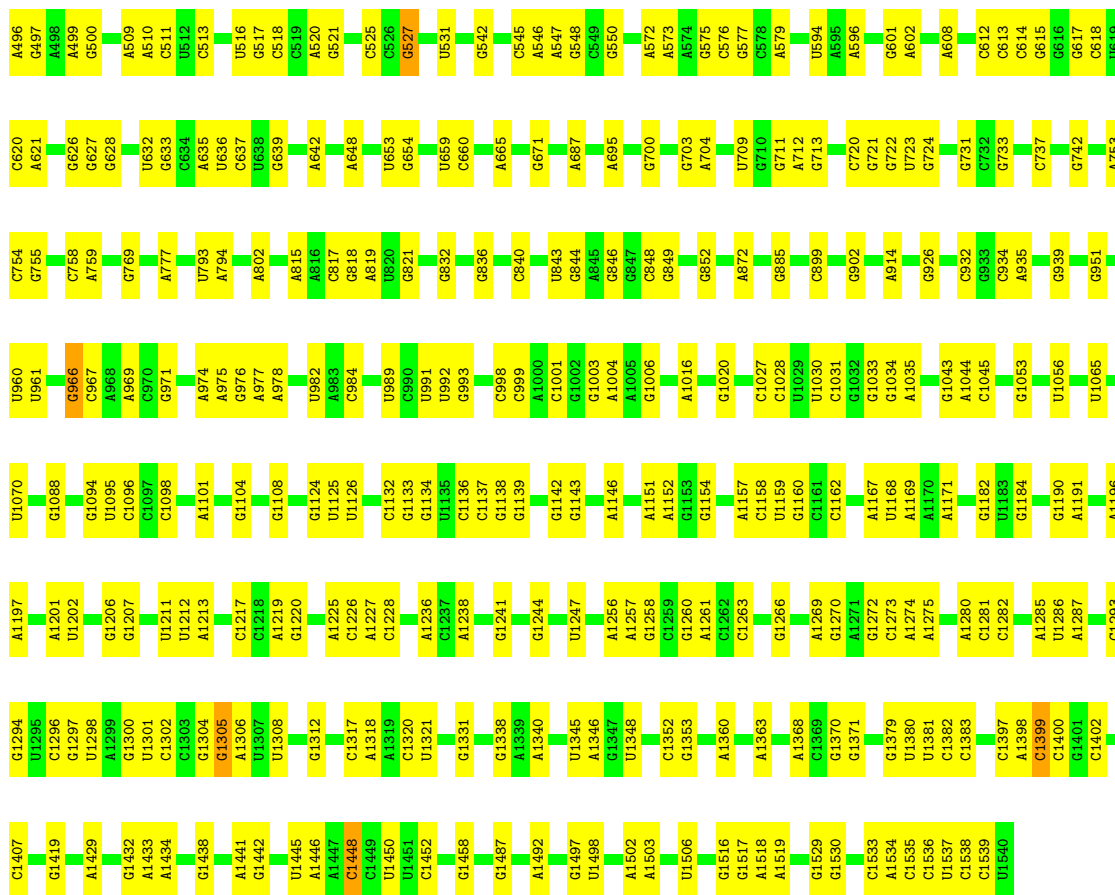
Chain 6: 95% 5%



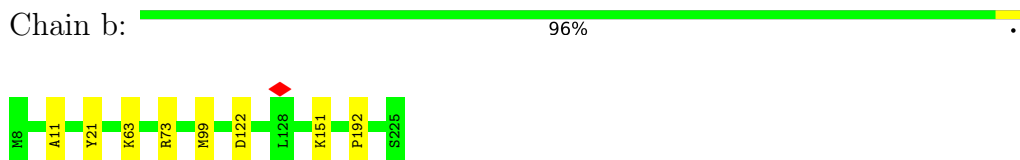
- Molecule 34: 16S rRNA

Chain a: 67% 32%

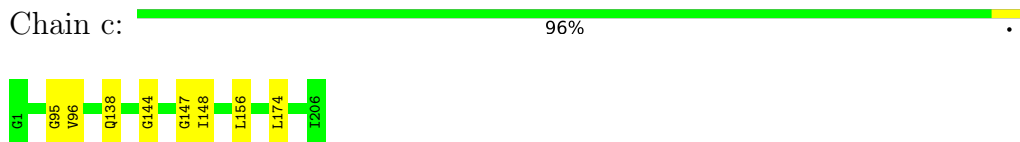




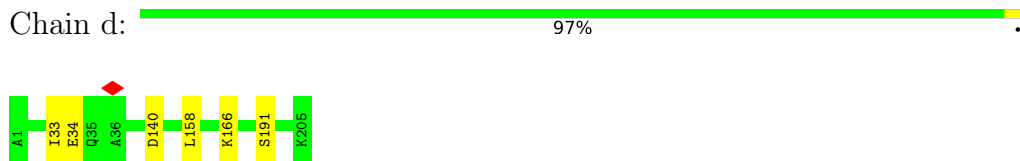
• Molecule 35: 30S ribosomal protein S2



• Molecule 36: 30S ribosomal protein S3

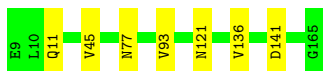


• Molecule 37: 30S ribosomal protein S4



• Molecule 38: 30S ribosomal protein S5

Chain e:  96%



- Molecule 39: 30S ribosomal protein S6

Chain f:  93% 7%



- Molecule 40: 30S ribosomal protein S7

Chain g:  92% 8%



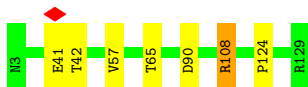
- Molecule 41: 30S ribosomal protein S8

Chain h:  98%



- Molecule 42: 30S ribosomal protein S9

Chain i:  94% 5%



- Molecule 43: 30S ribosomal protein S10

Chain j:  94% 6%




- Molecule 44: 30S ribosomal protein S11

Chain k:  93% 7%



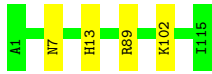
- Molecule 45: 30S ribosomal protein S12

Chain l:  93% 7%



- Molecule 46: 30S ribosomal protein S13

Chain m:  97%



- Molecule 47: 30S ribosomal protein S14

Chain n:  94% 6%



- Molecule 48: 30S ribosomal protein S15

Chain o:  94% 6%



- Molecule 49: 30S ribosomal protein S16

Chain p:  95% 5%




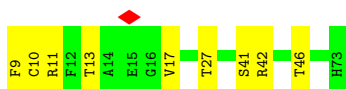
- Molecule 50: 30S ribosomal protein S17

Chain q:  92% 8%



- Molecule 51: 30S ribosomal protein S18

Chain r:  86% 14%



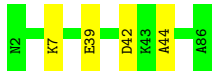
- Molecule 52: 30S ribosomal protein S19

Chain s:  97%




- Molecule 53: 30S ribosomal protein S20

Chain t:  95%



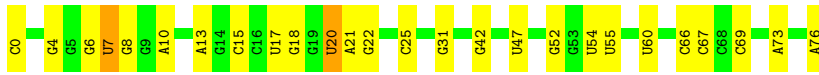
- Molecule 54: 30S ribosomal protein S21

Chain u:  82%



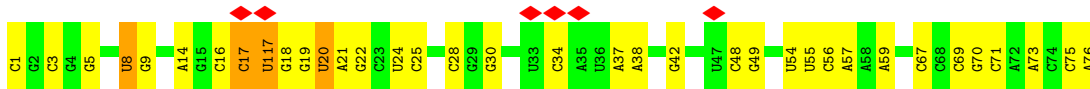
- Molecule 55: tRNA-fMet

Chain v:  66%



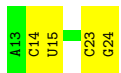
- Molecule 55: tRNA-fMet

Chain w:  8%



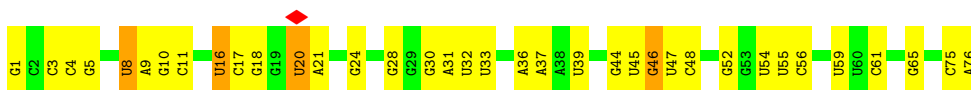
- Molecule 56: mRNA

Chain x:  67%



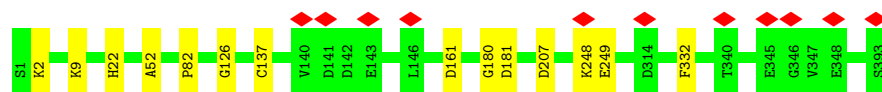
- Molecule 57: Phe-tRNA-Phe

Chain y:  53%



- Molecule 58: Elongation factor Tu 2

Chain z:  96%



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|---|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, C1                               | Depositor |
| Number of particles used             | 58475                                   | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | FEI POLARA 300                          | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 67                                      | Depositor |
| Minimum defocus (nm)                 | 300                                     | Depositor |
| Maximum defocus (nm)                 | 4000                                    | Depositor |
| Magnification                        | 51020                                   | Depositor |
| Image detector                       | GATAN K2 SUMMIT (4k x 4k)               | Depositor |
| Maximum map value                    | 0.288                                   | Depositor |
| Minimum map value                    | -0.143                                  | Depositor |
| Average map value                    | 0.001                                   | Depositor |
| Map value standard deviation         | 0.010                                   | Depositor |
| Recommended contour level            | 0.00532                                 | Depositor |
| Map size ( $\text{\AA}$ )            | 390.04, 390.04, 390.04                  | wwPDB     |
| Map dimensions                       | 398, 398, 398                           | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 0.98, 0.98, 0.98                        | Depositor |



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, PSU, H2U, 5MU, 2MA, OMU, MA6, K, 7MG, 2MG, 6MZ, FME, OMG, 3TD, UR3, 4SU, 5MC, MG, OMC, 4OC, 1MG, MIA

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   | A     | 0.25         | 1/69174 (0.0%) | 0.70        | 16/107907 (0.0%) |
| 2   | B     | 0.30         | 1/2876 (0.0%)  | 0.71        | 0/4483           |
| 3   | C     | 0.35         | 0/2121         | 0.70        | 0/2852           |
| 4   | D     | 0.35         | 0/1578         | 0.60        | 0/2124           |
| 5   | E     | 0.35         | 0/1563         | 0.64        | 0/2103           |
| 6   | F     | 0.38         | 0/1434         | 0.61        | 0/1926           |
| 7   | G     | 0.35         | 0/1324         | 0.56        | 0/1794           |
| 8   | H     | 0.39         | 0/1122         | 0.57        | 0/1515           |
| 9   | I     | 0.43         | 0/1046         | 0.60        | 0/1410           |
| 10  | J     | 0.34         | 0/1143         | 0.61        | 0/1540           |
| 11  | K     | 0.35         | 0/947          | 0.68        | 0/1268           |
| 12  | L     | 0.36         | 0/1052         | 0.71        | 0/1401           |
| 13  | M     | 0.37         | 0/1093         | 0.63        | 0/1460           |
| 14  | N     | 0.38         | 0/964          | 0.71        | 0/1289           |
| 15  | O     | 0.36         | 0/902          | 0.63        | 0/1209           |
| 16  | P     | 0.36         | 0/929          | 0.64        | 0/1242           |
| 17  | Q     | 0.36         | 0/946          | 0.67        | 0/1260           |
| 18  | R     | 0.35         | 0/823          | 0.60        | 0/1100           |
| 19  | S     | 0.33         | 0/852          | 0.67        | 0/1142           |
| 20  | T     | 0.35         | 0/736          | 0.61        | 0/984            |
| 21  | U     | 0.34         | 0/787          | 0.57        | 0/1051           |
| 22  | V     | 0.35         | 0/752          | 0.55        | 0/1008           |
| 23  | W     | 0.35         | 0/579          | 0.64        | 0/767            |
| 24  | X     | 0.36         | 0/635          | 0.65        | 0/848            |
| 25  | Y     | 0.38         | 0/495          | 0.59        | 0/658            |
| 26  | Z     | 0.36         | 0/438          | 0.60        | 0/586            |
| 27  | 0     | 0.33         | 0/440          | 0.67        | 0/588            |
| 28  | 1     | 0.35         | 0/424          | 0.56        | 0/565            |
| 29  | 2     | 0.38         | 0/370          | 0.78        | 0/487            |
| 30  | 3     | 0.33         | 0/513          | 0.62        | 0/676            |
| 31  | 4     | 0.33         | 0/303          | 0.65        | 0/397            |

| Mol | Chain | Bond lengths |                  | Bond angles |                  |
|-----|-------|--------------|------------------|-------------|------------------|
|     |       | RMSZ         | # Z  >5          | RMSZ        | # Z  >5          |
| 32  | 5     | 0.43         | 0/1001           | 0.58        | 0/1350           |
| 33  | 6     | 0.40         | 0/531            | 0.54        | 0/709            |
| 34  | a     | 0.26         | 7/36725 (0.0%)   | 0.71        | 10/57285 (0.0%)  |
| 35  | b     | 0.37         | 0/1735           | 0.54        | 0/2338           |
| 36  | c     | 0.36         | 0/1651           | 0.59        | 0/2225           |
| 37  | d     | 0.40         | 0/1665           | 0.61        | 0/2227           |
| 38  | e     | 0.35         | 0/1180           | 0.61        | 0/1587           |
| 39  | f     | 0.36         | 0/835            | 0.59        | 0/1128           |
| 40  | g     | 0.36         | 0/1195           | 0.60        | 0/1602           |
| 41  | h     | 0.34         | 0/989            | 0.61        | 0/1326           |
| 42  | i     | 0.38         | 0/1034           | 0.69        | 0/1375           |
| 43  | j     | 0.36         | 0/796            | 0.65        | 0/1077           |
| 44  | k     | 0.36         | 0/885            | 0.60        | 0/1195           |
| 45  | l     | 0.37         | 0/954            | 0.67        | 0/1282           |
| 46  | m     | 0.36         | 0/900            | 0.64        | 0/1204           |
| 47  | n     | 0.37         | 0/822            | 0.66        | 0/1095           |
| 48  | o     | 0.35         | 0/722            | 0.61        | 0/964            |
| 49  | p     | 0.38         | 0/659            | 0.58        | 0/884            |
| 50  | q     | 0.37         | 0/657            | 0.65        | 0/881            |
| 51  | r     | 0.40         | 0/544            | 0.61        | 0/731            |
| 52  | s     | 0.37         | 0/652            | 0.62        | 0/877            |
| 53  | t     | 0.36         | 0/671            | 0.61        | 0/888            |
| 54  | u     | 0.45         | 0/550            | 0.75        | 0/728            |
| 55  | v     | 0.33         | 1/1747 (0.1%)    | 0.68        | 0/2721           |
| 55  | w     | 0.34         | 1/1747 (0.1%)    | 0.96        | 4/2721 (0.1%)    |
| 56  | x     | 0.23         | 0/280            | 0.73        | 0/433            |
| 57  | y     | 0.33         | 1/1607 (0.1%)    | 0.68        | 0/2501           |
| 58  | z     | 0.37         | 0/3086           | 0.56        | 0/4175           |
| All | All   | 0.30         | 12/164181 (0.0%) | 0.69        | 30/245149 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | A     | 0                   | 1                   |
| 34  | a     | 0                   | 2                   |
| All | All   | 0                   | 3                   |

All (12) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 55  | v     | 0   | C    | OP3-P | -10.16 | 1.49        | 1.61     |
| 2   | B     | 1   | U    | OP3-P | -10.16 | 1.49        | 1.61     |
| 1   | A     | 1   | G    | OP3-P | -10.15 | 1.49        | 1.61     |
| 55  | w     | 1   | C    | OP3-P | -10.12 | 1.49        | 1.61     |
| 57  | y     | 1   | G    | OP3-P | -10.07 | 1.49        | 1.61     |
| 34  | a     | 141 | G    | C2-N2 | -6.71  | 1.27        | 1.34     |
| 34  | a     | 222 | C    | C4-N4 | -6.31  | 1.28        | 1.33     |
| 34  | a     | 141 | G    | N1-C2 | -6.20  | 1.32        | 1.37     |
| 34  | a     | 222 | C    | N3-C4 | -5.32  | 1.30        | 1.33     |
| 34  | a     | 222 | C    | N1-C2 | 5.26   | 1.45        | 1.40     |
| 34  | a     | 141 | G    | C6-N1 | -5.15  | 1.35        | 1.39     |
| 34  | a     | 141 | G    | C5-C6 | 5.05   | 1.47        | 1.42     |

All (30) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 55  | w     | 117  | U    | P-O3'-C3'   | 28.03 | 153.34      | 119.70   |
| 55  | w     | 117  | U    | O3'-P-O5'   | 18.55 | 139.25      | 104.00   |
| 55  | w     | 117  | U    | OP1-P-O3'   | -9.49 | 84.33       | 105.20   |
| 34  | a     | 222  | C    | N1-C2-O2    | 8.24  | 123.84      | 118.90   |
| 1   | A     | 1484 | U    | N1-C1'-C2'  | 8.16  | 124.61      | 114.00   |
| 1   | A     | 2407 | A    | C2'-C3'-O3' | 7.93  | 126.94      | 109.50   |
| 34  | a     | 222  | C    | C2-N1-C1'   | 6.92  | 126.41      | 118.80   |
| 34  | a     | 1399 | C    | C2'-C3'-O3' | 6.86  | 124.67      | 113.70   |
| 34  | a     | 141  | G    | O4'-C1'-N9  | 6.84  | 113.67      | 108.20   |
| 34  | a     | 141  | G    | C5-C6-O6    | 6.66  | 132.59      | 128.60   |
| 34  | a     | 1305 | G    | C2'-C3'-O3' | 6.60  | 124.27      | 113.70   |
| 1   | A     | 1051 | G    | N9-C1'-C2'  | 6.28  | 122.17      | 114.00   |
| 34  | a     | 384  | G    | N9-C1'-C2'  | 6.14  | 121.98      | 114.00   |
| 1   | A     | 242  | G    | C2'-C3'-O3' | 6.14  | 123.52      | 113.70   |
| 1   | A     | 614  | A    | C4'-C3'-O3' | -5.96 | 96.89       | 109.40   |
| 1   | A     | 1022 | G    | C2'-C3'-O3' | 5.96  | 123.23      | 113.70   |
| 1   | A     | 2475 | C    | N1-C1'-C2'  | 5.69  | 121.40      | 114.00   |
| 1   | A     | 2391 | G    | C4'-C3'-O3' | 5.59  | 124.17      | 113.00   |
| 34  | a     | 222  | C    | C6-N1-C1'   | -5.51 | 114.18      | 120.80   |
| 34  | a     | 1448 | C    | N1-C1'-C2'  | 5.32  | 120.92      | 114.00   |
| 1   | A     | 1475 | G    | C2'-C3'-O3' | 5.28  | 122.15      | 113.70   |
| 1   | A     | 301  | G    | C4'-C3'-O3' | 5.28  | 123.55      | 113.00   |
| 1   | A     | 1050 | A    | C2'-C3'-O3' | 5.27  | 122.14      | 113.70   |
| 1   | A     | 1536 | C    | C2'-C3'-O3' | 5.22  | 122.06      | 113.70   |
| 34  | a     | 1432 | G    | C2'-C3'-O3' | 5.18  | 121.99      | 113.70   |
| 1   | A     | 710  | U    | C2'-C3'-O3' | 5.14  | 121.93      | 113.70   |
| 55  | w     | 17   | C    | P-O3'-C3'   | 5.14  | 125.87      | 119.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | A     | 614  | A    | O4'-C1'-N9  | -5.08 | 104.14      | 108.20   |
| 1   | A     | 1126 | A    | N9-C1'-C2'  | 5.07  | 120.58      | 114.00   |
| 1   | A     | 204  | A    | C4'-C3'-O3' | 5.06  | 123.12      | 113.00   |

There are no chirality outliers.

All (3) planarity outliers are listed below:

| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 1   | A     | 1054 | A    | Sidechain |
| 34  | a     | 141  | G    | Sidechain |
| 34  | a     | 222  | C    | Sidechain |

## 5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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 |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 3   | C     | 269/271 (99%) | 239 (89%) | 27 (10%) | 3 (1%)   | 14          | 50  |
| 4   | D     | 206/208 (99%) | 190 (92%) | 15 (7%)  | 1 (0%)   | 29          | 68  |
| 5   | E     | 198/200 (99%) | 178 (90%) | 18 (9%)  | 2 (1%)   | 15          | 53  |
| 6   | F     | 175/177 (99%) | 157 (90%) | 16 (9%)  | 2 (1%)   | 14          | 50  |
| 7   | G     | 172/174 (99%) | 158 (92%) | 14 (8%)  | 0        | 100         | 100 |
| 8   | H     | 147/149 (99%) | 128 (87%) | 15 (10%) | 4 (3%)   | 5           | 26  |
| 9   | I     | 139/141 (99%) | 109 (78%) | 23 (16%) | 7 (5%)   | 2           | 12  |
| 10  | J     | 139/141 (99%) | 130 (94%) | 8 (6%)   | 1 (1%)   | 22          | 60  |
| 11  | K     | 120/122 (98%) | 106 (88%) | 10 (8%)  | 4 (3%)   | 4           | 21  |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 12  | L     | 141/143 (99%) | 117 (83%) | 18 (13%) | 6 (4%)   | 2           | 15  |
| 13  | M     | 134/136 (98%) | 128 (96%) | 5 (4%)   | 1 (1%)   | 22          | 60  |
| 14  | N     | 117/119 (98%) | 101 (86%) | 14 (12%) | 2 (2%)   | 9           | 39  |
| 15  | O     | 114/116 (98%) | 105 (92%) | 8 (7%)   | 1 (1%)   | 17          | 55  |
| 16  | P     | 112/114 (98%) | 99 (88%)  | 12 (11%) | 1 (1%)   | 17          | 55  |
| 17  | Q     | 113/115 (98%) | 111 (98%) | 2 (2%)   | 0        | 100         | 100 |
| 18  | R     | 100/102 (98%) | 85 (85%)  | 12 (12%) | 3 (3%)   | 4           | 24  |
| 19  | S     | 107/109 (98%) | 100 (94%) | 6 (6%)   | 1 (1%)   | 17          | 55  |
| 20  | T     | 90/92 (98%)   | 81 (90%)  | 7 (8%)   | 2 (2%)   | 6           | 31  |
| 21  | U     | 100/102 (98%) | 87 (87%)  | 9 (9%)   | 4 (4%)   | 3           | 17  |
| 22  | V     | 90/92 (98%)   | 86 (96%)  | 3 (3%)   | 1 (1%)   | 14          | 50  |
| 23  | W     | 73/75 (97%)   | 68 (93%)  | 5 (7%)   | 0        | 100         | 100 |
| 24  | X     | 75/77 (97%)   | 69 (92%)  | 6 (8%)   | 0        | 100         | 100 |
| 25  | Y     | 58/60 (97%)   | 54 (93%)  | 3 (5%)   | 1 (2%)   | 9           | 39  |
| 26  | Z     | 54/56 (96%)   | 51 (94%)  | 3 (6%)   | 0        | 100         | 100 |
| 27  | 0     | 53/55 (96%)   | 44 (83%)  | 8 (15%)  | 1 (2%)   | 8           | 36  |
| 28  | 1     | 49/51 (96%)   | 43 (88%)  | 6 (12%)  | 0        | 100         | 100 |
| 29  | 2     | 43/45 (96%)   | 40 (93%)  | 2 (5%)   | 1 (2%)   | 6           | 30  |
| 30  | 3     | 62/64 (97%)   | 59 (95%)  | 3 (5%)   | 0        | 100         | 100 |
| 31  | 4     | 36/38 (95%)   | 31 (86%)  | 5 (14%)  | 0        | 100         | 100 |
| 32  | 5     | 129/131 (98%) | 99 (77%)  | 21 (16%) | 9 (7%)   | 1           | 6   |
| 33  | 6     | 64/66 (97%)   | 58 (91%)  | 4 (6%)   | 2 (3%)   | 4           | 23  |
| 35  | b     | 216/218 (99%) | 186 (86%) | 25 (12%) | 5 (2%)   | 6           | 30  |
| 36  | c     | 204/206 (99%) | 183 (90%) | 15 (7%)  | 6 (3%)   | 4           | 24  |
| 37  | d     | 203/205 (99%) | 183 (90%) | 17 (8%)  | 3 (2%)   | 10          | 42  |
| 38  | e     | 156/157 (99%) | 133 (85%) | 21 (14%) | 2 (1%)   | 12          | 45  |
| 39  | f     | 98/100 (98%)  | 85 (87%)  | 9 (9%)   | 4 (4%)   | 3           | 16  |
| 40  | g     | 149/151 (99%) | 131 (88%) | 11 (7%)  | 7 (5%)   | 2           | 14  |
| 41  | h     | 127/129 (98%) | 116 (91%) | 11 (9%)  | 0        | 100         | 100 |
| 42  | i     | 125/127 (98%) | 97 (78%)  | 24 (19%) | 4 (3%)   | 4           | 22  |
| 43  | j     | 96/98 (98%)   | 73 (76%)  | 18 (19%) | 5 (5%)   | 2           | 12  |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 44  | k     | 114/116 (98%)   | 97 (85%)   | 11 (10%) | 6 (5%)   | 2           | 11  |
| 45  | l     | 119/121 (98%)   | 93 (78%)   | 19 (16%) | 7 (6%)   | 1           | 9   |
| 46  | m     | 113/115 (98%)   | 102 (90%)  | 9 (8%)   | 2 (2%)   | 8           | 37  |
| 47  | n     | 99/101 (98%)    | 84 (85%)   | 10 (10%) | 5 (5%)   | 2           | 12  |
| 48  | o     | 86/88 (98%)     | 79 (92%)   | 4 (5%)   | 3 (4%)   | 3           | 20  |
| 49  | p     | 80/82 (98%)     | 70 (88%)   | 8 (10%)  | 2 (2%)   | 5           | 28  |
| 50  | q     | 78/80 (98%)     | 67 (86%)   | 7 (9%)   | 4 (5%)   | 2           | 12  |
| 51  | r     | 63/65 (97%)     | 54 (86%)   | 6 (10%)  | 3 (5%)   | 2           | 13  |
| 52  | s     | 77/79 (98%)     | 67 (87%)   | 10 (13%) | 0        | 100         | 100 |
| 53  | t     | 83/85 (98%)     | 77 (93%)   | 4 (5%)   | 2 (2%)   | 6           | 29  |
| 54  | u     | 63/65 (97%)     | 41 (65%)   | 12 (19%) | 10 (16%) | 0           | 1   |
| 58  | z     | 391/393 (100%)  | 357 (91%)  | 22 (6%)  | 12 (3%)  | 4           | 23  |
| All | All   | 6219/6322 (98%) | 5486 (88%) | 581 (9%) | 152 (2%) | 9           | 29  |

All (152) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | C     | 70  | LYS  |
| 5   | E     | 83  | VAL  |
| 6   | F     | 11  | VAL  |
| 11  | K     | 89  | ASN  |
| 16  | P     | 65  | ASN  |
| 32  | 5     | 123 | ILE  |
| 36  | c     | 96  | VAL  |
| 36  | c     | 156 | LEU  |
| 42  | i     | 90  | ASP  |
| 43  | j     | 57  | VAL  |
| 44  | k     | 88  | PRO  |
| 44  | k     | 94  | SER  |
| 53  | t     | 39  | GLU  |
| 54  | u     | 13  | VAL  |
| 54  | u     | 14  | ALA  |
| 54  | u     | 37  | TYR  |
| 5   | E     | 8   | ALA  |
| 8   | H     | 3   | VAL  |
| 8   | H     | 122 | LEU  |
| 9   | I     | 7   | TYR  |
| 9   | I     | 38  | CYS  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 10         | J            | 81         | ILE         |
| 12         | L            | 92         | LEU         |
| 14         | N            | 117        | ASP         |
| 15         | O            | 66         | GLY         |
| 18         | R            | 54         | VAL         |
| 18         | R            | 55         | ASP         |
| 20         | T            | 37         | ASP         |
| 32         | 5            | 60         | LEU         |
| 38         | e            | 77         | ASN         |
| 40         | g            | 20         | GLU         |
| 40         | g            | 64         | ALA         |
| 40         | g            | 129        | ASN         |
| 42         | i            | 57         | VAL         |
| 42         | i            | 108        | ARG         |
| 43         | j            | 29         | ALA         |
| 44         | k            | 51         | PHE         |
| 44         | k            | 103        | GLY         |
| 45         | l            | 75         | GLU         |
| 46         | m            | 7          | ASN         |
| 47         | n            | 22         | LYS         |
| 47         | n            | 55         | SER         |
| 47         | n            | 90         | ARG         |
| 48         | o            | 2          | LEU         |
| 51         | r            | 10         | CYS         |
| 51         | r            | 17         | VAL         |
| 54         | u            | 9          | GLU         |
| 54         | u            | 30         | GLU         |
| 58         | z            | 161        | ASP         |
| 8          | H            | 15         | LEU         |
| 8          | H            | 41         | LYS         |
| 9          | I            | 6          | ALA         |
| 9          | I            | 64         | ARG         |
| 11         | K            | 110        | GLU         |
| 13         | M            | 69         | PRO         |
| 14         | N            | 59         | SER         |
| 22         | V            | 58         | SER         |
| 25         | Y            | 24         | GLU         |
| 27         | 0            | 2          | VAL         |
| 32         | 5            | 48         | ALA         |
| 32         | 5            | 88         | HIS         |
| 33         | 6            | 4          | ASP         |
| 35         | b            | 63         | LYS         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 35         | b            | 73         | ARG         |
| 36         | c            | 95         | GLY         |
| 37         | d            | 191        | SER         |
| 39         | f            | 33         | GLU         |
| 42         | i            | 124        | PRO         |
| 44         | k            | 118        | ASN         |
| 45         | l            | 42         | LYS         |
| 45         | l            | 88         | ASP         |
| 47         | n            | 2          | LYS         |
| 47         | n            | 38         | ASP         |
| 50         | q            | 17         | GLU         |
| 51         | r            | 46         | THR         |
| 54         | u            | 11         | PHE         |
| 58         | z            | 249        | GLU         |
| 3          | C            | 150        | GLY         |
| 4          | D            | 149        | ASN         |
| 6          | F            | 20         | ASN         |
| 9          | I            | 10         | LEU         |
| 12         | L            | 15         | ALA         |
| 12         | L            | 29         | LYS         |
| 12         | L            | 31         | GLY         |
| 18         | R            | 43         | ASN         |
| 20         | T            | 38         | ALA         |
| 21         | U            | 6          | ARG         |
| 21         | U            | 97         | SER         |
| 32         | 5            | 118        | ILE         |
| 35         | b            | 151        | LYS         |
| 36         | c            | 147        | GLY         |
| 37         | d            | 166        | LYS         |
| 38         | e            | 93         | VAL         |
| 39         | f            | 63         | ASN         |
| 40         | g            | 18         | GLY         |
| 40         | g            | 19         | SER         |
| 40         | g            | 112        | ASP         |
| 43         | j            | 35         | GLN         |
| 44         | k            | 13         | LYS         |
| 45         | l            | 46         | SER         |
| 48         | o            | 13         | GLU         |
| 50         | q            | 49         | ASN         |
| 50         | q            | 69         | THR         |
| 50         | q            | 79         | GLU         |
| 58         | z            | 332        | PHE         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 9          | I            | 92         | PRO         |
| 11         | K            | 35         | VAL         |
| 19         | S            | 65         | ASP         |
| 29         | 2            | 2          | LYS         |
| 32         | 5            | 55         | VAL         |
| 32         | 5            | 113        | PHE         |
| 35         | b            | 11         | ALA         |
| 35         | b            | 192        | PRO         |
| 36         | c            | 144        | GLY         |
| 37         | d            | 34         | GLU         |
| 39         | f            | 92         | THR         |
| 40         | g            | 56         | SER         |
| 45         | l            | 33         | CYS         |
| 45         | l            | 77         | SER         |
| 48         | o            | 45         | HIS         |
| 49         | p            | 64         | GLY         |
| 53         | t            | 44         | ALA         |
| 54         | u            | 12         | ASP         |
| 54         | u            | 36         | PHE         |
| 54         | u            | 65         | ARG         |
| 58         | z            | 9          | LYS         |
| 58         | z            | 82         | PRO         |
| 58         | z            | 126        | GLY         |
| 58         | z            | 137        | CYS         |
| 58         | z            | 180        | GLY         |
| 12         | L            | 115        | GLU         |
| 21         | U            | 75         | ALA         |
| 32         | 5            | 22         | ALA         |
| 32         | 5            | 108        | VAL         |
| 39         | f            | 56         | LYS         |
| 43         | j            | 6          | ILE         |
| 43         | j            | 75         | ASP         |
| 45         | l            | 2          | THR         |
| 46         | m            | 102        | LYS         |
| 49         | p            | 49         | GLY         |
| 54         | u            | 24         | LYS         |
| 58         | z            | 2          | LYS         |
| 58         | z            | 207        | ASP         |
| 58         | z            | 248        | LYS         |
| 11         | K            | 93         | GLN         |
| 12         | L            | 85         | VAL         |
| 36         | c            | 148        | ILE         |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | C     | 168 | GLY  |
| 58  | z     | 52  | ALA  |
| 9   | I     | 12  | VAL  |
| 21  | U     | 38  | ILE  |
| 33  | 6     | 55  | GLY  |

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

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

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

| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |     |
|-----|-------|----------------|-----------|----------|-------------|-----|
| 3   | C     | 216/216 (100%) | 207 (96%) | 9 (4%)   | 30          | 66  |
| 4   | D     | 163/163 (100%) | 154 (94%) | 9 (6%)   | 21          | 57  |
| 5   | E     | 164/164 (100%) | 154 (94%) | 10 (6%)  | 18          | 53  |
| 6   | F     | 148/148 (100%) | 145 (98%) | 3 (2%)   | 55          | 83  |
| 7   | G     | 135/135 (100%) | 133 (98%) | 2 (2%)   | 65          | 87  |
| 8   | H     | 114/114 (100%) | 108 (95%) | 6 (5%)   | 22          | 58  |
| 9   | I     | 109/109 (100%) | 104 (95%) | 5 (5%)   | 27          | 64  |
| 10  | J     | 115/115 (100%) | 113 (98%) | 2 (2%)   | 60          | 85  |
| 11  | K     | 103/103 (100%) | 100 (97%) | 3 (3%)   | 42          | 76  |
| 12  | L     | 102/102 (100%) | 93 (91%)  | 9 (9%)   | 10          | 36  |
| 13  | M     | 109/109 (100%) | 106 (97%) | 3 (3%)   | 43          | 77  |
| 14  | N     | 99/99 (100%)   | 95 (96%)  | 4 (4%)   | 31          | 68  |
| 15  | O     | 86/86 (100%)   | 86 (100%) | 0        | 100         | 100 |
| 16  | P     | 99/99 (100%)   | 98 (99%)  | 1 (1%)   | 76          | 91  |
| 17  | Q     | 88/88 (100%)   | 85 (97%)  | 3 (3%)   | 37          | 72  |
| 18  | R     | 84/84 (100%)   | 82 (98%)  | 2 (2%)   | 49          | 79  |
| 19  | S     | 92/92 (100%)   | 91 (99%)  | 1 (1%)   | 73          | 90  |
| 20  | T     | 79/79 (100%)   | 76 (96%)  | 3 (4%)   | 33          | 69  |
| 21  | U     | 83/83 (100%)   | 81 (98%)  | 2 (2%)   | 49          | 79  |
| 22  | V     | 77/77 (100%)   | 76 (99%)  | 1 (1%)   | 69          | 89  |

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| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |     |
|-----|-------|----------------|-----------|----------|-------------|-----|
| 23  | W     | 57/57 (100%)   | 55 (96%)  | 2 (4%)   | 36          | 71  |
| 24  | X     | 67/67 (100%)   | 66 (98%)  | 1 (2%)   | 65          | 87  |
| 25  | Y     | 55/55 (100%)   | 54 (98%)  | 1 (2%)   | 59          | 85  |
| 26  | Z     | 47/47 (100%)   | 47 (100%) | 0        | 100         | 100 |
| 27  | 0     | 46/46 (100%)   | 45 (98%)  | 1 (2%)   | 52          | 81  |
| 28  | 1     | 46/46 (100%)   | 46 (100%) | 0        | 100         | 100 |
| 29  | 2     | 37/37 (100%)   | 36 (97%)  | 1 (3%)   | 44          | 77  |
| 30  | 3     | 51/51 (100%)   | 49 (96%)  | 2 (4%)   | 32          | 69  |
| 31  | 4     | 34/34 (100%)   | 34 (100%) | 0        | 100         | 100 |
| 32  | 5     | 100/100 (100%) | 99 (99%)  | 1 (1%)   | 76          | 91  |
| 33  | 6     | 59/59 (100%)   | 58 (98%)  | 1 (2%)   | 60          | 85  |
| 35  | b     | 180/180 (100%) | 177 (98%) | 3 (2%)   | 60          | 85  |
| 36  | c     | 170/170 (100%) | 168 (99%) | 2 (1%)   | 71          | 90  |
| 37  | d     | 172/172 (100%) | 169 (98%) | 3 (2%)   | 60          | 85  |
| 38  | e     | 120/119 (101%) | 115 (96%) | 5 (4%)   | 30          | 66  |
| 39  | f     | 87/87 (100%)   | 84 (97%)  | 3 (3%)   | 37          | 72  |
| 40  | g     | 124/124 (100%) | 119 (96%) | 5 (4%)   | 31          | 68  |
| 41  | h     | 104/104 (100%) | 102 (98%) | 2 (2%)   | 57          | 84  |
| 42  | i     | 105/105 (100%) | 101 (96%) | 4 (4%)   | 33          | 69  |
| 43  | j     | 86/86 (100%)   | 85 (99%)  | 1 (1%)   | 71          | 90  |
| 44  | k     | 89/89 (100%)   | 87 (98%)  | 2 (2%)   | 52          | 81  |
| 45  | l     | 102/102 (100%) | 99 (97%)  | 3 (3%)   | 42          | 76  |
| 46  | m     | 93/93 (100%)   | 91 (98%)  | 2 (2%)   | 52          | 81  |
| 47  | n     | 83/83 (100%)   | 82 (99%)  | 1 (1%)   | 71          | 90  |
| 48  | o     | 76/76 (100%)   | 74 (97%)  | 2 (3%)   | 46          | 78  |
| 49  | p     | 65/65 (100%)   | 63 (97%)  | 2 (3%)   | 40          | 75  |
| 50  | q     | 74/74 (100%)   | 72 (97%)  | 2 (3%)   | 44          | 77  |
| 51  | r     | 56/56 (100%)   | 50 (89%)  | 6 (11%)  | 6           | 26  |
| 52  | s     | 70/70 (100%)   | 68 (97%)  | 2 (3%)   | 42          | 76  |
| 53  | t     | 65/65 (100%)   | 63 (97%)  | 2 (3%)   | 40          | 75  |
| 54  | u     | 55/55 (100%)   | 53 (96%)  | 2 (4%)   | 35          | 70  |

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| Mol | Chain | Analysed         | Rotameric  | Outliers | Percentiles |    |
|-----|-------|------------------|------------|----------|-------------|----|
| 58  | z     | 325/325 (100%)   | 323 (99%)  | 2 (1%)   | 86          | 95 |
| All | All   | 5165/5164 (100%) | 5021 (97%) | 144 (3%) | 46          | 77 |

All (144) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | C     | 35  | LYS  |
| 3   | C     | 42  | ARG  |
| 3   | C     | 69  | ASN  |
| 3   | C     | 101 | ARG  |
| 3   | C     | 104 | LEU  |
| 3   | C     | 110 | LYS  |
| 3   | C     | 200 | MET  |
| 3   | C     | 212 | TRP  |
| 3   | C     | 263 | ASP  |
| 4   | D     | 12  | THR  |
| 4   | D     | 30  | GLU  |
| 4   | D     | 33  | ARG  |
| 4   | D     | 39  | ASP  |
| 4   | D     | 51  | THR  |
| 4   | D     | 55  | LYS  |
| 4   | D     | 151 | THR  |
| 4   | D     | 189 | VAL  |
| 4   | D     | 204 | LYS  |
| 5   | E     | 2   | GLU  |
| 5   | E     | 57  | LYS  |
| 5   | E     | 69  | ARG  |
| 5   | E     | 117 | ARG  |
| 5   | E     | 136 | GLN  |
| 5   | E     | 139 | LYS  |
| 5   | E     | 144 | GLU  |
| 5   | E     | 158 | PHE  |
| 5   | E     | 165 | HIS  |
| 5   | E     | 188 | MET  |
| 6   | F     | 11  | VAL  |
| 6   | F     | 67  | THR  |
| 6   | F     | 114 | ARG  |
| 7   | G     | 94  | ARG  |
| 7   | G     | 169 | ARG  |
| 8   | H     | 17  | ASP  |
| 8   | H     | 77  | THR  |
| 8   | H     | 96  | THR  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 8          | H            | 122        | LEU         |
| 8          | H            | 134        | VAL         |
| 8          | H            | 145        | ASN         |
| 9          | I            | 9          | LYS         |
| 9          | I            | 12         | VAL         |
| 9          | I            | 30         | GLN         |
| 9          | I            | 67         | THR         |
| 9          | I            | 134        | SER         |
| 10         | J            | 12         | LYS         |
| 10         | J            | 138        | GLN         |
| 11         | K            | 31         | ARG         |
| 11         | K            | 58         | LEU         |
| 11         | K            | 61         | VAL         |
| 12         | L            | 1          | MET         |
| 12         | L            | 2          | ARG         |
| 12         | L            | 3          | LEU         |
| 12         | L            | 14         | LYS         |
| 12         | L            | 41         | ARG         |
| 12         | L            | 60         | ARG         |
| 12         | L            | 63         | LYS         |
| 12         | L            | 92         | LEU         |
| 12         | L            | 125        | LEU         |
| 13         | M            | 6          | ARG         |
| 13         | M            | 40         | ARG         |
| 13         | M            | 100        | LYS         |
| 14         | N            | 34         | ILE         |
| 14         | N            | 46         | ARG         |
| 14         | N            | 117        | ASP         |
| 14         | N            | 118        | ARG         |
| 16         | P            | 67         | GLU         |
| 17         | Q            | 8          | ILE         |
| 17         | Q            | 40         | LYS         |
| 17         | Q            | 101        | ASP         |
| 18         | R            | 66         | HIS         |
| 18         | R            | 73         | LYS         |
| 19         | S            | 29         | VAL         |
| 20         | T            | 69         | ARG         |
| 20         | T            | 76         | ARG         |
| 20         | T            | 91         | GLN         |
| 21         | U            | 65         | GLN         |
| 21         | U            | 73         | ASN         |
| 22         | V            | 42         | LEU         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 23         | W            | 8          | ASN         |
| 23         | W            | 16         | ARG         |
| 24         | X            | 59         | ASP         |
| 25         | Y            | 2          | LYS         |
| 27         | 0            | 45         | ASP         |
| 29         | 2            | 22         | MET         |
| 30         | 3            | 53         | ASP         |
| 30         | 3            | 61         | LEU         |
| 32         | 5            | 29         | ASP         |
| 33         | 6            | 37         | CYS         |
| 35         | b            | 21         | TYR         |
| 35         | b            | 99         | MET         |
| 35         | b            | 122        | ASP         |
| 36         | c            | 138        | GLN         |
| 36         | c            | 174        | LEU         |
| 37         | d            | 33         | ILE         |
| 37         | d            | 140        | ASP         |
| 37         | d            | 158        | LEU         |
| 38         | e            | 11         | GLN         |
| 38         | e            | 45         | VAL         |
| 38         | e            | 121        | ASN         |
| 38         | e            | 136        | VAL         |
| 38         | e            | 141        | ASP         |
| 39         | f            | 38         | ARG         |
| 39         | f            | 39         | LEU         |
| 39         | f            | 91         | ARG         |
| 40         | g            | 2          | ARG         |
| 40         | g            | 11         | ILE         |
| 40         | g            | 76         | SER         |
| 40         | g            | 89         | GLU         |
| 40         | g            | 147        | ASN         |
| 41         | h            | 111        | THR         |
| 41         | h            | 120        | LEU         |
| 42         | i            | 41         | GLU         |
| 42         | i            | 42         | THR         |
| 42         | i            | 65         | THR         |
| 42         | i            | 108        | ARG         |
| 43         | j            | 45         | ARG         |
| 44         | k            | 28         | ASN         |
| 44         | k            | 126        | ARG         |
| 45         | l            | 38         | THR         |
| 45         | l            | 77         | SER         |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 45  | l     | 93  | ARG  |
| 46  | m     | 13  | HIS  |
| 46  | m     | 89  | ARG  |
| 47  | n     | 17  | ASP  |
| 48  | o     | 17  | ASP  |
| 48  | o     | 88  | ARG  |
| 49  | p     | 31  | ARG  |
| 49  | p     | 34  | GLU  |
| 50  | q     | 3   | LYS  |
| 50  | q     | 52  | CYS  |
| 51  | r     | 9   | PHE  |
| 51  | r     | 11  | ARG  |
| 51  | r     | 13  | THR  |
| 51  | r     | 27  | THR  |
| 51  | r     | 41  | SER  |
| 51  | r     | 42  | ARG  |
| 52  | s     | 5   | LYS  |
| 52  | s     | 6   | LYS  |
| 53  | t     | 7   | LYS  |
| 53  | t     | 42  | ASP  |
| 54  | u     | 32  | ARG  |
| 54  | u     | 62  | GLU  |
| 58  | z     | 22  | HIS  |
| 58  | z     | 181 | ASP  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | C     | 59  | GLN  |
| 7   | G     | 37  | ASN  |
| 7   | G     | 103 | ASN  |
| 8   | H     | 18  | GLN  |
| 9   | I     | 42  | ASN  |
| 18  | R     | 11  | GLN  |
| 21  | U     | 65  | GLN  |
| 32  | 5     | 4   | ASN  |
| 35  | b     | 18  | GLN  |
| 37  | d     | 151 | GLN  |
| 39  | f     | 63  | ASN  |
| 44  | k     | 39  | ASN  |
| 48  | o     | 27  | GLN  |
| 53  | t     | 69  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 58  | z     | 135 | ASN  |

### 5.3.3 RNA [i](#)

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1   | A     | 2893/2903 (99%) | 815 (28%)         | 91 (3%)         |
| 2   | B     | 119/120 (99%)   | 44 (36%)          | 7 (5%)          |
| 34  | a     | 1536/1540 (99%) | 492 (32%)         | 0               |
| 55  | v     | 76/77 (98%)     | 23 (30%)          | 0               |
| 55  | w     | 76/77 (98%)     | 33 (43%)          | 0               |
| 56  | x     | 11/12 (91%)     | 4 (36%)           | 0               |
| 57  | y     | 74/76 (97%)     | 30 (40%)          | 0               |
| All | All   | 4785/4805 (99%) | 1441 (30%)        | 98 (2%)         |

All (1441) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 2   | G    |
| 1   | A     | 3   | U    |
| 1   | A     | 5   | A    |
| 1   | A     | 10  | A    |
| 1   | A     | 12  | U    |
| 1   | A     | 13  | A    |
| 1   | A     | 15  | G    |
| 1   | A     | 23  | G    |
| 1   | A     | 26  | G    |
| 1   | A     | 34  | U    |
| 1   | A     | 35  | G    |
| 1   | A     | 36  | G    |
| 1   | A     | 45  | G    |
| 1   | A     | 46  | G    |
| 1   | A     | 52  | A    |
| 1   | A     | 60  | G    |
| 1   | A     | 63  | A    |
| 1   | A     | 71  | A    |
| 1   | A     | 74  | A    |
| 1   | A     | 75  | G    |
| 1   | A     | 76  | C    |
| 1   | A     | 80  | G    |
| 1   | A     | 81  | G    |
| 1   | A     | 85  | G    |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 1          | A            | 86         | G           |
| 1          | A            | 96         | C           |
| 1          | A            | 100        | U           |
| 1          | A            | 101        | A           |
| 1          | A            | 102        | U           |
| 1          | A            | 103        | A           |
| 1          | A            | 118        | A           |
| 1          | A            | 119        | A           |
| 1          | A            | 120        | U           |
| 1          | A            | 125        | A           |
| 1          | A            | 126        | A           |
| 1          | A            | 135        | U           |
| 1          | A            | 138        | U           |
| 1          | A            | 139        | U           |
| 1          | A            | 140        | C           |
| 1          | A            | 141        | G           |
| 1          | A            | 146        | A           |
| 1          | A            | 147        | C           |
| 1          | A            | 148        | U           |
| 1          | A            | 149        | A           |
| 1          | A            | 157        | C           |
| 1          | A            | 158        | U           |
| 1          | A            | 159        | G           |
| 1          | A            | 160        | A           |
| 1          | A            | 161        | A           |
| 1          | A            | 162        | U           |
| 1          | A            | 163        | C           |
| 1          | A            | 166        | U           |
| 1          | A            | 170        | U           |
| 1          | A            | 171        | U           |
| 1          | A            | 181        | A           |
| 1          | A            | 196        | A           |
| 1          | A            | 199        | A           |
| 1          | A            | 205        | G           |
| 1          | A            | 215        | G           |
| 1          | A            | 216        | A           |
| 1          | A            | 219        | A           |
| 1          | A            | 221        | A           |
| 1          | A            | 222        | A           |
| 1          | A            | 228        | C           |
| 1          | A            | 229        | C           |
| 1          | A            | 231        | A           |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 1          | A            | 233        | A           |
| 1          | A            | 242        | G           |
| 1          | A            | 243        | U           |
| 1          | A            | 248        | G           |
| 1          | A            | 249        | C           |
| 1          | A            | 255        | A           |
| 1          | A            | 266        | G           |
| 1          | A            | 267        | C           |
| 1          | A            | 272        | A           |
| 1          | A            | 275        | C           |
| 1          | A            | 276        | U           |
| 1          | A            | 277        | G           |
| 1          | A            | 278        | A           |
| 1          | A            | 280        | U           |
| 1          | A            | 281        | C           |
| 1          | A            | 282        | A           |
| 1          | A            | 283        | G           |
| 1          | A            | 284        | U           |
| 1          | A            | 285        | G           |
| 1          | A            | 287        | G           |
| 1          | A            | 288        | U           |
| 1          | A            | 289        | G           |
| 1          | A            | 291        | G           |
| 1          | A            | 294        | A           |
| 1          | A            | 301        | G           |
| 1          | A            | 302        | C           |
| 1          | A            | 305        | C           |
| 1          | A            | 306        | U           |
| 1          | A            | 311        | A           |
| 1          | A            | 313        | G           |
| 1          | A            | 315        | G           |
| 1          | A            | 317        | G           |
| 1          | A            | 323        | C           |
| 1          | A            | 329        | G           |
| 1          | A            | 330        | A           |
| 1          | A            | 343        | C           |
| 1          | A            | 350        | G           |
| 1          | A            | 351        | C           |
| 1          | A            | 352        | A           |
| 1          | A            | 354        | A           |
| 1          | A            | 357        | C           |
| 1          | A            | 358        | U           |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 1          | A            | 361        | G           |
| 1          | A            | 362        | A           |
| 1          | A            | 365        | U           |
| 1          | A            | 366        | C           |
| 1          | A            | 367        | G           |
| 1          | A            | 368        | A           |
| 1          | A            | 369        | U           |
| 1          | A            | 371        | A           |
| 1          | A            | 372        | G           |
| 1          | A            | 383        | C           |
| 1          | A            | 386        | G           |
| 1          | A            | 387        | U           |
| 1          | A            | 390        | U           |
| 1          | A            | 396        | G           |
| 1          | A            | 404        | A           |
| 1          | A            | 405        | U           |
| 1          | A            | 406        | G           |
| 1          | A            | 411        | G           |
| 1          | A            | 412        | A           |
| 1          | A            | 417        | C           |
| 1          | A            | 420        | C           |
| 1          | A            | 422        | A           |
| 1          | A            | 451        | U           |
| 1          | A            | 455        | C           |
| 1          | A            | 456        | C           |
| 1          | A            | 457        | A           |
| 1          | A            | 459        | U           |
| 1          | A            | 473        | G           |
| 1          | A            | 474        | G           |
| 1          | A            | 479        | A           |
| 1          | A            | 481        | G           |
| 1          | A            | 487        | C           |
| 1          | A            | 491        | G           |
| 1          | A            | 492        | A           |
| 1          | A            | 496        | G           |
| 1          | A            | 503        | A           |
| 1          | A            | 504        | A           |
| 1          | A            | 505        | A           |
| 1          | A            | 509        | C           |
| 1          | A            | 513        | A           |
| 1          | A            | 518        | G           |
| 1          | A            | 526        | A           |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 1          | A            | 527        | C           |
| 1          | A            | 529        | A           |
| 1          | A            | 532        | A           |
| 1          | A            | 533        | G           |
| 1          | A            | 535        | G           |
| 1          | A            | 542        | U           |
| 1          | A            | 543        | G           |
| 1          | A            | 544        | C           |
| 1          | A            | 545        | U           |
| 1          | A            | 546        | U           |
| 1          | A            | 547        | A           |
| 1          | A            | 548        | G           |
| 1          | A            | 549        | G           |
| 1          | A            | 550        | C           |
| 1          | A            | 557        | C           |
| 1          | A            | 563        | A           |
| 1          | A            | 573        | U           |
| 1          | A            | 575        | A           |
| 1          | A            | 586        | A           |
| 1          | A            | 603        | A           |
| 1          | A            | 613        | A           |
| 1          | A            | 614        | A           |
| 1          | A            | 615        | U           |
| 1          | A            | 616        | A           |
| 1          | A            | 622        | G           |
| 1          | A            | 627        | A           |
| 1          | A            | 637        | A           |
| 1          | A            | 640        | C           |
| 1          | A            | 644        | A           |
| 1          | A            | 645        | C           |
| 1          | A            | 646        | U           |
| 1          | A            | 647        | G           |
| 1          | A            | 651        | G           |
| 1          | A            | 652        | U           |
| 1          | A            | 653        | U           |
| 1          | A            | 654        | A           |
| 1          | A            | 655        | A           |
| 1          | A            | 656        | G           |
| 1          | A            | 659        | G           |
| 1          | A            | 661        | A           |
| 1          | A            | 668        | A           |
| 1          | A            | 678        | C           |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 1          | A            | 685        | A           |
| 1          | A            | 686        | U           |
| 1          | A            | 694        | U           |
| 1          | A            | 695        | G           |
| 1          | A            | 696        | G           |
| 1          | A            | 710        | U           |
| 1          | A            | 711        | G           |
| 1          | A            | 713        | G           |
| 1          | A            | 714        | U           |
| 1          | A            | 717        | C           |
| 1          | A            | 730        | A           |
| 1          | A            | 734        | A           |
| 1          | A            | 738        | G           |
| 1          | A            | 747        | 5MC         |
| 1          | A            | 752        | A           |
| 1          | A            | 763        | G           |
| 1          | A            | 765        | C           |
| 1          | A            | 771        | G           |
| 1          | A            | 775        | G           |
| 1          | A            | 776        | G           |
| 1          | A            | 782        | A           |
| 1          | A            | 783        | A           |
| 1          | A            | 784        | G           |
| 1          | A            | 785        | G           |
| 1          | A            | 788        | A           |
| 1          | A            | 805        | G           |
| 1          | A            | 812        | C           |
| 1          | A            | 816        | C           |
| 1          | A            | 819        | A           |
| 1          | A            | 827        | U           |
| 1          | A            | 828        | U           |
| 1          | A            | 830        | G           |
| 1          | A            | 843        | G           |
| 1          | A            | 844        | A           |
| 1          | A            | 845        | A           |
| 1          | A            | 846        | C           |
| 1          | A            | 847        | U           |
| 1          | A            | 858        | G           |
| 1          | A            | 859        | G           |
| 1          | A            | 860        | U           |
| 1          | A            | 866        | A           |
| 1          | A            | 868        | U           |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 1          | A            | 869        | G           |
| 1          | A            | 870        | U           |
| 1          | A            | 872        | U           |
| 1          | A            | 873        | C           |
| 1          | A            | 877        | A           |
| 1          | A            | 878        | A           |
| 1          | A            | 880        | G           |
| 1          | A            | 882        | G           |
| 1          | A            | 892        | A           |
| 1          | A            | 896        | A           |
| 1          | A            | 897        | C           |
| 1          | A            | 899        | A           |
| 1          | A            | 900        | A           |
| 1          | A            | 901        | C           |
| 1          | A            | 903        | C           |
| 1          | A            | 906        | U           |
| 1          | A            | 907        | G           |
| 1          | A            | 909        | A           |
| 1          | A            | 910        | A           |
| 1          | A            | 914        | G           |
| 1          | A            | 915        | C           |
| 1          | A            | 925        | A           |
| 1          | A            | 934        | U           |
| 1          | A            | 935        | C           |
| 1          | A            | 940        | G           |
| 1          | A            | 941        | A           |
| 1          | A            | 946        | C           |
| 1          | A            | 951        | C           |
| 1          | A            | 961        | C           |
| 1          | A            | 968        | C           |
| 1          | A            | 974        | G           |
| 1          | A            | 982        | C           |
| 1          | A            | 983        | A           |
| 1          | A            | 984        | A           |
| 1          | A            | 985        | C           |
| 1          | A            | 989        | G           |
| 1          | A            | 990        | A           |
| 1          | A            | 995        | C           |
| 1          | A            | 996        | A           |
| 1          | A            | 999        | U           |
| 1          | A            | 1003       | G           |
| 1          | A            | 1005       | C           |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 1          | A            | 1009       | A           |
| 1          | A            | 1012       | U           |
| 1          | A            | 1013       | C           |
| 1          | A            | 1019       | U           |
| 1          | A            | 1020       | A           |
| 1          | A            | 1021       | A           |
| 1          | A            | 1022       | G           |
| 1          | A            | 1023       | U           |
| 1          | A            | 1025       | G           |
| 1          | A            | 1026       | G           |
| 1          | A            | 1033       | U           |
| 1          | A            | 1042       | G           |
| 1          | A            | 1043       | C           |
| 1          | A            | 1044       | C           |
| 1          | A            | 1045       | C           |
| 1          | A            | 1046       | A           |
| 1          | A            | 1047       | G           |
| 1          | A            | 1049       | C           |
| 1          | A            | 1050       | A           |
| 1          | A            | 1051       | G           |
| 1          | A            | 1052       | C           |
| 1          | A            | 1053       | C           |
| 1          | A            | 1054       | A           |
| 1          | A            | 1055       | G           |
| 1          | A            | 1057       | A           |
| 1          | A            | 1059       | G           |
| 1          | A            | 1060       | U           |
| 1          | A            | 1061       | U           |
| 1          | A            | 1062       | G           |
| 1          | A            | 1064       | C           |
| 1          | A            | 1065       | U           |
| 1          | A            | 1066       | U           |
| 1          | A            | 1067       | A           |
| 1          | A            | 1068       | G           |
| 1          | A            | 1069       | A           |
| 1          | A            | 1070       | A           |
| 1          | A            | 1071       | G           |
| 1          | A            | 1073       | A           |
| 1          | A            | 1075       | C           |
| 1          | A            | 1076       | C           |
| 1          | A            | 1079       | C           |
| 1          | A            | 1084       | A           |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 1          | A            | 1087       | G           |
| 1          | A            | 1088       | A           |
| 1          | A            | 1090       | A           |
| 1          | A            | 1096       | A           |
| 1          | A            | 1097       | U           |
| 1          | A            | 1101       | U           |
| 1          | A            | 1103       | A           |
| 1          | A            | 1104       | C           |
| 1          | A            | 1105       | U           |
| 1          | A            | 1106       | G           |
| 1          | A            | 1110       | G           |
| 1          | A            | 1112       | G           |
| 1          | A            | 1114       | C           |
| 1          | A            | 1115       | G           |
| 1          | A            | 1116       | G           |
| 1          | A            | 1117       | C           |
| 1          | A            | 1119       | U           |
| 1          | A            | 1121       | C           |
| 1          | A            | 1130       | U           |
| 1          | A            | 1131       | G           |
| 1          | A            | 1132       | U           |
| 1          | A            | 1135       | C           |
| 1          | A            | 1136       | G           |
| 1          | A            | 1139       | G           |
| 1          | A            | 1140       | C           |
| 1          | A            | 1141       | U           |
| 1          | A            | 1142       | A           |
| 1          | A            | 1144       | A           |
| 1          | A            | 1149       | G           |
| 1          | A            | 1151       | A           |
| 1          | A            | 1168       | G           |
| 1          | A            | 1169       | A           |
| 1          | A            | 1171       | G           |
| 1          | A            | 1172       | C           |
| 1          | A            | 1174       | U           |
| 1          | A            | 1175       | A           |
| 1          | A            | 1176       | U           |
| 1          | A            | 1177       | G           |
| 1          | A            | 1178       | C           |
| 1          | A            | 1180       | U           |
| 1          | A            | 1195       | G           |
| 1          | A            | 1203       | U           |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 1          | A            | 1204       | A           |
| 1          | A            | 1205       | A           |
| 1          | A            | 1218       | G           |
| 1          | A            | 1236       | G           |
| 1          | A            | 1248       | G           |
| 1          | A            | 1250       | G           |
| 1          | A            | 1253       | A           |
| 1          | A            | 1256       | G           |
| 1          | A            | 1271       | G           |
| 1          | A            | 1272       | A           |
| 1          | A            | 1273       | U           |
| 1          | A            | 1287       | A           |
| 1          | A            | 1289       | C           |
| 1          | A            | 1300       | G           |
| 1          | A            | 1301       | A           |
| 1          | A            | 1306       | C           |
| 1          | A            | 1321       | A           |
| 1          | A            | 1343       | G           |
| 1          | A            | 1345       | C           |
| 1          | A            | 1346       | G           |
| 1          | A            | 1350       | C           |
| 1          | A            | 1352       | U           |
| 1          | A            | 1353       | A           |
| 1          | A            | 1360       | G           |
| 1          | A            | 1365       | A           |
| 1          | A            | 1368       | G           |
| 1          | A            | 1378       | A           |
| 1          | A            | 1379       | U           |
| 1          | A            | 1386       | C           |
| 1          | A            | 1387       | A           |
| 1          | A            | 1392       | A           |
| 1          | A            | 1395       | A           |
| 1          | A            | 1397       | U           |
| 1          | A            | 1403       | A           |
| 1          | A            | 1407       | G           |
| 1          | A            | 1409       | U           |
| 1          | A            | 1410       | G           |
| 1          | A            | 1416       | G           |
| 1          | A            | 1418       | G           |
| 1          | A            | 1419       | A           |
| 1          | A            | 1420       | A           |
| 1          | A            | 1427       | A           |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 1          | A            | 1428       | C           |
| 1          | A            | 1434       | A           |
| 1          | A            | 1437       | C           |
| 1          | A            | 1451       | C           |
| 1          | A            | 1452       | G           |
| 1          | A            | 1453       | A           |
| 1          | A            | 1456       | G           |
| 1          | A            | 1458       | U           |
| 1          | A            | 1459       | G           |
| 1          | A            | 1461       | C           |
| 1          | A            | 1476       | U           |
| 1          | A            | 1478       | G           |
| 1          | A            | 1479       | G           |
| 1          | A            | 1480       | C           |
| 1          | A            | 1481       | U           |
| 1          | A            | 1482       | G           |
| 1          | A            | 1484       | U           |
| 1          | A            | 1485       | U           |
| 1          | A            | 1490       | A           |
| 1          | A            | 1491       | G           |
| 1          | A            | 1493       | C           |
| 1          | A            | 1494       | A           |
| 1          | A            | 1498       | C           |
| 1          | A            | 1503       | A           |
| 1          | A            | 1504       | A           |
| 1          | A            | 1506       | U           |
| 1          | A            | 1508       | A           |
| 1          | A            | 1509       | A           |
| 1          | A            | 1510       | G           |
| 1          | A            | 1515       | A           |
| 1          | A            | 1519       | G           |
| 1          | A            | 1522       | A           |
| 1          | A            | 1524       | G           |
| 1          | A            | 1528       | A           |
| 1          | A            | 1529       | G           |
| 1          | A            | 1533       | C           |
| 1          | A            | 1535       | A           |
| 1          | A            | 1536       | C           |
| 1          | A            | 1537       | G           |
| 1          | A            | 1538       | G           |
| 1          | A            | 1540       | G           |
| 1          | A            | 1542       | U           |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 1          | A            | 1543       | G           |
| 1          | A            | 1546       | G           |
| 1          | A            | 1555       | G           |
| 1          | A            | 1558       | C           |
| 1          | A            | 1559       | U           |
| 1          | A            | 1566       | A           |
| 1          | A            | 1569       | A           |
| 1          | A            | 1572       | A           |
| 1          | A            | 1578       | U           |
| 1          | A            | 1579       | A           |
| 1          | A            | 1581       | G           |
| 1          | A            | 1582       | C           |
| 1          | A            | 1584       | U           |
| 1          | A            | 1585       | C           |
| 1          | A            | 1589       | U           |
| 1          | A            | 1590       | A           |
| 1          | A            | 1591       | A           |
| 1          | A            | 1607       | C           |
| 1          | A            | 1608       | A           |
| 1          | A            | 1609       | A           |
| 1          | A            | 1610       | A           |
| 1          | A            | 1612       | C           |
| 1          | A            | 1616       | A           |
| 1          | A            | 1617       | C           |
| 1          | A            | 1622       | G           |
| 1          | A            | 1644       | C           |
| 1          | A            | 1647       | U           |
| 1          | A            | 1648       | U           |
| 1          | A            | 1649       | G           |
| 1          | A            | 1651       | G           |
| 1          | A            | 1654       | A           |
| 1          | A            | 1672       | A           |
| 1          | A            | 1674       | G           |
| 1          | A            | 1675       | C           |
| 1          | A            | 1678       | A           |
| 1          | A            | 1679       | A           |
| 1          | A            | 1693       | U           |
| 1          | A            | 1695       | G           |
| 1          | A            | 1703       | G           |
| 1          | A            | 1715       | G           |
| 1          | A            | 1716       | U           |
| 1          | A            | 1717       | A           |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 1          | A            | 1721       | G           |
| 1          | A            | 1722       | A           |
| 1          | A            | 1723       | G           |
| 1          | A            | 1724       | G           |
| 1          | A            | 1725       | C           |
| 1          | A            | 1726       | G           |
| 1          | A            | 1728       | C           |
| 1          | A            | 1729       | U           |
| 1          | A            | 1731       | G           |
| 1          | A            | 1733       | U           |
| 1          | A            | 1734       | C           |
| 1          | A            | 1735       | G           |
| 1          | A            | 1738       | G           |
| 1          | A            | 1739       | A           |
| 1          | A            | 1750       | G           |
| 1          | A            | 1764       | C           |
| 1          | A            | 1773       | A           |
| 1          | A            | 1776       | G           |
| 1          | A            | 1780       | A           |
| 1          | A            | 1782       | U           |
| 1          | A            | 1784       | A           |
| 1          | A            | 1791       | A           |
| 1          | A            | 1800       | C           |
| 1          | A            | 1801       | A           |
| 1          | A            | 1802       | A           |
| 1          | A            | 1808       | A           |
| 1          | A            | 1811       | G           |
| 1          | A            | 1812       | U           |
| 1          | A            | 1816       | C           |
| 1          | A            | 1818       | U           |
| 1          | A            | 1819       | A           |
| 1          | A            | 1839       | G           |
| 1          | A            | 1842       | G           |
| 1          | A            | 1847       | G           |
| 1          | A            | 1853       | A           |
| 1          | A            | 1857       | G           |
| 1          | A            | 1858       | A           |
| 1          | A            | 1863       | G           |
| 1          | A            | 1866       | A           |
| 1          | A            | 1867       | G           |
| 1          | A            | 1870       | C           |
| 1          | A            | 1871       | A           |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 1          | A            | 1872       | A           |
| 1          | A            | 1873       | G           |
| 1          | A            | 1875       | G           |
| 1          | A            | 1876       | A           |
| 1          | A            | 1877       | A           |
| 1          | A            | 1878       | G           |
| 1          | A            | 1881       | C           |
| 1          | A            | 1884       | G           |
| 1          | A            | 1885       | A           |
| 1          | A            | 1890       | A           |
| 1          | A            | 1896       | G           |
| 1          | A            | 1902       | C           |
| 1          | A            | 1905       | C           |
| 1          | A            | 1906       | G           |
| 1          | A            | 1907       | G           |
| 1          | A            | 1913       | A           |
| 1          | A            | 1914       | C           |
| 1          | A            | 1916       | A           |
| 1          | A            | 1927       | A           |
| 1          | A            | 1929       | G           |
| 1          | A            | 1930       | G           |
| 1          | A            | 1936       | A           |
| 1          | A            | 1937       | A           |
| 1          | A            | 1938       | A           |
| 1          | A            | 1939       | 5MU         |
| 1          | A            | 1940       | U           |
| 1          | A            | 1941       | C           |
| 1          | A            | 1942       | C           |
| 1          | A            | 1955       | U           |
| 1          | A            | 1962       | 5MC         |
| 1          | A            | 1964       | G           |
| 1          | A            | 1965       | C           |
| 1          | A            | 1967       | C           |
| 1          | A            | 1970       | A           |
| 1          | A            | 1971       | U           |
| 1          | A            | 1972       | G           |
| 1          | A            | 1982       | U           |
| 1          | A            | 1991       | U           |
| 1          | A            | 1993       | U           |
| 1          | A            | 1997       | C           |
| 1          | A            | 2004       | G           |
| 1          | A            | 2021       | C           |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 1          | A            | 2022       | U           |
| 1          | A            | 2023       | C           |
| 1          | A            | 2027       | G           |
| 1          | A            | 2029       | G           |
| 1          | A            | 2033       | A           |
| 1          | A            | 2036       | C           |
| 1          | A            | 2043       | C           |
| 1          | A            | 2049       | G           |
| 1          | A            | 2051       | A           |
| 1          | A            | 2055       | C           |
| 1          | A            | 2056       | G           |
| 1          | A            | 2059       | A           |
| 1          | A            | 2060       | A           |
| 1          | A            | 2061       | G           |
| 1          | A            | 2062       | A           |
| 1          | A            | 2063       | C           |
| 1          | A            | 2067       | G           |
| 1          | A            | 2069       | 7MG         |
| 1          | A            | 2072       | C           |
| 1          | A            | 2077       | A           |
| 1          | A            | 2080       | A           |
| 1          | A            | 2092       | U           |
| 1          | A            | 2093       | G           |
| 1          | A            | 2095       | A           |
| 1          | A            | 2097       | A           |
| 1          | A            | 2098       | U           |
| 1          | A            | 2099       | U           |
| 1          | A            | 2100       | G           |
| 1          | A            | 2106       | U           |
| 1          | A            | 2108       | A           |
| 1          | A            | 2110       | G           |
| 1          | A            | 2111       | U           |
| 1          | A            | 2112       | G           |
| 1          | A            | 2113       | U           |
| 1          | A            | 2118       | U           |
| 1          | A            | 2119       | A           |
| 1          | A            | 2121       | G           |
| 1          | A            | 2127       | G           |
| 1          | A            | 2131       | U           |
| 1          | A            | 2132       | U           |
| 1          | A            | 2133       | G           |
| 1          | A            | 2134       | A           |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 1          | A            | 2141       | G           |
| 1          | A            | 2145       | C           |
| 1          | A            | 2147       | A           |
| 1          | A            | 2157       | G           |
| 1          | A            | 2162       | G           |
| 1          | A            | 2164       | C           |
| 1          | A            | 2170       | A           |
| 1          | A            | 2172       | U           |
| 1          | A            | 2173       | A           |
| 1          | A            | 2186       | G           |
| 1          | A            | 2189       | U           |
| 1          | A            | 2190       | G           |
| 1          | A            | 2191       | A           |
| 1          | A            | 2192       | U           |
| 1          | A            | 2193       | G           |
| 1          | A            | 2194       | U           |
| 1          | A            | 2198       | A           |
| 1          | A            | 2199       | A           |
| 1          | A            | 2204       | G           |
| 1          | A            | 2211       | A           |
| 1          | A            | 2214       | C           |
| 1          | A            | 2220       | U           |
| 1          | A            | 2223       | G           |
| 1          | A            | 2225       | A           |
| 1          | A            | 2226       | C           |
| 1          | A            | 2238       | G           |
| 1          | A            | 2239       | G           |
| 1          | A            | 2246       | G           |
| 1          | A            | 2263       | C           |
| 1          | A            | 2267       | A           |
| 1          | A            | 2268       | A           |
| 1          | A            | 2278       | A           |
| 1          | A            | 2283       | C           |
| 1          | A            | 2286       | G           |
| 1          | A            | 2287       | A           |
| 1          | A            | 2292       | U           |
| 1          | A            | 2293       | G           |
| 1          | A            | 2295       | C           |
| 1          | A            | 2296       | U           |
| 1          | A            | 2297       | A           |
| 1          | A            | 2302       | U           |
| 1          | A            | 2305       | U           |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 1          | A            | 2307       | G           |
| 1          | A            | 2309       | A           |
| 1          | A            | 2311       | A           |
| 1          | A            | 2315       | G           |
| 1          | A            | 2319       | G           |
| 1          | A            | 2321       | U           |
| 1          | A            | 2322       | A           |
| 1          | A            | 2325       | G           |
| 1          | A            | 2326       | C           |
| 1          | A            | 2327       | A           |
| 1          | A            | 2331       | G           |
| 1          | A            | 2333       | A           |
| 1          | A            | 2336       | A           |
| 1          | A            | 2337       | G           |
| 1          | A            | 2345       | G           |
| 1          | A            | 2347       | C           |
| 1          | A            | 2350       | C           |
| 1          | A            | 2352       | A           |
| 1          | A            | 2357       | G           |
| 1          | A            | 2361       | G           |
| 1          | A            | 2373       | G           |
| 1          | A            | 2377       | A           |
| 1          | A            | 2378       | A           |
| 1          | A            | 2383       | G           |
| 1          | A            | 2385       | C           |
| 1          | A            | 2391       | G           |
| 1          | A            | 2392       | A           |
| 1          | A            | 2396       | G           |
| 1          | A            | 2402       | U           |
| 1          | A            | 2403       | C           |
| 1          | A            | 2404       | U           |
| 1          | A            | 2406       | A           |
| 1          | A            | 2407       | A           |
| 1          | A            | 2408       | U           |
| 1          | A            | 2409       | G           |
| 1          | A            | 2410       | G           |
| 1          | A            | 2414       | G           |
| 1          | A            | 2423       | U           |
| 1          | A            | 2424       | C           |
| 1          | A            | 2429       | G           |
| 1          | A            | 2430       | A           |
| 1          | A            | 2435       | A           |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 1          | A            | 2436       | G           |
| 1          | A            | 2441       | U           |
| 1          | A            | 2445       | 2MG         |
| 1          | A            | 2447       | G           |
| 1          | A            | 2448       | A           |
| 1          | A            | 2459       | A           |
| 1          | A            | 2469       | A           |
| 1          | A            | 2472       | G           |
| 1          | A            | 2473       | U           |
| 1          | A            | 2474       | U           |
| 1          | A            | 2475       | C           |
| 1          | A            | 2476       | A           |
| 1          | A            | 2481       | G           |
| 1          | A            | 2491       | U           |
| 1          | A            | 2492       | U           |
| 1          | A            | 2494       | G           |
| 1          | A            | 2502       | G           |
| 1          | A            | 2504       | PSU         |
| 1          | A            | 2505       | G           |
| 1          | A            | 2506       | U           |
| 1          | A            | 2518       | A           |
| 1          | A            | 2523       | G           |
| 1          | A            | 2529       | G           |
| 1          | A            | 2530       | A           |
| 1          | A            | 2535       | G           |
| 1          | A            | 2547       | A           |
| 1          | A            | 2554       | U           |
| 1          | A            | 2566       | A           |
| 1          | A            | 2567       | G           |
| 1          | A            | 2572       | A           |
| 1          | A            | 2573       | C           |
| 1          | A            | 2574       | G           |
| 1          | A            | 2577       | A           |
| 1          | A            | 2585       | U           |
| 1          | A            | 2586       | U           |
| 1          | A            | 2602       | A           |
| 1          | A            | 2609       | U           |
| 1          | A            | 2610       | C           |
| 1          | A            | 2613       | U           |
| 1          | A            | 2623       | G           |
| 1          | A            | 2624       | G           |
| 1          | A            | 2629       | U           |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 1          | A            | 2636       | C           |
| 1          | A            | 2647       | U           |
| 1          | A            | 2649       | C           |
| 1          | A            | 2654       | A           |
| 1          | A            | 2656       | U           |
| 1          | A            | 2668       | G           |
| 1          | A            | 2669       | G           |
| 1          | A            | 2671       | G           |
| 1          | A            | 2685       | G           |
| 1          | A            | 2689       | U           |
| 1          | A            | 2690       | U           |
| 1          | A            | 2692       | G           |
| 1          | A            | 2702       | G           |
| 1          | A            | 2707       | U           |
| 1          | A            | 2708       | G           |
| 1          | A            | 2713       | U           |
| 1          | A            | 2714       | G           |
| 1          | A            | 2718       | G           |
| 1          | A            | 2721       | A           |
| 1          | A            | 2722       | G           |
| 1          | A            | 2724       | U           |
| 1          | A            | 2726       | A           |
| 1          | A            | 2729       | G           |
| 1          | A            | 2732       | G           |
| 1          | A            | 2739       | U           |
| 1          | A            | 2740       | A           |
| 1          | A            | 2744       | G           |
| 1          | A            | 2748       | A           |
| 1          | A            | 2753       | A           |
| 1          | A            | 2758       | A           |
| 1          | A            | 2759       | G           |
| 1          | A            | 2761       | A           |
| 1          | A            | 2764       | A           |
| 1          | A            | 2765       | A           |
| 1          | A            | 2769       | U           |
| 1          | A            | 2771       | C           |
| 1          | A            | 2778       | A           |
| 1          | A            | 2782       | G           |
| 1          | A            | 2783       | U           |
| 1          | A            | 2784       | U           |
| 1          | A            | 2790       | U           |
| 1          | A            | 2791       | G           |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 1          | A            | 2793       | C           |
| 1          | A            | 2796       | C           |
| 1          | A            | 2798       | U           |
| 1          | A            | 2799       | G           |
| 1          | A            | 2801       | G           |
| 1          | A            | 2803       | G           |
| 1          | A            | 2806       | C           |
| 1          | A            | 2809       | A           |
| 1          | A            | 2818       | U           |
| 1          | A            | 2820       | A           |
| 1          | A            | 2821       | A           |
| 1          | A            | 2835       | A           |
| 1          | A            | 2837       | A           |
| 1          | A            | 2845       | U           |
| 1          | A            | 2853       | C           |
| 1          | A            | 2857       | G           |
| 1          | A            | 2859       | G           |
| 1          | A            | 2861       | U           |
| 1          | A            | 2867       | G           |
| 1          | A            | 2868       | A           |
| 1          | A            | 2872       | A           |
| 1          | A            | 2874       | C           |
| 1          | A            | 2879       | A           |
| 1          | A            | 2880       | C           |
| 1          | A            | 2881       | U           |
| 1          | A            | 2883       | A           |
| 1          | A            | 2884       | U           |
| 1          | A            | 2886       | A           |
| 1          | A            | 2891       | U           |
| 1          | A            | 2894       | G           |
| 1          | A            | 2897       | U           |
| 1          | A            | 2900       | A           |
| 1          | A            | 2901       | C           |
| 1          | A            | 2902       | C           |
| 1          | A            | 2903       | U           |
| 2          | B            | 4          | C           |
| 2          | B            | 5          | U           |
| 2          | B            | 6          | G           |
| 2          | B            | 11         | C           |
| 2          | B            | 12         | C           |
| 2          | B            | 13         | G           |
| 2          | B            | 15         | A           |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 2          | B            | 22         | U           |
| 2          | B            | 23         | G           |
| 2          | B            | 24         | G           |
| 2          | B            | 33         | G           |
| 2          | B            | 34         | A           |
| 2          | B            | 35         | C           |
| 2          | B            | 36         | C           |
| 2          | B            | 40         | U           |
| 2          | B            | 42         | C           |
| 2          | B            | 44         | G           |
| 2          | B            | 46         | A           |
| 2          | B            | 51         | G           |
| 2          | B            | 53         | A           |
| 2          | B            | 56         | G           |
| 2          | B            | 57         | A           |
| 2          | B            | 59         | A           |
| 2          | B            | 61         | G           |
| 2          | B            | 64         | G           |
| 2          | B            | 66         | A           |
| 2          | B            | 67         | G           |
| 2          | B            | 70         | C           |
| 2          | B            | 81         | G           |
| 2          | B            | 87         | U           |
| 2          | B            | 88         | C           |
| 2          | B            | 89         | U           |
| 2          | B            | 90         | C           |
| 2          | B            | 91         | C           |
| 2          | B            | 95         | U           |
| 2          | B            | 96         | G           |
| 2          | B            | 100        | G           |
| 2          | B            | 105        | G           |
| 2          | B            | 106        | G           |
| 2          | B            | 109        | A           |
| 2          | B            | 112        | G           |
| 2          | B            | 117        | G           |
| 2          | B            | 118        | C           |
| 2          | B            | 119        | A           |
| 34         | a            | 2          | A           |
| 34         | a            | 3          | A           |
| 34         | a            | 4          | U           |
| 34         | a            | 5          | U           |
| 34         | a            | 6          | G           |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 34         | a            | 7          | A           |
| 34         | a            | 9          | G           |
| 34         | a            | 10         | A           |
| 34         | a            | 28         | A           |
| 34         | a            | 31         | G           |
| 34         | a            | 32         | A           |
| 34         | a            | 38         | G           |
| 34         | a            | 39         | G           |
| 34         | a            | 41         | G           |
| 34         | a            | 45         | G           |
| 34         | a            | 47         | C           |
| 34         | a            | 48         | C           |
| 34         | a            | 50         | A           |
| 34         | a            | 51         | A           |
| 34         | a            | 61         | G           |
| 34         | a            | 63         | C           |
| 34         | a            | 64         | G           |
| 34         | a            | 66         | A           |
| 34         | a            | 67         | C           |
| 34         | a            | 68         | G           |
| 34         | a            | 69         | G           |
| 34         | a            | 70         | U           |
| 34         | a            | 72         | A           |
| 34         | a            | 73         | C           |
| 34         | a            | 76         | G           |
| 34         | a            | 77         | A           |
| 34         | a            | 78         | A           |
| 34         | a            | 79         | G           |
| 34         | a            | 80         | A           |
| 34         | a            | 83         | C           |
| 34         | a            | 85         | U           |
| 34         | a            | 86         | G           |
| 34         | a            | 87         | C           |
| 34         | a            | 89         | U           |
| 34         | a            | 94         | G           |
| 34         | a            | 95         | C           |
| 34         | a            | 96         | U           |
| 34         | a            | 97         | G           |
| 34         | a            | 98         | A           |
| 34         | a            | 99         | C           |
| 34         | a            | 100        | G           |
| 34         | a            | 102        | G           |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 34         | a            | 107        | G           |
| 34         | a            | 112        | G           |
| 34         | a            | 115        | G           |
| 34         | a            | 116        | A           |
| 34         | a            | 121        | U           |
| 34         | a            | 122        | G           |
| 34         | a            | 129        | A           |
| 34         | a            | 130        | A           |
| 34         | a            | 131        | A           |
| 34         | a            | 140        | U           |
| 34         | a            | 141        | G           |
| 34         | a            | 142        | G           |
| 34         | a            | 144        | G           |
| 34         | a            | 145        | G           |
| 34         | a            | 146        | G           |
| 34         | a            | 149        | A           |
| 34         | a            | 151        | A           |
| 34         | a            | 152        | A           |
| 34         | a            | 161        | A           |
| 34         | a            | 163        | C           |
| 34         | a            | 164        | G           |
| 34         | a            | 165        | G           |
| 34         | a            | 166        | U           |
| 34         | a            | 169        | C           |
| 34         | a            | 173        | U           |
| 34         | a            | 179        | A           |
| 34         | a            | 181        | A           |
| 34         | a            | 182        | A           |
| 34         | a            | 183        | C           |
| 34         | a            | 184        | G           |
| 34         | a            | 185        | U           |
| 34         | a            | 187        | G           |
| 34         | a            | 188        | C           |
| 34         | a            | 189        | A           |
| 34         | a            | 191        | G           |
| 34         | a            | 193        | C           |
| 34         | a            | 195        | A           |
| 34         | a            | 196        | A           |
| 34         | a            | 197        | A           |
| 34         | a            | 202        | G           |
| 34         | a            | 203        | G           |
| 34         | a            | 207        | C           |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 34         | a            | 209        | U           |
| 34         | a            | 210        | C           |
| 34         | a            | 211        | G           |
| 34         | a            | 212        | G           |
| 34         | a            | 213        | G           |
| 34         | a            | 215        | C           |
| 34         | a            | 216        | U           |
| 34         | a            | 218        | U           |
| 34         | a            | 222        | C           |
| 34         | a            | 226        | G           |
| 34         | a            | 230        | G           |
| 34         | a            | 232        | G           |
| 34         | a            | 245        | U           |
| 34         | a            | 247        | G           |
| 34         | a            | 248        | C           |
| 34         | a            | 251        | G           |
| 34         | a            | 254        | G           |
| 34         | a            | 255        | G           |
| 34         | a            | 264        | C           |
| 34         | a            | 266        | G           |
| 34         | a            | 267        | C           |
| 34         | a            | 271        | C           |
| 34         | a            | 279        | A           |
| 34         | a            | 280        | C           |
| 34         | a            | 281        | G           |
| 34         | a            | 282        | A           |
| 34         | a            | 289        | G           |
| 34         | a            | 300        | A           |
| 34         | a            | 305        | G           |
| 34         | a            | 306        | A           |
| 34         | a            | 308        | C           |
| 34         | a            | 319        | G           |
| 34         | a            | 321        | A           |
| 34         | a            | 323        | U           |
| 34         | a            | 324        | G           |
| 34         | a            | 328        | C           |
| 34         | a            | 329        | A           |
| 34         | a            | 330        | C           |
| 34         | a            | 331        | G           |
| 34         | a            | 335        | C           |
| 34         | a            | 341        | C           |
| 34         | a            | 343        | U           |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 34         | a            | 345        | C           |
| 34         | a            | 346        | G           |
| 34         | a            | 349        | A           |
| 34         | a            | 352        | C           |
| 34         | a            | 354        | G           |
| 34         | a            | 366        | A           |
| 34         | a            | 367        | U           |
| 34         | a            | 368        | U           |
| 34         | a            | 370        | C           |
| 34         | a            | 372        | C           |
| 34         | a            | 373        | A           |
| 34         | a            | 376        | G           |
| 34         | a            | 380        | G           |
| 34         | a            | 381        | C           |
| 34         | a            | 382        | A           |
| 34         | a            | 383        | A           |
| 34         | a            | 384        | G           |
| 34         | a            | 385        | C           |
| 34         | a            | 386        | C           |
| 34         | a            | 387        | U           |
| 34         | a            | 388        | G           |
| 34         | a            | 392        | C           |
| 34         | a            | 394        | G           |
| 34         | a            | 397        | A           |
| 34         | a            | 398        | U           |
| 34         | a            | 404        | G           |
| 34         | a            | 405        | U           |
| 34         | a            | 406        | G           |
| 34         | a            | 411        | A           |
| 34         | a            | 412        | A           |
| 34         | a            | 413        | G           |
| 34         | a            | 414        | A           |
| 34         | a            | 415        | A           |
| 34         | a            | 418        | C           |
| 34         | a            | 420        | U           |
| 34         | a            | 421        | U           |
| 34         | a            | 422        | C           |
| 34         | a            | 424        | G           |
| 34         | a            | 425        | G           |
| 34         | a            | 428        | G           |
| 34         | a            | 429        | U           |
| 34         | a            | 433        | G           |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 34         | a            | 434        | U           |
| 34         | a            | 435        | A           |
| 34         | a            | 436        | C           |
| 34         | a            | 437        | U           |
| 34         | a            | 439        | U           |
| 34         | a            | 441        | A           |
| 34         | a            | 443        | C           |
| 34         | a            | 445        | G           |
| 34         | a            | 446        | G           |
| 34         | a            | 447        | G           |
| 34         | a            | 449        | G           |
| 34         | a            | 453        | G           |
| 34         | a            | 458        | U           |
| 34         | a            | 464        | U           |
| 34         | a            | 466        | A           |
| 34         | a            | 467        | U           |
| 34         | a            | 468        | A           |
| 34         | a            | 475        | C           |
| 34         | a            | 477        | C           |
| 34         | a            | 480        | U           |
| 34         | a            | 484        | G           |
| 34         | a            | 485        | U           |
| 34         | a            | 486        | U           |
| 34         | a            | 490        | C           |
| 34         | a            | 491        | G           |
| 34         | a            | 492        | C           |
| 34         | a            | 495        | A           |
| 34         | a            | 496        | A           |
| 34         | a            | 497        | G           |
| 34         | a            | 499        | A           |
| 34         | a            | 500        | G           |
| 34         | a            | 509        | A           |
| 34         | a            | 510        | A           |
| 34         | a            | 511        | C           |
| 34         | a            | 513        | C           |
| 34         | a            | 517        | G           |
| 34         | a            | 518        | C           |
| 34         | a            | 520        | A           |
| 34         | a            | 521        | G           |
| 34         | a            | 525        | C           |
| 34         | a            | 527        | 7MG         |
| 34         | a            | 531        | U           |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 34         | a            | 542        | G           |
| 34         | a            | 545        | C           |
| 34         | a            | 546        | A           |
| 34         | a            | 547        | A           |
| 34         | a            | 548        | G           |
| 34         | a            | 550        | G           |
| 34         | a            | 572        | A           |
| 34         | a            | 573        | A           |
| 34         | a            | 575        | G           |
| 34         | a            | 576        | C           |
| 34         | a            | 577        | G           |
| 34         | a            | 579        | A           |
| 34         | a            | 594        | U           |
| 34         | a            | 596        | A           |
| 34         | a            | 601        | G           |
| 34         | a            | 602        | A           |
| 34         | a            | 608        | A           |
| 34         | a            | 612        | C           |
| 34         | a            | 613        | C           |
| 34         | a            | 614        | C           |
| 34         | a            | 615        | G           |
| 34         | a            | 617        | G           |
| 34         | a            | 618        | C           |
| 34         | a            | 620        | C           |
| 34         | a            | 621        | A           |
| 34         | a            | 626        | G           |
| 34         | a            | 627        | G           |
| 34         | a            | 628        | G           |
| 34         | a            | 632        | U           |
| 34         | a            | 633        | G           |
| 34         | a            | 635        | A           |
| 34         | a            | 636        | U           |
| 34         | a            | 637        | C           |
| 34         | a            | 639        | G           |
| 34         | a            | 642        | A           |
| 34         | a            | 648        | A           |
| 34         | a            | 653        | U           |
| 34         | a            | 654        | G           |
| 34         | a            | 659        | U           |
| 34         | a            | 660        | C           |
| 34         | a            | 665        | A           |
| 34         | a            | 671        | G           |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 34         | a            | 687        | A           |
| 34         | a            | 695        | A           |
| 34         | a            | 700        | G           |
| 34         | a            | 703        | G           |
| 34         | a            | 704        | A           |
| 34         | a            | 709        | U           |
| 34         | a            | 711        | G           |
| 34         | a            | 712        | A           |
| 34         | a            | 713        | G           |
| 34         | a            | 720        | C           |
| 34         | a            | 721        | G           |
| 34         | a            | 722        | G           |
| 34         | a            | 723        | U           |
| 34         | a            | 724        | G           |
| 34         | a            | 731        | G           |
| 34         | a            | 733        | G           |
| 34         | a            | 737        | C           |
| 34         | a            | 742        | G           |
| 34         | a            | 753        | A           |
| 34         | a            | 754        | C           |
| 34         | a            | 755        | G           |
| 34         | a            | 758        | C           |
| 34         | a            | 759        | A           |
| 34         | a            | 769        | G           |
| 34         | a            | 777        | A           |
| 34         | a            | 793        | U           |
| 34         | a            | 794        | A           |
| 34         | a            | 802        | A           |
| 34         | a            | 815        | A           |
| 34         | a            | 817        | C           |
| 34         | a            | 818        | G           |
| 34         | a            | 819        | A           |
| 34         | a            | 821        | G           |
| 34         | a            | 832        | G           |
| 34         | a            | 836        | G           |
| 34         | a            | 840        | C           |
| 34         | a            | 843        | U           |
| 34         | a            | 844        | G           |
| 34         | a            | 846        | G           |
| 34         | a            | 848        | C           |
| 34         | a            | 849        | G           |
| 34         | a            | 852        | G           |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 34         | a            | 872        | A           |
| 34         | a            | 885        | G           |
| 34         | a            | 899        | C           |
| 34         | a            | 902        | G           |
| 34         | a            | 914        | A           |
| 34         | a            | 926        | G           |
| 34         | a            | 932        | C           |
| 34         | a            | 934        | C           |
| 34         | a            | 935        | A           |
| 34         | a            | 939        | G           |
| 34         | a            | 951        | G           |
| 34         | a            | 960        | U           |
| 34         | a            | 961        | U           |
| 34         | a            | 966        | 2MG         |
| 34         | a            | 969        | A           |
| 34         | a            | 971        | G           |
| 34         | a            | 974        | A           |
| 34         | a            | 975        | A           |
| 34         | a            | 976        | G           |
| 34         | a            | 977        | A           |
| 34         | a            | 978        | A           |
| 34         | a            | 982        | U           |
| 34         | a            | 984        | C           |
| 34         | a            | 989        | U           |
| 34         | a            | 991        | U           |
| 34         | a            | 992        | U           |
| 34         | a            | 993        | G           |
| 34         | a            | 998        | C           |
| 34         | a            | 999        | C           |
| 34         | a            | 1001       | C           |
| 34         | a            | 1003       | G           |
| 34         | a            | 1004       | A           |
| 34         | a            | 1006       | G           |
| 34         | a            | 1016       | A           |
| 34         | a            | 1020       | G           |
| 34         | a            | 1027       | C           |
| 34         | a            | 1028       | C           |
| 34         | a            | 1030       | U           |
| 34         | a            | 1031       | C           |
| 34         | a            | 1033       | G           |
| 34         | a            | 1034       | G           |
| 34         | a            | 1035       | A           |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 34         | a            | 1043       | G           |
| 34         | a            | 1044       | A           |
| 34         | a            | 1045       | C           |
| 34         | a            | 1053       | G           |
| 34         | a            | 1056       | U           |
| 34         | a            | 1065       | U           |
| 34         | a            | 1070       | U           |
| 34         | a            | 1088       | G           |
| 34         | a            | 1094       | G           |
| 34         | a            | 1095       | U           |
| 34         | a            | 1096       | C           |
| 34         | a            | 1098       | C           |
| 34         | a            | 1101       | A           |
| 34         | a            | 1104       | G           |
| 34         | a            | 1108       | G           |
| 34         | a            | 1124       | G           |
| 34         | a            | 1125       | U           |
| 34         | a            | 1126       | U           |
| 34         | a            | 1132       | C           |
| 34         | a            | 1133       | G           |
| 34         | a            | 1134       | G           |
| 34         | a            | 1136       | C           |
| 34         | a            | 1137       | C           |
| 34         | a            | 1138       | G           |
| 34         | a            | 1139       | G           |
| 34         | a            | 1142       | G           |
| 34         | a            | 1143       | G           |
| 34         | a            | 1146       | A           |
| 34         | a            | 1151       | A           |
| 34         | a            | 1152       | A           |
| 34         | a            | 1154       | G           |
| 34         | a            | 1157       | A           |
| 34         | a            | 1158       | C           |
| 34         | a            | 1159       | U           |
| 34         | a            | 1160       | G           |
| 34         | a            | 1162       | C           |
| 34         | a            | 1167       | A           |
| 34         | a            | 1168       | U           |
| 34         | a            | 1169       | A           |
| 34         | a            | 1171       | A           |
| 34         | a            | 1182       | G           |
| 34         | a            | 1184       | G           |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 34         | a            | 1190       | G           |
| 34         | a            | 1191       | A           |
| 34         | a            | 1196       | A           |
| 34         | a            | 1197       | A           |
| 34         | a            | 1201       | A           |
| 34         | a            | 1202       | U           |
| 34         | a            | 1206       | G           |
| 34         | a            | 1211       | U           |
| 34         | a            | 1212       | U           |
| 34         | a            | 1213       | A           |
| 34         | a            | 1217       | C           |
| 34         | a            | 1219       | A           |
| 34         | a            | 1220       | G           |
| 34         | a            | 1225       | A           |
| 34         | a            | 1226       | C           |
| 34         | a            | 1227       | A           |
| 34         | a            | 1228       | C           |
| 34         | a            | 1236       | A           |
| 34         | a            | 1238       | A           |
| 34         | a            | 1241       | G           |
| 34         | a            | 1244       | G           |
| 34         | a            | 1247       | U           |
| 34         | a            | 1256       | A           |
| 34         | a            | 1257       | A           |
| 34         | a            | 1258       | G           |
| 34         | a            | 1260       | G           |
| 34         | a            | 1261       | A           |
| 34         | a            | 1263       | C           |
| 34         | a            | 1266       | G           |
| 34         | a            | 1269       | A           |
| 34         | a            | 1270       | G           |
| 34         | a            | 1272       | G           |
| 34         | a            | 1273       | C           |
| 34         | a            | 1274       | A           |
| 34         | a            | 1275       | A           |
| 34         | a            | 1280       | A           |
| 34         | a            | 1281       | C           |
| 34         | a            | 1282       | C           |
| 34         | a            | 1285       | A           |
| 34         | a            | 1286       | U           |
| 34         | a            | 1287       | A           |
| 34         | a            | 1293       | C           |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 34         | a            | 1294       | G           |
| 34         | a            | 1296       | C           |
| 34         | a            | 1297       | G           |
| 34         | a            | 1298       | U           |
| 34         | a            | 1300       | G           |
| 34         | a            | 1301       | U           |
| 34         | a            | 1302       | C           |
| 34         | a            | 1304       | G           |
| 34         | a            | 1305       | G           |
| 34         | a            | 1306       | A           |
| 34         | a            | 1308       | U           |
| 34         | a            | 1312       | G           |
| 34         | a            | 1317       | C           |
| 34         | a            | 1318       | A           |
| 34         | a            | 1320       | C           |
| 34         | a            | 1321       | U           |
| 34         | a            | 1331       | G           |
| 34         | a            | 1338       | G           |
| 34         | a            | 1340       | A           |
| 34         | a            | 1345       | U           |
| 34         | a            | 1346       | A           |
| 34         | a            | 1348       | U           |
| 34         | a            | 1352       | C           |
| 34         | a            | 1353       | G           |
| 34         | a            | 1360       | A           |
| 34         | a            | 1363       | A           |
| 34         | a            | 1368       | A           |
| 34         | a            | 1370       | G           |
| 34         | a            | 1371       | G           |
| 34         | a            | 1379       | G           |
| 34         | a            | 1380       | U           |
| 34         | a            | 1381       | U           |
| 34         | a            | 1382       | C           |
| 34         | a            | 1383       | C           |
| 34         | a            | 1397       | C           |
| 34         | a            | 1398       | A           |
| 34         | a            | 1399       | C           |
| 34         | a            | 1400       | C           |
| 34         | a            | 1419       | G           |
| 34         | a            | 1429       | A           |
| 34         | a            | 1433       | A           |
| 34         | a            | 1434       | A           |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 34         | a            | 1438       | G           |
| 34         | a            | 1441       | A           |
| 34         | a            | 1442       | G           |
| 34         | a            | 1445       | U           |
| 34         | a            | 1446       | A           |
| 34         | a            | 1448       | C           |
| 34         | a            | 1450       | U           |
| 34         | a            | 1452       | C           |
| 34         | a            | 1458       | G           |
| 34         | a            | 1487       | G           |
| 34         | a            | 1492       | A           |
| 34         | a            | 1497       | G           |
| 34         | a            | 1502       | A           |
| 34         | a            | 1503       | A           |
| 34         | a            | 1506       | U           |
| 34         | a            | 1517       | G           |
| 34         | a            | 1529       | G           |
| 34         | a            | 1530       | G           |
| 34         | a            | 1533       | C           |
| 34         | a            | 1534       | A           |
| 34         | a            | 1535       | C           |
| 34         | a            | 1536       | C           |
| 34         | a            | 1537       | U           |
| 34         | a            | 1538       | C           |
| 34         | a            | 1539       | C           |
| 55         | v            | 4          | G           |
| 55         | v            | 6          | G           |
| 55         | v            | 7          | 4SU         |
| 55         | v            | 8          | G           |
| 55         | v            | 10         | A           |
| 55         | v            | 13         | A           |
| 55         | v            | 15         | C           |
| 55         | v            | 17         | U           |
| 55         | v            | 18         | G           |
| 55         | v            | 20         | H2U         |
| 55         | v            | 21         | A           |
| 55         | v            | 22         | G           |
| 55         | v            | 25         | C           |
| 55         | v            | 31         | G           |
| 55         | v            | 42         | G           |
| 55         | v            | 47         | U           |
| 55         | v            | 52         | G           |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 55         | v            | 60         | U           |
| 55         | v            | 66         | C           |
| 55         | v            | 67         | C           |
| 55         | v            | 69         | C           |
| 55         | v            | 73         | A           |
| 55         | v            | 76         | A           |
| 55         | w            | 3          | C           |
| 55         | w            | 5          | G           |
| 55         | w            | 8          | 4SU         |
| 55         | w            | 9          | G           |
| 55         | w            | 14         | A           |
| 55         | w            | 16         | C           |
| 55         | w            | 17         | C           |
| 55         | w            | 117        | U           |
| 55         | w            | 18         | G           |
| 55         | w            | 19         | G           |
| 55         | w            | 20         | H2U         |
| 55         | w            | 21         | A           |
| 55         | w            | 22         | G           |
| 55         | w            | 24         | U           |
| 55         | w            | 25         | C           |
| 55         | w            | 28         | C           |
| 55         | w            | 30         | G           |
| 55         | w            | 34         | C           |
| 55         | w            | 37         | A           |
| 55         | w            | 38         | A           |
| 55         | w            | 42         | G           |
| 55         | w            | 48         | C           |
| 55         | w            | 49         | G           |
| 55         | w            | 56         | C           |
| 55         | w            | 57         | A           |
| 55         | w            | 59         | A           |
| 55         | w            | 67         | C           |
| 55         | w            | 69         | C           |
| 55         | w            | 70         | G           |
| 55         | w            | 71         | C           |
| 55         | w            | 73         | A           |
| 55         | w            | 75         | C           |
| 55         | w            | 76         | A           |
| 56         | x            | 14         | C           |
| 56         | x            | 15         | U           |
| 56         | x            | 23         | C           |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 56         | x            | 24         | G           |
| 57         | y            | 3          | C           |
| 57         | y            | 4          | C           |
| 57         | y            | 5          | G           |
| 57         | y            | 8          | 4SU         |
| 57         | y            | 9          | A           |
| 57         | y            | 10         | G           |
| 57         | y            | 11         | C           |
| 57         | y            | 16         | H2U         |
| 57         | y            | 17         | C           |
| 57         | y            | 18         | G           |
| 57         | y            | 20         | H2U         |
| 57         | y            | 21         | A           |
| 57         | y            | 24         | G           |
| 57         | y            | 28         | G           |
| 57         | y            | 30         | G           |
| 57         | y            | 31         | A           |
| 57         | y            | 33         | U           |
| 57         | y            | 36         | A           |
| 57         | y            | 44         | G           |
| 57         | y            | 45         | U           |
| 57         | y            | 46         | 7MG         |
| 57         | y            | 47         | U           |
| 57         | y            | 48         | C           |
| 57         | y            | 52         | G           |
| 57         | y            | 56         | C           |
| 57         | y            | 59         | U           |
| 57         | y            | 61         | C           |
| 57         | y            | 65         | G           |
| 57         | y            | 75         | C           |
| 57         | y            | 76         | A           |

All (98) RNA pucker outliers are listed below:

| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 1          | A            | 51         | G           |
| 1          | A            | 84         | A           |
| 1          | A            | 85         | G           |
| 1          | A            | 101        | A           |
| 1          | A            | 119        | A           |
| 1          | A            | 141        | G           |
| 1          | A            | 162        | U           |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 1          | A            | 196        | A           |
| 1          | A            | 204        | A           |
| 1          | A            | 242        | G           |
| 1          | A            | 265        | A           |
| 1          | A            | 282        | A           |
| 1          | A            | 290        | U           |
| 1          | A            | 301        | G           |
| 1          | A            | 362        | A           |
| 1          | A            | 411        | G           |
| 1          | A            | 547        | A           |
| 1          | A            | 555        | G           |
| 1          | A            | 645        | C           |
| 1          | A            | 652        | U           |
| 1          | A            | 653        | U           |
| 1          | A            | 710        | U           |
| 1          | A            | 747        | 5MC         |
| 1          | A            | 764        | A           |
| 1          | A            | 775        | G           |
| 1          | A            | 784        | G           |
| 1          | A            | 859        | G           |
| 1          | A            | 872        | U           |
| 1          | A            | 884        | U           |
| 1          | A            | 899        | A           |
| 1          | A            | 984        | A           |
| 1          | A            | 1020       | A           |
| 1          | A            | 1022       | G           |
| 1          | A            | 1046       | A           |
| 1          | A            | 1050       | A           |
| 1          | A            | 1069       | A           |
| 1          | A            | 1070       | A           |
| 1          | A            | 1089       | A           |
| 1          | A            | 1124       | G           |
| 1          | A            | 1130       | U           |
| 1          | A            | 1140       | C           |
| 1          | A            | 1190       | G           |
| 1          | A            | 1211       | U           |
| 1          | A            | 1240       | U           |
| 1          | A            | 1399       | C           |
| 1          | A            | 1419       | A           |
| 1          | A            | 1420       | A           |
| 1          | A            | 1432       | G           |
| 1          | A            | 1451       | C           |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 1          | A            | 1452       | G           |
| 1          | A            | 1458       | U           |
| 1          | A            | 1475       | G           |
| 1          | A            | 1481       | U           |
| 1          | A            | 1490       | A           |
| 1          | A            | 1507       | C           |
| 1          | A            | 1508       | A           |
| 1          | A            | 1536       | C           |
| 1          | A            | 1538       | G           |
| 1          | A            | 1555       | G           |
| 1          | A            | 1607       | C           |
| 1          | A            | 1608       | A           |
| 1          | A            | 1730       | U           |
| 1          | A            | 1818       | U           |
| 1          | A            | 1857       | G           |
| 1          | A            | 1875       | G           |
| 1          | A            | 1884       | G           |
| 1          | A            | 1939       | 5MU         |
| 1          | A            | 1940       | U           |
| 1          | A            | 1964       | G           |
| 1          | A            | 1976       | U           |
| 1          | A            | 2099       | U           |
| 1          | A            | 2192       | U           |
| 1          | A            | 2296       | U           |
| 1          | A            | 2326       | C           |
| 1          | A            | 2391       | G           |
| 1          | A            | 2401       | U           |
| 1          | A            | 2407       | A           |
| 1          | A            | 2430       | A           |
| 1          | A            | 2517       | C           |
| 1          | A            | 2529       | G           |
| 1          | A            | 2566       | A           |
| 1          | A            | 2645       | G           |
| 1          | A            | 2712       | C           |
| 1          | A            | 2790       | U           |
| 1          | A            | 2808       | G           |
| 1          | A            | 2820       | A           |
| 1          | A            | 2849       | U           |
| 1          | A            | 2873       | A           |
| 1          | A            | 2893       | A           |
| 1          | A            | 2900       | A           |
| 1          | A            | 2902       | C           |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 4   | C    |
| 2   | B     | 34  | A    |
| 2   | B     | 41  | G    |
| 2   | B     | 44  | G    |
| 2   | B     | 46  | A    |
| 2   | B     | 56  | G    |
| 2   | B     | 89  | U    |

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

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

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

| Mol | Type | Chain | Res  | Link    | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|------|---------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |      |         | Counts       | RMSZ | # $ Z  > 2$ | Counts      | RMSZ | # $ Z  > 2$ |
| 34  | UR3  | a     | 1498 | 34      | 19,22,23     | 1.08 | 2 (10%)     | 26,32,35    | 1.72 | 3 (11%)     |
| 1   | PSU  | A     | 746  | 1,60    | 18,21,22     | 1.38 | 3 (16%)     | 22,30,33    | 1.92 | 4 (18%)     |
| 34  | MA6  | a     | 1519 | 34      | 19,26,27     | 1.22 | 2 (10%)     | 18,38,41    | 1.68 | 4 (22%)     |
| 34  | 2MG  | a     | 966  | 34      | 18,26,27     | 0.93 | 0           | 16,38,41    | 1.32 | 3 (18%)     |
| 1   | OMU  | A     | 2552 | 1,60    | 19,22,23     | 1.36 | 3 (15%)     | 26,31,34    | 2.14 | 8 (30%)     |
| 34  | 7MG  | a     | 527  | 34      | 22,26,27     | 1.48 | 4 (18%)     | 29,39,42    | 2.39 | 8 (27%)     |
| 57  | 7MG  | y     | 46   | 57      | 22,26,27     | 1.44 | 4 (18%)     | 29,39,42    | 2.36 | 7 (24%)     |
| 55  | 4SU  | w     | 8    | 55      | 18,21,22     | 1.71 | 5 (27%)     | 26,30,33    | 2.14 | 5 (19%)     |
| 1   | 2MG  | A     | 2445 | 1       | 18,26,27     | 1.11 | 1 (5%)      | 16,38,41    | 1.20 | 2 (12%)     |
| 34  | 2MG  | a     | 1516 | 34      | 18,26,27     | 0.96 | 1 (5%)      | 16,38,41    | 1.16 | 2 (12%)     |
| 57  | PSU  | y     | 55   | 57      | 18,21,22     | 1.36 | 2 (11%)     | 22,30,33    | 1.90 | 5 (22%)     |
| 34  | PSU  | a     | 516  | 34      | 18,21,22     | 1.40 | 2 (11%)     | 22,30,33    | 1.96 | 5 (22%)     |
| 34  | 4OC  | a     | 1402 | 34,60   | 20,23,24     | 0.81 | 0           | 26,32,35    | 1.31 | 5 (19%)     |
| 1   | 5MU  | A     | 1939 | 1       | 19,22,23     | 1.38 | 5 (26%)     | 28,32,35    | 2.00 | 8 (28%)     |
| 1   | OMG  | A     | 2251 | 1,55,60 | 18,26,27     | 1.04 | 2 (11%)     | 19,38,41    | 1.22 | 3 (15%)     |
| 1   | 7MG  | A     | 2069 | 1,60    | 22,26,27     | 1.53 | 4 (18%)     | 29,39,42    | 2.45 | 10 (34%)    |
| 57  | 5MU  | y     | 54   | 57      | 19,22,23     | 1.40 | 4 (21%)     | 28,32,35    | 2.09 | 8 (28%)     |

| Mol | Type | Chain | Res  | Link  | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|-------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 57  | PSU  | y     | 39   | 57    | 18,21,22     | 1.41 | 2 (11%)  | 22,30,33    | 1.86 | 4 (18%)  |
| 57  | H2U  | y     | 20   | 57    | 18,21,22     | 0.84 | 1 (5%)   | 21,30,33    | 1.58 | 4 (19%)  |
| 57  | MIA  | y     | 37   | 57    | 24,31,32     | 2.37 | 6 (25%)  | 26,44,47    | 2.65 | 10 (38%) |
| 1   | PSU  | A     | 2605 | 1,60  | 18,21,22     | 1.39 | 2 (11%)  | 22,30,33    | 2.04 | 4 (18%)  |
| 1   | PSU  | A     | 2580 | 1     | 18,21,22     | 1.47 | 3 (16%)  | 22,30,33    | 1.93 | 5 (22%)  |
| 1   | PSU  | A     | 2604 | 1     | 18,21,22     | 1.40 | 3 (16%)  | 22,30,33    | 1.85 | 4 (18%)  |
| 55  | 4SU  | v     | 7    | 55    | 18,21,22     | 1.66 | 4 (22%)  | 26,30,33    | 2.34 | 5 (19%)  |
| 1   | PSU  | A     | 955  | 1     | 18,21,22     | 1.38 | 2 (11%)  | 22,30,33    | 1.95 | 4 (18%)  |
| 55  | PSU  | v     | 55   | 55,60 | 18,21,22     | 1.34 | 3 (16%)  | 22,30,33    | 1.85 | 5 (22%)  |
| 1   | OMC  | A     | 2498 | 1,60  | 19,22,23     | 0.90 | 1 (5%)   | 26,31,34    | 1.18 | 2 (7%)   |
| 1   | 6MZ  | A     | 2030 | 1     | 18,25,26     | 1.01 | 1 (5%)   | 16,36,39    | 2.28 | 5 (31%)  |
| 55  | H2U  | v     | 20   | 55    | 18,21,22     | 0.90 | 1 (5%)   | 21,30,33    | 1.59 | 5 (23%)  |
| 1   | PSU  | A     | 1911 | 1     | 18,21,22     | 1.35 | 2 (11%)  | 22,30,33    | 1.93 | 4 (18%)  |
| 1   | 3TD  | A     | 1915 | 1,60  | 18,22,23     | 7.19 | 13 (72%) | 22,32,35    | 1.96 | 3 (13%)  |
| 1   | PSU  | A     | 2457 | 1     | 18,21,22     | 1.52 | 3 (16%)  | 22,30,33    | 1.85 | 5 (22%)  |
| 55  | H2U  | w     | 20   | 55    | 18,21,22     | 0.81 | 0        | 21,30,33    | 1.69 | 3 (14%)  |
| 57  | PSU  | y     | 32   | 57    | 18,21,22     | 1.33 | 2 (11%)  | 22,30,33    | 1.91 | 5 (22%)  |
| 1   | 6MZ  | A     | 1618 | 1     | 18,25,26     | 1.03 | 1 (5%)   | 16,36,39    | 2.29 | 5 (31%)  |
| 55  | PSU  | w     | 55   | 55    | 18,21,22     | 1.30 | 2 (11%)  | 22,30,33    | 1.93 | 5 (22%)  |
| 1   | 5MC  | A     | 1962 | 1     | 18,22,23     | 0.90 | 1 (5%)   | 26,32,35    | 1.19 | 3 (11%)  |
| 1   | H2U  | A     | 2449 | 1     | 18,21,22     | 1.02 | 2 (11%)  | 21,30,33    | 1.51 | 4 (19%)  |
| 55  | 5MU  | w     | 54   | 55    | 19,22,23     | 1.48 | 4 (21%)  | 28,32,35    | 2.04 | 10 (35%) |
| 1   | PSU  | A     | 2504 | 1     | 18,21,22     | 1.37 | 2 (11%)  | 22,30,33    | 1.79 | 4 (18%)  |
| 34  | 2MG  | a     | 1207 | 34,60 | 18,26,27     | 0.98 | 0        | 16,38,41    | 1.11 | 2 (12%)  |
| 34  | 5MC  | a     | 1407 | 34    | 18,22,23     | 1.00 | 1 (5%)   | 26,32,35    | 1.29 | 4 (15%)  |
| 34  | MA6  | a     | 1518 | 34    | 19,26,27     | 1.34 | 3 (15%)  | 18,38,41    | 1.77 | 4 (22%)  |
| 1   | 2MG  | A     | 1835 | 1     | 18,26,27     | 1.01 | 1 (5%)   | 16,38,41    | 1.14 | 1 (6%)   |
| 1   | PSU  | A     | 1917 | 1     | 18,21,22     | 1.38 | 2 (11%)  | 22,30,33    | 1.94 | 4 (18%)  |
| 1   | 5MC  | A     | 747  | 1     | 18,22,23     | 0.97 | 2 (11%)  | 26,32,35    | 1.60 | 6 (23%)  |
| 57  | 4SU  | y     | 8    | 57    | 18,21,22     | 1.71 | 5 (27%)  | 26,30,33    | 2.28 | 7 (26%)  |
| 1   | 2MA  | A     | 2503 | 1,60  | 17,25,26     | 1.02 | 1 (5%)   | 17,37,40    | 1.15 | 2 (11%)  |
| 55  | 5MU  | v     | 54   | 55    | 19,22,23     | 1.48 | 5 (26%)  | 28,32,35    | 1.88 | 8 (28%)  |
| 1   | 1MG  | A     | 745  | 1     | 18,26,27     | 0.89 | 0        | 19,39,42    | 1.48 | 3 (15%)  |
| 34  | 5MC  | a     | 967  | 34    | 18,22,23     | 1.06 | 1 (5%)   | 26,32,35    | 1.23 | 4 (15%)  |
| 57  | H2U  | y     | 16   | 57    | 18,21,22     | 0.81 | 1 (5%)   | 21,30,33    | 1.49 | 4 (19%)  |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res  | Link    | Chirals | Torsions   | Rings   |
|-----|------|-------|------|---------|---------|------------|---------|
| 34  | UR3  | a     | 1498 | 34      | -       | 2/7/25/26  | 0/2/2/2 |
| 1   | PSU  | A     | 746  | 1,60    | -       | 3/7/25/26  | 0/2/2/2 |
| 34  | MA6  | a     | 1519 | 34      | -       | 3/7/29/30  | 0/3/3/3 |
| 34  | 2MG  | a     | 966  | 34      | -       | 3/5/27/28  | 0/3/3/3 |
| 1   | OMU  | A     | 2552 | 1,60    | -       | 2/9/27/28  | 0/2/2/2 |
| 34  | 7MG  | a     | 527  | 34      | -       | 2/7/37/38  | 0/3/3/3 |
| 57  | 7MG  | y     | 46   | 57      | -       | 4/7/37/38  | 0/3/3/3 |
| 55  | 4SU  | w     | 8    | 55      | -       | 6/7/25/26  | 0/2/2/2 |
| 1   | 2MG  | A     | 2445 | 1       | -       | 2/5/27/28  | 0/3/3/3 |
| 34  | 2MG  | a     | 1516 | 34      | -       | 0/5/27/28  | 0/3/3/3 |
| 57  | PSU  | y     | 55   | 57      | -       | 0/7/25/26  | 0/2/2/2 |
| 34  | PSU  | a     | 516  | 34      | -       | 0/7/25/26  | 0/2/2/2 |
| 34  | 4OC  | a     | 1402 | 34,60   | -       | 2/9/29/30  | 0/2/2/2 |
| 1   | 5MU  | A     | 1939 | 1       | -       | 2/7/25/26  | 0/2/2/2 |
| 1   | OMG  | A     | 2251 | 1,55,60 | -       | 0/5/27/28  | 0/3/3/3 |
| 1   | 7MG  | A     | 2069 | 1,60    | -       | 2/7/37/38  | 0/3/3/3 |
| 57  | 5MU  | y     | 54   | 57      | -       | 0/7/25/26  | 0/2/2/2 |
| 57  | PSU  | y     | 39   | 57      | -       | 2/7/25/26  | 0/2/2/2 |
| 57  | H2U  | y     | 20   | 57      | -       | 2/7/38/39  | 0/2/2/2 |
| 57  | MIA  | y     | 37   | 57      | -       | 5/11/33/34 | 0/3/3/3 |
| 1   | PSU  | A     | 2605 | 1,60    | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | PSU  | A     | 2580 | 1       | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | PSU  | A     | 2604 | 1       | -       | 2/7/25/26  | 0/2/2/2 |
| 55  | 4SU  | v     | 7    | 55      | -       | 2/7/25/26  | 0/2/2/2 |
| 1   | PSU  | A     | 955  | 1       | -       | 0/7/25/26  | 0/2/2/2 |
| 55  | PSU  | v     | 55   | 55,60   | -       | 2/7/25/26  | 0/2/2/2 |
| 1   | OMC  | A     | 2498 | 1,60    | -       | 0/9/27/28  | 0/2/2/2 |
| 1   | 6MZ  | A     | 2030 | 1       | -       | 3/5/27/28  | 0/3/3/3 |
| 55  | H2U  | v     | 20   | 55      | -       | 5/7/38/39  | 0/2/2/2 |
| 1   | PSU  | A     | 1911 | 1       | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | 3TD  | A     | 1915 | 1,60    | -       | 2/7/25/26  | 0/2/2/2 |
| 1   | PSU  | A     | 2457 | 1       | -       | 2/7/25/26  | 0/2/2/2 |
| 55  | H2U  | w     | 20   | 55      | -       | 2/7/38/39  | 0/2/2/2 |

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| Mol | Type | Chain | Res  | Link  | Chirals | Torsions  | Rings   |
|-----|------|-------|------|-------|---------|-----------|---------|
| 57  | PSU  | y     | 32   | 57    | -       | 2/7/25/26 | 0/2/2/2 |
| 1   | 6MZ  | A     | 1618 | 1     | -       | 3/5/27/28 | 0/3/3/3 |
| 55  | PSU  | w     | 55   | 55    | -       | 1/7/25/26 | 0/2/2/2 |
| 1   | 5MC  | A     | 1962 | 1     | -       | 2/7/25/26 | 0/2/2/2 |
| 1   | H2U  | A     | 2449 | 1     | -       | 0/7/38/39 | 0/2/2/2 |
| 55  | 5MU  | w     | 54   | 55    | -       | 0/7/25/26 | 0/2/2/2 |
| 1   | PSU  | A     | 2504 | 1     | -       | 2/7/25/26 | 0/2/2/2 |
| 34  | 2MG  | a     | 1207 | 34,60 | -       | 0/5/27/28 | 0/3/3/3 |
| 34  | 5MC  | a     | 1407 | 34    | -       | 0/7/25/26 | 0/2/2/2 |
| 34  | MA6  | a     | 1518 | 34    | -       | 2/7/29/30 | 0/3/3/3 |
| 1   | 2MG  | A     | 1835 | 1     | -       | 0/5/27/28 | 0/3/3/3 |
| 1   | PSU  | A     | 1917 | 1     | -       | 2/7/25/26 | 0/2/2/2 |
| 1   | 5MC  | A     | 747  | 1     | -       | 0/7/25/26 | 0/2/2/2 |
| 57  | 4SU  | y     | 8    | 57    | -       | 2/7/25/26 | 0/2/2/2 |
| 1   | 2MA  | A     | 2503 | 1,60  | -       | 0/3/25/26 | 0/3/3/3 |
| 55  | 5MU  | v     | 54   | 55    | -       | 0/7/25/26 | 0/2/2/2 |
| 1   | 1MG  | A     | 745  | 1     | -       | 0/3/25/26 | 0/3/3/3 |
| 34  | 5MC  | a     | 967  | 34    | -       | 0/7/25/26 | 0/2/2/2 |
| 57  | H2U  | y     | 16   | 57    | -       | 2/7/38/39 | 0/2/2/2 |

All (127) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|--------|-------------|----------|
| 1   | A     | 1915 | 3TD  | O4'-C1' | 16.38  | 1.66        | 1.43     |
| 1   | A     | 1915 | 3TD  | C6-C5   | 15.22  | 1.53        | 1.35     |
| 1   | A     | 1915 | 3TD  | C2'-C1' | -15.08 | 1.34        | 1.53     |
| 1   | A     | 1915 | 3TD  | C2-N1   | 7.61   | 1.47        | 1.37     |
| 57  | y     | 37   | MIA  | C13-C14 | 7.49   | 1.53        | 1.32     |
| 57  | y     | 37   | MIA  | C2-S10  | -6.46  | 1.70        | 1.75     |
| 1   | A     | 1915 | 3TD  | C2-N3   | 6.08   | 1.52        | 1.38     |
| 1   | A     | 1915 | 3TD  | O4'-C4' | -6.00  | 1.31        | 1.45     |
| 1   | A     | 1915 | 3TD  | C6-N1   | 4.96   | 1.44        | 1.36     |
| 1   | A     | 2069 | 7MG  | C4-N9   | -4.70  | 1.32        | 1.37     |
| 55  | w     | 8    | 4SU  | C4-S4   | -4.43  | 1.60        | 1.68     |
| 57  | y     | 8    | 4SU  | C4-S4   | -4.37  | 1.60        | 1.68     |
| 55  | v     | 7    | 4SU  | C4-S4   | -4.28  | 1.60        | 1.68     |
| 34  | a     | 516  | PSU  | C6-C5   | 4.23   | 1.40        | 1.35     |
| 57  | y     | 39   | PSU  | C6-C5   | 4.19   | 1.40        | 1.35     |
| 57  | y     | 55   | PSU  | C6-C5   | 4.11   | 1.40        | 1.35     |
| 1   | A     | 1911 | PSU  | C6-C5   | 4.04   | 1.40        | 1.35     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | A     | 2457 | PSU  | C6-C5   | 4.01  | 1.40        | 1.35     |
| 55  | v     | 55   | PSU  | C6-C5   | 4.00  | 1.40        | 1.35     |
| 1   | A     | 2580 | PSU  | C6-C5   | 3.95  | 1.39        | 1.35     |
| 1   | A     | 1917 | PSU  | C6-C5   | 3.94  | 1.39        | 1.35     |
| 1   | A     | 2605 | PSU  | C6-C5   | 3.89  | 1.39        | 1.35     |
| 57  | y     | 32   | PSU  | C6-C5   | 3.88  | 1.39        | 1.35     |
| 55  | w     | 55   | PSU  | C6-C5   | 3.87  | 1.39        | 1.35     |
| 1   | A     | 2504 | PSU  | C6-C5   | 3.78  | 1.39        | 1.35     |
| 34  | a     | 527  | 7MG  | C4-N9   | -3.77 | 1.33        | 1.37     |
| 1   | A     | 746  | PSU  | C6-C5   | 3.52  | 1.39        | 1.35     |
| 1   | A     | 955  | PSU  | C6-C5   | 3.49  | 1.39        | 1.35     |
| 1   | A     | 2604 | PSU  | C6-C5   | 3.43  | 1.39        | 1.35     |
| 34  | a     | 967  | 5MC  | C6-C5   | 3.40  | 1.40        | 1.34     |
| 57  | y     | 46   | 7MG  | C4-N9   | -3.38 | 1.33        | 1.37     |
| 55  | v     | 54   | 5MU  | C6-C5   | 3.30  | 1.40        | 1.34     |
| 1   | A     | 2552 | OMU  | C2-N1   | 3.17  | 1.43        | 1.38     |
| 57  | y     | 46   | 7MG  | C5-C4   | 3.16  | 1.48        | 1.38     |
| 55  | w     | 54   | 5MU  | C6-C5   | 3.14  | 1.39        | 1.34     |
| 34  | a     | 1407 | 5MC  | C6-C5   | 3.09  | 1.39        | 1.34     |
| 1   | A     | 1915 | 3TD  | O2'-C2' | 3.07  | 1.50        | 1.43     |
| 34  | a     | 527  | 7MG  | C5-C4   | 3.03  | 1.48        | 1.38     |
| 55  | w     | 54   | 5MU  | C2-N1   | 3.01  | 1.43        | 1.38     |
| 34  | a     | 1518 | MA6  | C5-C4   | 3.00  | 1.48        | 1.40     |
| 57  | y     | 54   | 5MU  | C2-N1   | 2.96  | 1.43        | 1.38     |
| 55  | w     | 8    | 4SU  | C2-N1   | 2.96  | 1.43        | 1.38     |
| 57  | y     | 8    | 4SU  | C2-N1   | 2.88  | 1.43        | 1.38     |
| 1   | A     | 1915 | 3TD  | O2-C2   | -2.81 | 1.17        | 1.23     |
| 57  | y     | 8    | 4SU  | C4-N3   | -2.75 | 1.34        | 1.37     |
| 1   | A     | 2552 | OMU  | C4-N3   | -2.75 | 1.33        | 1.38     |
| 1   | A     | 2580 | PSU  | C4-N3   | -2.75 | 1.33        | 1.38     |
| 55  | w     | 8    | 4SU  | C4-N3   | -2.74 | 1.34        | 1.37     |
| 1   | A     | 2604 | PSU  | C4-N3   | -2.73 | 1.33        | 1.38     |
| 57  | y     | 54   | 5MU  | C6-C5   | 2.72  | 1.39        | 1.34     |
| 1   | A     | 1915 | 3TD  | C10-N3  | -2.72 | 1.42        | 1.47     |
| 1   | A     | 746  | PSU  | C4-N3   | -2.71 | 1.33        | 1.38     |
| 1   | A     | 2069 | 7MG  | C5-C4   | 2.71  | 1.46        | 1.38     |
| 55  | w     | 54   | 5MU  | C4-C5   | 2.70  | 1.49        | 1.44     |
| 55  | v     | 7    | 4SU  | C2-N1   | 2.70  | 1.42        | 1.38     |
| 1   | A     | 2504 | PSU  | C4-N3   | -2.69 | 1.33        | 1.38     |
| 1   | A     | 1915 | 3TD  | O3'-C3' | -2.69 | 1.36        | 1.43     |
| 57  | y     | 37   | MIA  | C5-C4   | 2.65  | 1.47        | 1.40     |
| 1   | A     | 747  | 5MC  | C6-C5   | 2.64  | 1.38        | 1.34     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 55  | v     | 7    | 4SU  | C4-N3   | -2.64 | 1.34        | 1.37     |
| 55  | v     | 54   | 5MU  | C4-N3   | -2.63 | 1.34        | 1.38     |
| 1   | A     | 2605 | PSU  | C4-N3   | -2.57 | 1.34        | 1.38     |
| 1   | A     | 2457 | PSU  | C4-N3   | -2.56 | 1.34        | 1.38     |
| 34  | a     | 1518 | MA6  | C6-N1   | 2.53  | 1.36        | 1.33     |
| 34  | a     | 1519 | MA6  | C5-C4   | 2.53  | 1.47        | 1.40     |
| 1   | A     | 1915 | 3TD  | C4-N3   | 2.53  | 1.45        | 1.40     |
| 55  | v     | 54   | 5MU  | C2-N1   | 2.52  | 1.42        | 1.38     |
| 1   | A     | 1618 | 6MZ  | C5-C4   | 2.51  | 1.47        | 1.40     |
| 1   | A     | 955  | PSU  | C4-N3   | -2.51 | 1.34        | 1.38     |
| 1   | A     | 2030 | 6MZ  | C5-C4   | 2.50  | 1.47        | 1.40     |
| 57  | y     | 37   | MIA  | C6-N1   | 2.50  | 1.36        | 1.32     |
| 1   | A     | 2445 | 2MG  | C6-N1   | -2.47 | 1.34        | 1.37     |
| 1   | A     | 1939 | 5MU  | C6-C5   | 2.46  | 1.38        | 1.34     |
| 55  | v     | 54   | 5MU  | C4-C5   | 2.46  | 1.48        | 1.44     |
| 1   | A     | 2580 | PSU  | C2-N3   | -2.46 | 1.33        | 1.37     |
| 1   | A     | 1939 | 5MU  | C6-N1   | -2.41 | 1.33        | 1.38     |
| 1   | A     | 2449 | H2U  | C2-N3   | -2.40 | 1.33        | 1.38     |
| 57  | y     | 8    | 4SU  | C5-C4   | -2.40 | 1.39        | 1.42     |
| 1   | A     | 2069 | 7MG  | C5-N7   | -2.40 | 1.32        | 1.35     |
| 1   | A     | 1939 | 5MU  | C4-N3   | -2.39 | 1.34        | 1.38     |
| 57  | y     | 54   | 5MU  | C4-C5   | 2.38  | 1.48        | 1.44     |
| 1   | A     | 1915 | 3TD  | C3'-C4' | 2.38  | 1.59        | 1.53     |
| 1   | A     | 1962 | 5MC  | C6-C5   | 2.36  | 1.38        | 1.34     |
| 1   | A     | 2449 | H2U  | C4-N3   | -2.36 | 1.33        | 1.37     |
| 1   | A     | 2457 | PSU  | C2-N3   | -2.36 | 1.33        | 1.37     |
| 1   | A     | 2503 | 2MA  | C2-N3   | 2.34  | 1.36        | 1.31     |
| 1   | A     | 1835 | 2MG  | C6-N1   | -2.34 | 1.34        | 1.37     |
| 1   | A     | 747  | 5MC  | C6-N1   | -2.30 | 1.34        | 1.38     |
| 55  | v     | 7    | 4SU  | C5-C4   | -2.29 | 1.39        | 1.42     |
| 57  | y     | 54   | 5MU  | C4-N3   | -2.29 | 1.34        | 1.38     |
| 34  | a     | 516  | PSU  | C4-N3   | -2.28 | 1.34        | 1.38     |
| 1   | A     | 1917 | PSU  | C4-N3   | -2.27 | 1.34        | 1.38     |
| 55  | w     | 54   | 5MU  | C4-N3   | -2.26 | 1.34        | 1.38     |
| 57  | y     | 32   | PSU  | C4-N3   | -2.25 | 1.34        | 1.38     |
| 34  | a     | 527  | 7MG  | C8-N9   | 2.25  | 1.47        | 1.46     |
| 1   | A     | 1911 | PSU  | C4-N3   | -2.25 | 1.34        | 1.38     |
| 57  | y     | 46   | 7MG  | C8-N9   | 2.25  | 1.47        | 1.46     |
| 55  | w     | 8    | 4SU  | C5-C4   | -2.24 | 1.39        | 1.42     |
| 57  | y     | 55   | PSU  | C4-N3   | -2.23 | 1.34        | 1.38     |
| 55  | v     | 55   | PSU  | C4-N3   | -2.22 | 1.34        | 1.38     |
| 1   | A     | 2251 | OMG  | O4'-C1' | 2.21  | 1.44        | 1.41     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 34  | a     | 1519 | MA6  | O4'-C1' | 2.21  | 1.44        | 1.41     |
| 1   | A     | 1939 | 5MU  | C4-C5   | 2.21  | 1.48        | 1.44     |
| 55  | w     | 55   | PSU  | C4-N3   | -2.18 | 1.34        | 1.38     |
| 57  | y     | 37   | MIA  | C2-N1   | 2.17  | 1.37        | 1.34     |
| 1   | A     | 2069 | 7MG  | C6-N1   | -2.17 | 1.34        | 1.38     |
| 1   | A     | 2251 | OMG  | C6-N1   | -2.15 | 1.34        | 1.37     |
| 1   | A     | 746  | PSU  | C2-N3   | -2.12 | 1.33        | 1.37     |
| 57  | y     | 37   | MIA  | O4'-C1' | 2.10  | 1.44        | 1.41     |
| 57  | y     | 39   | PSU  | C4-N3   | -2.10 | 1.34        | 1.38     |
| 55  | w     | 8    | 4SU  | C6-C5   | 2.09  | 1.39        | 1.35     |
| 1   | A     | 2498 | OMC  | C5-C4   | -2.08 | 1.38        | 1.42     |
| 57  | y     | 20   | H2U  | C2-N3   | -2.08 | 1.34        | 1.38     |
| 57  | y     | 16   | H2U  | C2-N3   | -2.07 | 1.34        | 1.38     |
| 55  | v     | 54   | 5MU  | C2-N3   | -2.05 | 1.34        | 1.38     |
| 57  | y     | 46   | 7MG  | C5-C6   | 2.04  | 1.48        | 1.43     |
| 1   | A     | 1939 | 5MU  | C2-N1   | 2.04  | 1.41        | 1.38     |
| 1   | A     | 2604 | PSU  | C2-N3   | -2.04 | 1.34        | 1.37     |
| 55  | v     | 55   | PSU  | C4-C5   | 2.04  | 1.50        | 1.44     |
| 34  | a     | 1498 | UR3  | C2-N1   | 2.03  | 1.41        | 1.38     |
| 34  | a     | 1518 | MA6  | O4'-C1' | 2.03  | 1.43        | 1.41     |
| 55  | v     | 20   | H2U  | C2-N3   | -2.03 | 1.34        | 1.38     |
| 57  | y     | 8    | 4SU  | C6-C5   | 2.02  | 1.39        | 1.35     |
| 34  | a     | 527  | 7MG  | C6-N1   | -2.02 | 1.35        | 1.38     |
| 34  | a     | 1498 | UR3  | C5-C4   | -2.02 | 1.38        | 1.43     |
| 34  | a     | 1516 | 2MG  | C6-N1   | -2.02 | 1.34        | 1.37     |
| 1   | A     | 2552 | OMU  | C6-C5   | 2.02  | 1.39        | 1.35     |

All (247) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 57  | y     | 46   | 7MG  | N9-C4-N3    | 7.89  | 137.26      | 125.47   |
| 34  | a     | 527  | 7MG  | N9-C4-N3    | 7.73  | 137.04      | 125.47   |
| 57  | y     | 37   | MIA  | C12-C13-C14 | -7.64 | 112.26      | 127.14   |
| 1   | A     | 2069 | 7MG  | N9-C4-N3    | 7.18  | 136.21      | 125.47   |
| 55  | v     | 7    | 4SU  | C4-N3-C2    | -6.84 | 120.70      | 127.34   |
| 57  | y     | 8    | 4SU  | C4-N3-C2    | -6.32 | 121.20      | 127.34   |
| 1   | A     | 2605 | PSU  | N1-C2-N3    | 6.12  | 122.07      | 115.13   |
| 55  | w     | 8    | 4SU  | C4-N3-C2    | -6.05 | 121.47      | 127.34   |
| 1   | A     | 1618 | 6MZ  | C2-N1-C6    | 5.96  | 121.70      | 116.59   |
| 1   | A     | 2030 | 6MZ  | C2-N1-C6    | 5.96  | 121.70      | 116.59   |
| 1   | A     | 2580 | PSU  | N1-C2-N3    | 5.90  | 121.82      | 115.13   |
| 1   | A     | 2457 | PSU  | N1-C2-N3    | 5.82  | 121.72      | 115.13   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | A     | 2504 | PSU  | N1-C2-N3   | 5.81  | 121.71      | 115.13   |
| 55  | w     | 55   | PSU  | N1-C2-N3   | 5.74  | 121.64      | 115.13   |
| 1   | A     | 1911 | PSU  | N1-C2-N3   | 5.74  | 121.64      | 115.13   |
| 1   | A     | 1917 | PSU  | N1-C2-N3   | 5.74  | 121.63      | 115.13   |
| 57  | y     | 32   | PSU  | N1-C2-N3   | 5.73  | 121.62      | 115.13   |
| 34  | a     | 1498 | UR3  | C4-N3-C2   | -5.68 | 119.22      | 124.56   |
| 55  | v     | 7    | 4SU  | C5-C4-N3   | 5.67  | 119.95      | 114.69   |
| 1   | A     | 1915 | 3TD  | N1-C2-N3   | 5.66  | 120.60      | 116.14   |
| 1   | A     | 746  | PSU  | N1-C2-N3   | 5.63  | 121.51      | 115.13   |
| 57  | y     | 55   | PSU  | N1-C2-N3   | 5.55  | 121.42      | 115.13   |
| 1   | A     | 955  | PSU  | N1-C2-N3   | 5.55  | 121.42      | 115.13   |
| 1   | A     | 2604 | PSU  | N1-C2-N3   | 5.54  | 121.40      | 115.13   |
| 57  | y     | 39   | PSU  | N1-C2-N3   | 5.53  | 121.39      | 115.13   |
| 1   | A     | 1915 | 3TD  | C4-N3-C2   | -5.53 | 118.61      | 124.61   |
| 55  | v     | 55   | PSU  | N1-C2-N3   | 5.47  | 121.33      | 115.13   |
| 57  | y     | 8    | 4SU  | C5-C4-N3   | 5.36  | 119.66      | 114.69   |
| 34  | a     | 516  | PSU  | N1-C2-N3   | 5.34  | 121.18      | 115.13   |
| 55  | w     | 8    | 4SU  | C5-C4-N3   | 5.33  | 119.63      | 114.69   |
| 1   | A     | 2552 | OMU  | N3-C2-N1   | 5.31  | 121.93      | 114.89   |
| 55  | v     | 54   | 5MU  | N3-C2-N1   | 5.09  | 121.64      | 114.89   |
| 1   | A     | 2552 | OMU  | C4-N3-C2   | -4.98 | 120.01      | 126.58   |
| 57  | y     | 46   | 7MG  | C5-C4-N3   | -4.96 | 118.68      | 128.13   |
| 1   | A     | 2069 | 7MG  | C5-C4-N3   | -4.93 | 118.73      | 128.13   |
| 34  | a     | 527  | 7MG  | C5-C4-N3   | -4.88 | 118.83      | 128.13   |
| 1   | A     | 1939 | 5MU  | C4-N3-C2   | -4.87 | 121.05      | 127.35   |
| 1   | A     | 1939 | 5MU  | N3-C2-N1   | 4.86  | 121.34      | 114.89   |
| 55  | w     | 54   | 5MU  | N3-C2-N1   | 4.79  | 121.25      | 114.89   |
| 57  | y     | 8    | 4SU  | N3-C2-N1   | 4.73  | 121.17      | 114.89   |
| 55  | v     | 7    | 4SU  | N3-C2-N1   | 4.66  | 121.08      | 114.89   |
| 55  | w     | 20   | H2U  | O4'-C1'-N1 | 4.63  | 115.61      | 109.30   |
| 1   | A     | 2069 | 7MG  | C2-N3-C4   | 4.59  | 120.49      | 112.30   |
| 1   | A     | 2069 | 7MG  | N9-C8-N7   | -4.55 | 96.87       | 103.38   |
| 57  | y     | 37   | MIA  | C5-C6-N1   | -4.53 | 117.05      | 120.81   |
| 57  | y     | 54   | 5MU  | N3-C2-N1   | 4.50  | 120.87      | 114.89   |
| 57  | y     | 46   | 7MG  | N9-C8-N7   | -4.49 | 96.96       | 103.38   |
| 57  | y     | 37   | MIA  | C2-N3-C4   | 4.47  | 121.49      | 115.32   |
| 55  | w     | 54   | 5MU  | C4-N3-C2   | -4.46 | 121.58      | 127.35   |
| 57  | y     | 46   | 7MG  | C2-N3-C4   | 4.46  | 120.24      | 112.30   |
| 57  | y     | 54   | 5MU  | C4-N3-C2   | -4.44 | 121.61      | 127.35   |
| 55  | w     | 8    | 4SU  | N3-C2-N1   | 4.38  | 120.70      | 114.89   |
| 57  | y     | 54   | 5MU  | C5-C4-N3   | 4.37  | 119.04      | 115.31   |
| 1   | A     | 2605 | PSU  | C4-N3-C2   | -4.34 | 120.09      | 126.34   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 34  | a     | 527  | 7MG  | N9-C8-N7    | -4.30 | 97.23       | 103.38   |
| 55  | v     | 54   | 5MU  | C4-N3-C2    | -4.25 | 121.85      | 127.35   |
| 34  | a     | 527  | 7MG  | C2-N3-C4    | 4.19  | 119.77      | 112.30   |
| 55  | w     | 54   | 5MU  | C5-C4-N3    | 4.17  | 118.87      | 115.31   |
| 1   | A     | 747  | 5MC  | CM5-C5-C6   | -4.11 | 117.36      | 122.85   |
| 1   | A     | 955  | PSU  | C6-C5-C4    | -4.04 | 115.37      | 118.20   |
| 55  | v     | 54   | 5MU  | C5-C4-N3    | 4.04  | 118.76      | 115.31   |
| 34  | a     | 1519 | MA6  | C4-C5-N7    | -3.98 | 105.25      | 109.40   |
| 57  | y     | 37   | MIA  | C16-C14-C13 | -3.94 | 111.25      | 122.65   |
| 1   | A     | 2449 | H2U  | N3-C2-N1    | 3.94  | 120.82      | 116.65   |
| 57  | y     | 39   | PSU  | O2-C2-N1    | -3.92 | 118.47      | 122.79   |
| 1   | A     | 746  | PSU  | C4-N3-C2    | -3.91 | 120.70      | 126.34   |
| 57  | y     | 54   | 5MU  | O4-C4-C5    | -3.91 | 120.37      | 124.90   |
| 1   | A     | 955  | PSU  | C4-N3-C2    | -3.90 | 120.72      | 126.34   |
| 55  | v     | 7    | 4SU  | C5-C4-S4    | -3.84 | 119.52      | 124.47   |
| 55  | w     | 20   | H2U  | C4-N3-C2    | -3.82 | 122.62      | 125.79   |
| 1   | A     | 1917 | PSU  | C4-N3-C2    | -3.82 | 120.84      | 126.34   |
| 1   | A     | 1911 | PSU  | C4-N3-C2    | -3.78 | 120.90      | 126.34   |
| 57  | y     | 55   | PSU  | C4-N3-C2    | -3.74 | 120.94      | 126.34   |
| 34  | a     | 1518 | MA6  | N3-C2-N1    | -3.74 | 122.83      | 128.68   |
| 57  | y     | 8    | 4SU  | C5-C4-S4    | -3.72 | 119.67      | 124.47   |
| 1   | A     | 1939 | 5MU  | C5-C4-N3    | 3.71  | 118.48      | 115.31   |
| 1   | A     | 1939 | 5MU  | O4-C4-C5    | -3.70 | 120.61      | 124.90   |
| 55  | w     | 55   | PSU  | C4-N3-C2    | -3.70 | 121.01      | 126.34   |
| 1   | A     | 2604 | PSU  | C4-N3-C2    | -3.69 | 121.02      | 126.34   |
| 1   | A     | 2552 | OMU  | C1'-N1-C2   | 3.66  | 124.19      | 117.57   |
| 1   | A     | 747  | 5MC  | C5-C4-N3    | -3.65 | 117.73      | 121.67   |
| 57  | y     | 32   | PSU  | C4-N3-C2    | -3.64 | 121.10      | 126.34   |
| 34  | a     | 1518 | MA6  | C3'-C2'-C1' | 3.63  | 106.44      | 100.98   |
| 57  | y     | 37   | MIA  | C4-C5-N7    | -3.59 | 105.66      | 109.40   |
| 55  | v     | 55   | PSU  | C4-N3-C2    | -3.57 | 121.20      | 126.34   |
| 34  | a     | 1498 | UR3  | C1'-N1-C2   | 3.54  | 122.97      | 116.99   |
| 57  | y     | 37   | MIA  | C15-C14-C13 | -3.52 | 112.49      | 122.65   |
| 57  | y     | 20   | H2U  | C4-N3-C2    | -3.51 | 122.88      | 125.79   |
| 1   | A     | 2504 | PSU  | C4-N3-C2    | -3.48 | 121.32      | 126.34   |
| 34  | a     | 516  | PSU  | C4-N3-C2    | -3.48 | 121.33      | 126.34   |
| 57  | y     | 54   | 5MU  | C5M-C5-C4   | 3.47  | 122.58      | 118.77   |
| 1   | A     | 1618 | 6MZ  | C3'-C2'-C1' | 3.44  | 106.16      | 100.98   |
| 1   | A     | 2030 | 6MZ  | C3'-C2'-C1' | 3.43  | 106.15      | 100.98   |
| 34  | a     | 516  | PSU  | C3'-C2'-C1' | 3.43  | 105.63      | 101.64   |
| 1   | A     | 746  | PSU  | O2-C2-N1    | -3.40 | 119.04      | 122.79   |
| 55  | w     | 8    | 4SU  | C5-C4-S4    | -3.40 | 120.09      | 124.47   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | A     | 1618 | 6MZ  | C9-N6-C6    | -3.38 | 119.96      | 122.87   |
| 57  | y     | 16   | H2U  | C4-N3-C2    | -3.37 | 123.00      | 125.79   |
| 1   | A     | 2605 | PSU  | O2-C2-N1    | -3.35 | 119.11      | 122.79   |
| 1   | A     | 2030 | 6MZ  | C9-N6-C6    | -3.34 | 120.00      | 122.87   |
| 1   | A     | 2552 | OMU  | C5-C4-N3    | 3.33  | 119.83      | 114.84   |
| 1   | A     | 2580 | PSU  | C4-N3-C2    | -3.32 | 121.55      | 126.34   |
| 1   | A     | 955  | PSU  | O2-C2-N1    | -3.31 | 119.15      | 122.79   |
| 1   | A     | 1911 | PSU  | O2-C2-N1    | -3.31 | 119.15      | 122.79   |
| 57  | y     | 39   | PSU  | C6-C5-C4    | -3.29 | 115.90      | 118.20   |
| 55  | w     | 55   | PSU  | O2-C2-N1    | -3.29 | 119.17      | 122.79   |
| 57  | y     | 39   | PSU  | C4-N3-C2    | -3.28 | 121.61      | 126.34   |
| 1   | A     | 1917 | PSU  | C6-C5-C4    | -3.27 | 115.91      | 118.20   |
| 57  | y     | 32   | PSU  | O2-C2-N1    | -3.26 | 119.20      | 122.79   |
| 55  | w     | 54   | 5MU  | C5M-C5-C4   | 3.23  | 122.32      | 118.77   |
| 34  | a     | 1519 | MA6  | N3-C2-N1    | -3.21 | 123.67      | 128.68   |
| 55  | v     | 20   | H2U  | C3'-C2'-C1' | 3.20  | 107.51      | 101.43   |
| 1   | A     | 1618 | 6MZ  | N3-C2-N1    | -3.18 | 123.71      | 128.68   |
| 57  | y     | 55   | PSU  | O2-C2-N1    | -3.17 | 119.30      | 122.79   |
| 1   | A     | 745  | 1MG  | O6-C6-C5    | -3.15 | 118.61      | 124.19   |
| 1   | A     | 2457 | PSU  | C4-N3-C2    | -3.15 | 121.80      | 126.34   |
| 1   | A     | 2030 | 6MZ  | N3-C2-N1    | -3.15 | 123.76      | 128.68   |
| 34  | a     | 516  | PSU  | C6-C5-C4    | -3.14 | 116.00      | 118.20   |
| 55  | w     | 54   | 5MU  | O4-C4-C5    | -3.14 | 121.26      | 124.90   |
| 57  | y     | 20   | H2U  | O4'-C1'-N1  | 3.13  | 113.57      | 109.30   |
| 1   | A     | 1911 | PSU  | C6-C5-C4    | -3.12 | 116.01      | 118.20   |
| 55  | v     | 55   | PSU  | O2-C2-N1    | -3.11 | 119.37      | 122.79   |
| 1   | A     | 1917 | PSU  | O2-C2-N1    | -3.09 | 119.39      | 122.79   |
| 1   | A     | 1962 | 5MC  | O2-C2-N3    | -3.05 | 117.37      | 122.33   |
| 1   | A     | 746  | PSU  | C6-C5-C4    | -3.04 | 116.07      | 118.20   |
| 34  | a     | 967  | 5MC  | O2-C2-N3    | -3.03 | 117.40      | 122.33   |
| 1   | A     | 2498 | OMC  | O2-C2-N3    | -3.03 | 117.41      | 122.33   |
| 34  | a     | 1407 | 5MC  | O2-C2-N3    | -3.02 | 117.42      | 122.33   |
| 1   | A     | 1939 | 5MU  | C5-C6-N1    | -3.00 | 120.25      | 123.34   |
| 55  | w     | 55   | PSU  | C3'-C2'-C1' | 2.97  | 105.10      | 101.64   |
| 55  | v     | 20   | H2U  | N3-C2-N1    | 2.97  | 119.80      | 116.65   |
| 57  | y     | 55   | PSU  | C6-C5-C4    | -2.95 | 116.13      | 118.20   |
| 1   | A     | 2457 | PSU  | O2-C2-N1    | -2.95 | 119.54      | 122.79   |
| 1   | A     | 2069 | 7MG  | C5-C6-N1    | 2.94  | 116.16      | 110.99   |
| 34  | a     | 527  | 7MG  | C5-C6-N1    | 2.92  | 116.14      | 110.99   |
| 55  | v     | 54   | 5MU  | O4-C4-C5    | -2.91 | 121.53      | 124.90   |
| 57  | y     | 8    | 4SU  | C6-N1-C2    | -2.90 | 117.28      | 120.99   |
| 1   | A     | 2605 | PSU  | C6-C5-C4    | -2.89 | 116.18      | 118.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 57  | y     | 46   | 7MG  | C5-C6-N1    | 2.89  | 116.08      | 110.99   |
| 1   | A     | 2552 | OMU  | O4-C4-C5    | -2.88 | 120.10      | 125.16   |
| 1   | A     | 2504 | PSU  | O2-C2-N1    | -2.86 | 119.64      | 122.79   |
| 1   | A     | 2503 | 2MA  | C5-C6-N1    | 2.85  | 118.94      | 114.02   |
| 57  | y     | 37   | MIA  | C2-N1-C6    | 2.84  | 122.28      | 117.19   |
| 34  | a     | 1407 | 5MC  | C5-C4-N3    | -2.84 | 118.61      | 121.67   |
| 1   | A     | 2552 | OMU  | O2-C2-N3    | -2.83 | 116.22      | 121.50   |
| 34  | a     | 967  | 5MC  | C5-C4-N3    | -2.83 | 118.62      | 121.67   |
| 34  | a     | 966  | 2MG  | C5-C6-N1    | 2.79  | 118.87      | 113.95   |
| 55  | v     | 20   | H2U  | C5-C4-N3    | 2.78  | 119.78      | 116.65   |
| 1   | A     | 2449 | H2U  | C4-N3-C2    | -2.78 | 123.49      | 125.79   |
| 1   | A     | 2580 | PSU  | C3'-C2'-C1' | 2.77  | 104.86      | 101.64   |
| 55  | v     | 55   | PSU  | C6-C5-C4    | -2.77 | 116.26      | 118.20   |
| 34  | a     | 1518 | MA6  | C4-C5-N7    | -2.77 | 106.52      | 109.40   |
| 1   | A     | 745  | 1MG  | C5-C6-N1    | 2.75  | 118.03      | 113.90   |
| 34  | a     | 1519 | MA6  | C10-N6-C6   | -2.70 | 111.35      | 119.51   |
| 34  | a     | 516  | PSU  | O2-C2-N1    | -2.70 | 119.82      | 122.79   |
| 1   | A     | 2030 | 6MZ  | C4-C5-N7    | -2.68 | 106.61      | 109.40   |
| 34  | a     | 1402 | 4OC  | C6-C5-C4    | 2.67  | 120.22      | 116.96   |
| 1   | A     | 1618 | 6MZ  | C4-C5-N7    | -2.66 | 106.63      | 109.40   |
| 1   | A     | 1962 | 5MC  | C5-C4-N3    | -2.65 | 118.81      | 121.67   |
| 55  | w     | 20   | H2U  | C5-C6-N1    | -2.64 | 102.91      | 111.61   |
| 57  | y     | 20   | H2U  | C5-C4-N3    | 2.61  | 119.58      | 116.65   |
| 34  | a     | 1207 | 2MG  | C8-N7-C5    | 2.61  | 107.96      | 102.99   |
| 57  | y     | 37   | MIA  | C16-C14-C15 | -2.60 | 108.86      | 114.60   |
| 34  | a     | 1516 | 2MG  | C5-C6-N1    | 2.59  | 118.52      | 113.95   |
| 1   | A     | 2604 | PSU  | C6-C5-C4    | -2.56 | 116.41      | 118.20   |
| 1   | A     | 2604 | PSU  | O2-C2-N1    | -2.56 | 119.97      | 122.79   |
| 1   | A     | 747  | 5MC  | O2-C2-N3    | -2.55 | 118.18      | 122.33   |
| 57  | y     | 32   | PSU  | C3'-C2'-C1' | 2.55  | 104.61      | 101.64   |
| 55  | v     | 20   | H2U  | O4'-C1'-N1  | 2.55  | 112.77      | 109.30   |
| 34  | a     | 1498 | UR3  | C3U-N3-C2   | 2.53  | 121.75      | 117.31   |
| 1   | A     | 747  | 5MC  | C5-C6-N1    | -2.53 | 120.73      | 123.34   |
| 34  | a     | 1516 | 2MG  | C8-N7-C5    | 2.50  | 107.75      | 102.99   |
| 1   | A     | 2251 | OMG  | O6-C6-C5    | -2.50 | 119.50      | 124.37   |
| 55  | w     | 8    | 4SU  | C6-N1-C2    | -2.49 | 117.81      | 120.99   |
| 1   | A     | 2445 | 2MG  | C5-C6-N1    | 2.48  | 118.34      | 113.95   |
| 1   | A     | 1835 | 2MG  | C5-C6-N1    | 2.48  | 118.32      | 113.95   |
| 57  | y     | 37   | MIA  | C3'-C2'-C1' | 2.47  | 104.70      | 100.98   |
| 34  | a     | 527  | 7MG  | CM7-N7-C5   | 2.47  | 132.77      | 126.40   |
| 57  | y     | 16   | H2U  | C5-C4-N3    | 2.47  | 119.42      | 116.65   |
| 57  | y     | 16   | H2U  | O4'-C1'-N1  | 2.46  | 112.65      | 109.30   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | A     | 2580 | PSU  | C6-C5-C4    | -2.45 | 116.49      | 118.20   |
| 34  | a     | 527  | 7MG  | O4'-C1'-N9  | 2.45  | 112.63      | 109.30   |
| 57  | y     | 32   | PSU  | C6-C5-C4    | -2.45 | 116.49      | 118.20   |
| 1   | A     | 2552 | OMU  | C6-N1-C2    | -2.45 | 117.86      | 120.99   |
| 34  | a     | 1518 | MA6  | C9-N6-C6    | -2.42 | 112.18      | 119.51   |
| 1   | A     | 747  | 5MC  | C3'-C2'-C1' | 2.42  | 106.03      | 101.43   |
| 1   | A     | 2580 | PSU  | O2-C2-N3    | -2.42 | 117.26      | 121.82   |
| 34  | a     | 1402 | 4OC  | O4'-C1'-N1  | 2.42  | 113.88      | 108.36   |
| 57  | y     | 20   | H2U  | C3'-C2'-C1' | 2.41  | 106.00      | 101.43   |
| 1   | A     | 2069 | 7MG  | O4'-C1'-N9  | 2.41  | 112.58      | 109.30   |
| 1   | A     | 2069 | 7MG  | N2-C2-N3    | -2.41 | 115.05      | 119.73   |
| 1   | A     | 1962 | 5MC  | CM5-C5-C6   | -2.40 | 119.64      | 122.85   |
| 34  | a     | 966  | 2MG  | C8-N7-C5    | 2.40  | 107.55      | 102.99   |
| 1   | A     | 2498 | OMC  | O4'-C1'-N1  | 2.39  | 113.83      | 108.36   |
| 57  | y     | 37   | MIA  | N3-C2-N1    | -2.38 | 122.59      | 126.98   |
| 34  | a     | 1207 | 2MG  | C5-C6-N1    | 2.38  | 118.15      | 113.95   |
| 1   | A     | 2457 | PSU  | C6-C5-C4    | -2.37 | 116.54      | 118.20   |
| 55  | v     | 7    | 4SU  | C6-N1-C2    | -2.37 | 117.96      | 120.99   |
| 34  | a     | 967  | 5MC  | C3'-C2'-C1' | 2.37  | 105.93      | 101.43   |
| 1   | A     | 2445 | 2MG  | C8-N7-C5    | 2.35  | 107.47      | 102.99   |
| 1   | A     | 1915 | 3TD  | C3'-C2'-C1' | 2.34  | 104.36      | 101.64   |
| 55  | w     | 55   | PSU  | C6-C5-C4    | -2.33 | 116.57      | 118.20   |
| 34  | a     | 1407 | 5MC  | C5-C6-N1    | -2.33 | 120.94      | 123.34   |
| 34  | a     | 1402 | 4OC  | C2'-C1'-N1  | -2.32 | 109.72      | 114.22   |
| 55  | w     | 54   | 5MU  | C5M-C5-C6   | -2.32 | 119.75      | 122.85   |
| 55  | v     | 54   | 5MU  | C5-C6-N1    | -2.31 | 120.96      | 123.34   |
| 55  | v     | 54   | 5MU  | C6-N1-C2    | -2.31 | 118.96      | 121.30   |
| 57  | y     | 54   | 5MU  | C1'-N1-C2   | 2.30  | 121.74      | 117.57   |
| 1   | A     | 2449 | H2U  | C5-C4-N3    | 2.29  | 119.23      | 116.65   |
| 57  | y     | 54   | 5MU  | C5M-C5-C6   | -2.29 | 119.79      | 122.85   |
| 1   | A     | 1939 | 5MU  | O2-C2-N1    | -2.29 | 119.75      | 122.79   |
| 34  | a     | 1402 | 4OC  | O2-C2-N3    | -2.28 | 118.62      | 122.33   |
| 1   | A     | 2552 | OMU  | O4'-C1'-N1  | 2.28  | 113.58      | 108.36   |
| 57  | y     | 8    | 4SU  | O2-C2-N3    | -2.28 | 117.26      | 121.50   |
| 57  | y     | 16   | H2U  | C3'-C2'-C1' | 2.28  | 105.75      | 101.43   |
| 34  | a     | 1407 | 5MC  | O4'-C1'-N1  | 2.27  | 113.55      | 108.36   |
| 55  | w     | 54   | 5MU  | C3'-C2'-C1' | 2.27  | 105.73      | 101.43   |
| 57  | y     | 46   | 7MG  | CM7-N7-C5   | 2.26  | 132.24      | 126.40   |
| 34  | a     | 527  | 7MG  | O6-C6-C5    | -2.25 | 122.01      | 127.54   |
| 34  | a     | 1402 | 4OC  | C5-C4-N3    | -2.25 | 118.97      | 122.59   |
| 55  | w     | 54   | 5MU  | O4'-C1'-N1  | 2.23  | 113.47      | 108.36   |
| 1   | A     | 745  | 1MG  | C8-N7-C5    | 2.23  | 107.23      | 102.99   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 57  | y     | 8    | 4SU  | C1'-N1-C2   | 2.22  | 121.58      | 117.57   |
| 1   | A     | 2504 | PSU  | C6-C5-C4    | -2.21 | 116.65      | 118.20   |
| 55  | w     | 54   | 5MU  | C5-C6-N1    | -2.20 | 121.07      | 123.34   |
| 1   | A     | 1939 | 5MU  | C5M-C5-C4   | 2.19  | 121.18      | 118.77   |
| 1   | A     | 2069 | 7MG  | N2-C2-N1    | 2.19  | 121.37      | 116.71   |
| 1   | A     | 2069 | 7MG  | O6-C6-C5    | -2.18 | 122.19      | 127.54   |
| 34  | a     | 966  | 2MG  | O6-C6-C5    | -2.18 | 120.12      | 124.37   |
| 34  | a     | 1519 | MA6  | C10-N6-C9   | -2.18 | 109.11      | 116.12   |
| 55  | v     | 20   | H2U  | C4-N3-C2    | -2.17 | 123.99      | 125.79   |
| 1   | A     | 2251 | OMG  | C5-C6-N1    | 2.16  | 117.76      | 113.95   |
| 57  | y     | 55   | PSU  | C3'-C2'-C1' | 2.13  | 104.12      | 101.64   |
| 1   | A     | 2251 | OMG  | O2'-C2'-C1' | 2.12  | 113.29      | 109.09   |
| 55  | v     | 55   | PSU  | C3'-C2'-C1' | 2.11  | 104.09      | 101.64   |
| 1   | A     | 2457 | PSU  | C3'-C2'-C1' | 2.10  | 104.08      | 101.64   |
| 1   | A     | 2503 | 2MA  | C8-N7-C5    | 2.10  | 106.99      | 102.99   |
| 34  | a     | 967  | 5MC  | C5-C6-N1    | -2.10 | 121.18      | 123.34   |
| 57  | y     | 46   | 7MG  | O6-C6-C5    | -2.10 | 122.39      | 127.54   |
| 55  | v     | 54   | 5MU  | O4'-C1'-N1  | 2.09  | 113.13      | 108.36   |
| 1   | A     | 2069 | 7MG  | CM7-N7-C5   | 2.08  | 131.77      | 126.40   |
| 55  | v     | 54   | 5MU  | O2-C2-N3    | -2.07 | 117.64      | 121.50   |
| 1   | A     | 2449 | H2U  | O4'-C1'-N1  | 2.05  | 112.10      | 109.30   |
| 57  | y     | 54   | 5MU  | C6-N1-C2    | -2.04 | 119.23      | 121.30   |
| 55  | w     | 54   | 5MU  | O2-C2-N3    | -2.04 | 117.71      | 121.50   |
| 1   | A     | 1939 | 5MU  | C5M-C5-C6   | -2.03 | 120.13      | 122.85   |
| 1   | A     | 747  | 5MC  | N1-C2-N3    | 2.03  | 122.51      | 118.81   |

There are no chirality outliers.

All (80) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 1   | A     | 746  | PSU  | C2'-C1'-C5-C4   |
| 1   | A     | 746  | PSU  | O4'-C1'-C5-C6   |
| 1   | A     | 2030 | 6MZ  | C4'-C5'-O5'-P   |
| 1   | A     | 2030 | 6MZ  | C3'-C4'-C5'-O5' |
| 1   | A     | 2069 | 7MG  | O4'-C4'-C5'-O5' |
| 1   | A     | 2069 | 7MG  | C3'-C4'-C5'-O5' |
| 1   | A     | 2445 | 2MG  | O4'-C4'-C5'-O5' |
| 1   | A     | 2445 | 2MG  | C3'-C4'-C5'-O5' |
| 1   | A     | 2552 | OMU  | O4'-C1'-N1-C2   |
| 1   | A     | 2552 | OMU  | O4'-C1'-N1-C6   |
| 34  | a     | 1498 | UR3  | O4'-C1'-N1-C6   |
| 34  | a     | 1498 | UR3  | O4'-C1'-N1-C2   |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 34  | a     | 1518 | MA6  | C5-C6-N6-C9     |
| 34  | a     | 1519 | MA6  | C5-C6-N6-C10    |
| 55  | v     | 20   | H2U  | O4'-C1'-N1-C2   |
| 55  | v     | 20   | H2U  | O4'-C1'-N1-C6   |
| 55  | v     | 55   | PSU  | O4'-C1'-C5-C4   |
| 55  | v     | 55   | PSU  | O4'-C1'-C5-C6   |
| 55  | w     | 8    | 4SU  | C3'-C4'-C5'-O5' |
| 55  | w     | 8    | 4SU  | O4'-C4'-C5'-O5' |
| 57  | y     | 20   | H2U  | O4'-C1'-N1-C2   |
| 57  | y     | 20   | H2U  | O4'-C1'-N1-C6   |
| 57  | y     | 37   | MIA  | O4'-C4'-C5'-O5' |
| 57  | y     | 37   | MIA  | C12-C13-C14-C15 |
| 57  | y     | 37   | MIA  | C12-C13-C14-C16 |
| 57  | y     | 46   | 7MG  | O4'-C4'-C5'-O5' |
| 1   | A     | 1962 | 5MC  | O4'-C4'-C5'-O5' |
| 1   | A     | 2504 | PSU  | O4'-C4'-C5'-O5' |
| 34  | a     | 1402 | 4OC  | O4'-C4'-C5'-O5' |
| 34  | a     | 1402 | 4OC  | C3'-C4'-C5'-O5' |
| 57  | y     | 37   | MIA  | C3'-C4'-C5'-O5' |
| 1   | A     | 1917 | PSU  | O4'-C4'-C5'-O5' |
| 1   | A     | 1962 | 5MC  | C3'-C4'-C5'-O5' |
| 1   | A     | 2030 | 6MZ  | O4'-C4'-C5'-O5' |
| 1   | A     | 2504 | PSU  | C3'-C4'-C5'-O5' |
| 57  | y     | 46   | 7MG  | C3'-C4'-C5'-O5' |
| 34  | a     | 1518 | MA6  | N1-C6-N6-C9     |
| 34  | a     | 1519 | MA6  | N1-C6-N6-C10    |
| 55  | w     | 8    | 4SU  | C2'-C1'-N1-C6   |
| 55  | w     | 8    | 4SU  | C2'-C1'-N1-C2   |
| 1   | A     | 1915 | 3TD  | C3'-C4'-C5'-O5' |
| 1   | A     | 1917 | PSU  | C3'-C4'-C5'-O5' |
| 1   | A     | 2604 | PSU  | O4'-C4'-C5'-O5' |
| 57  | y     | 16   | H2U  | O4'-C4'-C5'-O5' |
| 57  | y     | 16   | H2U  | C3'-C4'-C5'-O5' |
| 1   | A     | 1915 | 3TD  | O4'-C4'-C5'-O5' |
| 55  | v     | 7    | 4SU  | O4'-C4'-C5'-O5' |
| 55  | v     | 20   | H2U  | O4'-C4'-C5'-O5' |
| 55  | v     | 20   | H2U  | C4'-C5'-O5'-P   |
| 55  | w     | 8    | 4SU  | O4'-C1'-N1-C6   |
| 1   | A     | 2604 | PSU  | C3'-C4'-C5'-O5' |
| 57  | y     | 46   | 7MG  | C2'-C1'-N9-C8   |
| 55  | w     | 8    | 4SU  | O4'-C1'-N1-C2   |
| 1   | A     | 1618 | 6MZ  | C3'-C4'-C5'-O5' |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 55  | v     | 20   | H2U  | C3'-C4'-C5'-O5' |
| 1   | A     | 1618 | 6MZ  | O4'-C4'-C5'-O5' |
| 34  | a     | 527  | 7MG  | C3'-C4'-C5'-O5' |
| 34  | a     | 1519 | MA6  | C4'-C5'-O5'-P   |
| 34  | a     | 527  | 7MG  | C4'-C5'-O5'-P   |
| 34  | a     | 966  | 2MG  | C3'-C4'-C5'-O5' |
| 34  | a     | 966  | 2MG  | C4'-C5'-O5'-P   |
| 55  | v     | 7    | 4SU  | C3'-C4'-C5'-O5' |
| 55  | w     | 20   | H2U  | C2'-C1'-N1-C6   |
| 1   | A     | 746  | PSU  | O4'-C1'-C5-C4   |
| 57  | y     | 32   | PSU  | O4'-C1'-C5-C4   |
| 57  | y     | 39   | PSU  | O4'-C1'-C5-C4   |
| 57  | y     | 46   | 7MG  | O4'-C1'-N9-C8   |
| 1   | A     | 2457 | PSU  | O4'-C4'-C5'-O5' |
| 1   | A     | 1939 | 5MU  | O4'-C4'-C5'-O5' |
| 57  | y     | 37   | MIA  | N3-C2-S10-C11   |
| 57  | y     | 8    | 4SU  | C2'-C1'-N1-C2   |
| 55  | w     | 20   | H2U  | C2'-C1'-N1-C2   |
| 55  | w     | 55   | PSU  | O4'-C1'-C5-C6   |
| 57  | y     | 32   | PSU  | O4'-C1'-C5-C6   |
| 57  | y     | 39   | PSU  | O4'-C1'-C5-C6   |
| 1   | A     | 1939 | 5MU  | C3'-C4'-C5'-O5' |
| 1   | A     | 2457 | PSU  | C3'-C4'-C5'-O5' |
| 34  | a     | 966  | 2MG  | O4'-C4'-C5'-O5' |
| 57  | y     | 8    | 4SU  | O4'-C4'-C5'-O5' |
| 1   | A     | 1618 | 6MZ  | C4'-C5'-O5'-P   |

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 1481 ligands modelled in this entry, 1478 are monoatomic - leaving 3 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 |
| 59  | FME  | A     | 3001 | -    | 8,9,10       | 0.53 | 0        | 7,9,11      | 1.07 | 0        |
| 63  | GTP  | z     | 402  | 60   | 26,34,34     | 0.95 | 1 (3%)   | 32,54,54    | 1.47 | 5 (15%)  |
| 62  | PHE  | z     | 401  | -    | 10,11,12     | 0.38 | 0        | 10,13,15    | 0.29 | 0        |

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   |
|-----|------|-------|------|------|---------|------------|---------|
| 59  | FME  | A     | 3001 | -    | -       | 0/7/9/11   | -       |
| 63  | GTP  | z     | 402  | 60   | -       | 7/18/38/38 | 0/3/3/3 |
| 62  | PHE  | z     | 401  | -    | -       | 1/5/6/8    | 0/1/1/1 |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 63  | z     | 402 | GTP  | C6-N1 | -2.71 | 1.33        | 1.37     |

All (5) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 63  | z     | 402 | GTP  | PA-O3A-PB   | -3.58 | 120.55      | 132.83   |
| 63  | z     | 402 | GTP  | PB-O3B-PG   | -3.46 | 120.95      | 132.83   |
| 63  | z     | 402 | GTP  | C3'-C2'-C1' | 3.14  | 105.71      | 100.98   |
| 63  | z     | 402 | GTP  | C5-C6-N1    | 2.46  | 118.30      | 113.95   |
| 63  | z     | 402 | GTP  | C8-N7-C5    | 2.19  | 107.16      | 102.99   |

There are no chirality outliers.

All (8) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 62  | z     | 401 | PHE  | O-C-CA-CB       |
| 63  | z     | 402 | GTP  | C5'-O5'-PA-O1A  |
| 63  | z     | 402 | GTP  | C5'-O5'-PA-O2A  |
| 63  | z     | 402 | GTP  | C3'-C4'-C5'-O5' |

*Continued on next page...*

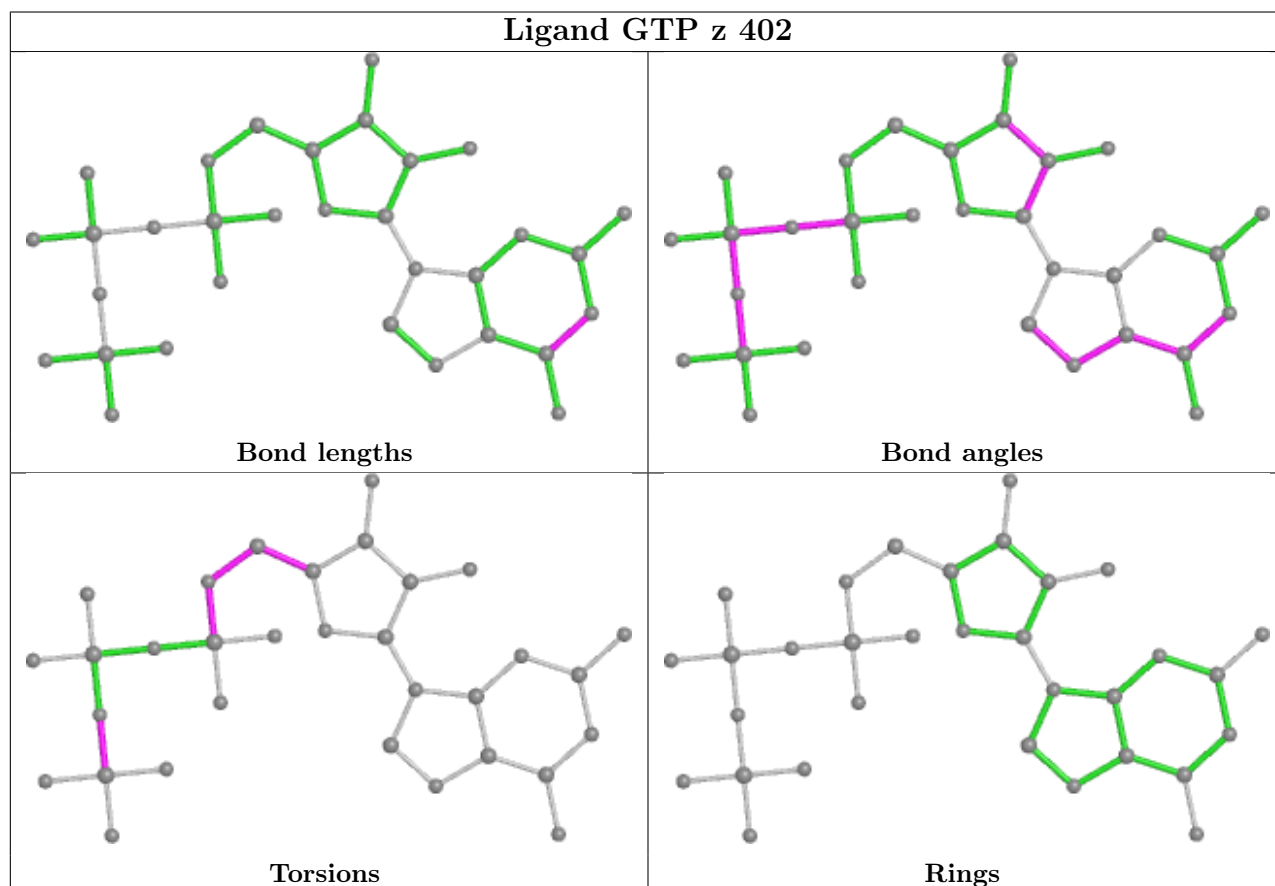
Continued from previous page...

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 63  | z     | 402 | GTP  | O4'-C4'-C5'-O5' |
| 63  | z     | 402 | GTP  | C4'-C5'-O5'-PA  |
| 63  | z     | 402 | GTP  | PB-O3B-PG-O1G   |
| 63  | z     | 402 | GTP  | C5'-O5'-PA-O3A  |

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

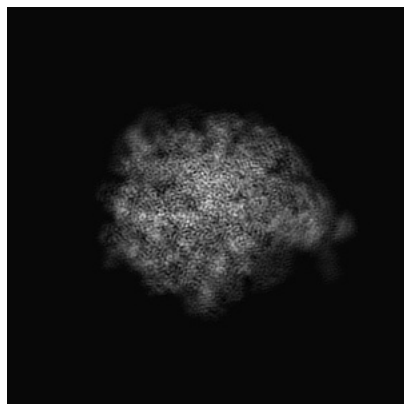
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8829. These allow visual inspection of the internal detail of the map and identification of artifacts.

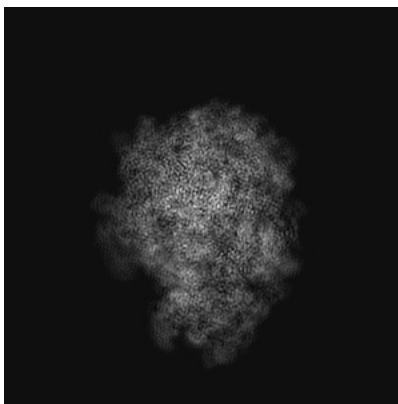
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

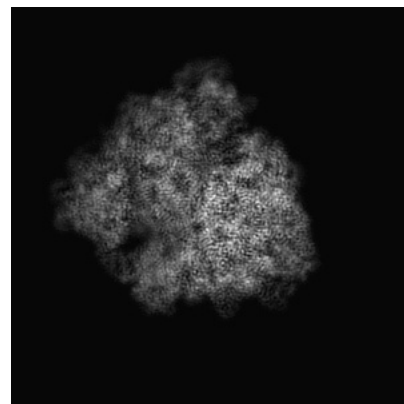
#### 6.1.1 Primary map



X

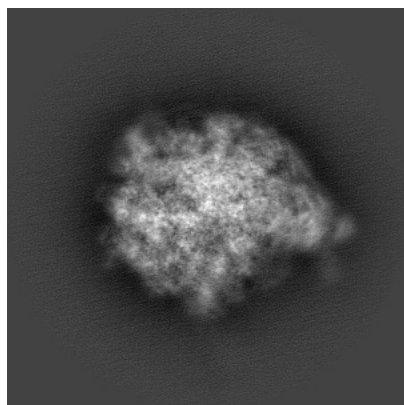


Y

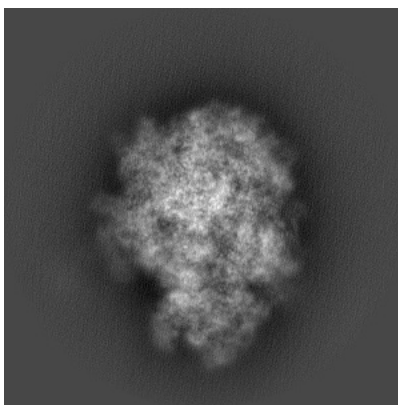


Z

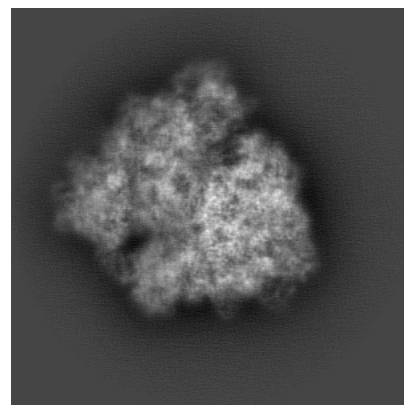
#### 6.1.2 Raw map



X



Y

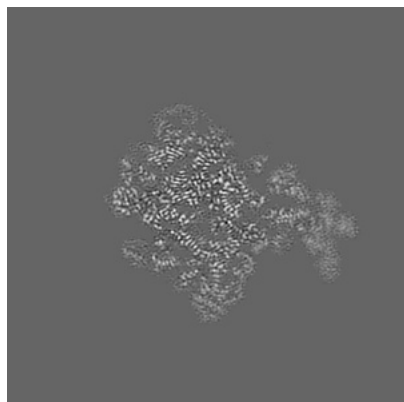


Z

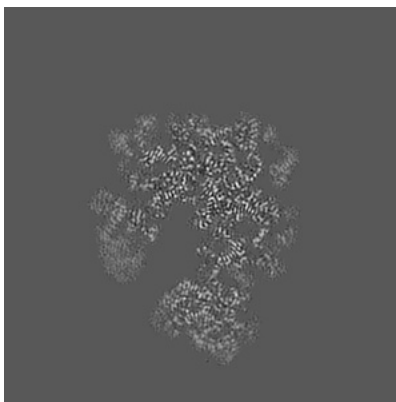
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

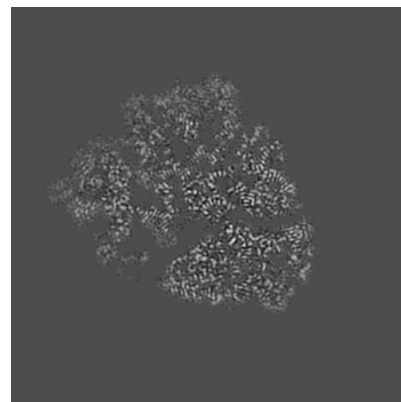
### 6.2.1 Primary map



X Index: 199

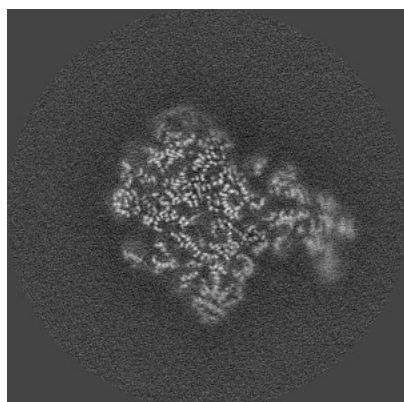


Y Index: 199

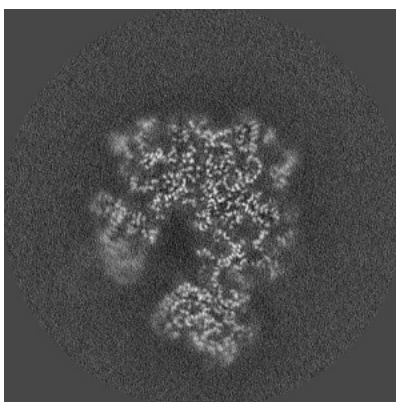


Z Index: 199

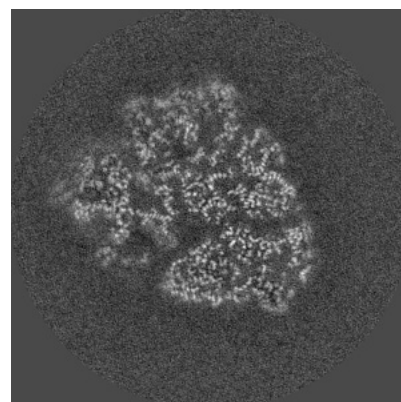
### 6.2.2 Raw map



X Index: 199



Y Index: 199



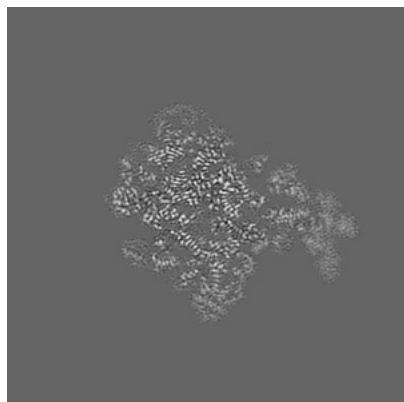
Z Index: 199

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

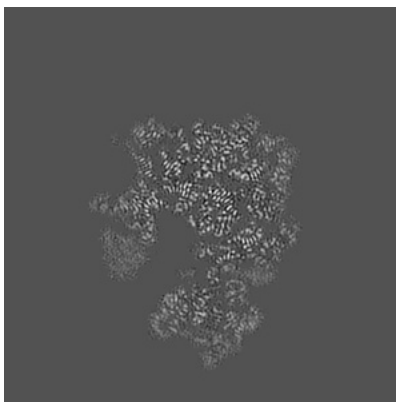


## 6.3 Largest variance slices [i](#)

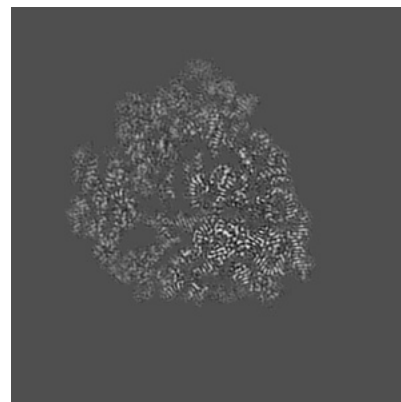
### 6.3.1 Primary map



X Index: 199

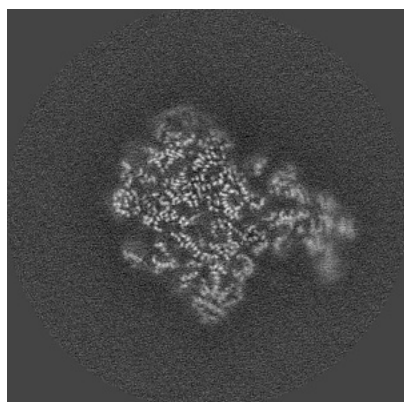


Y Index: 207

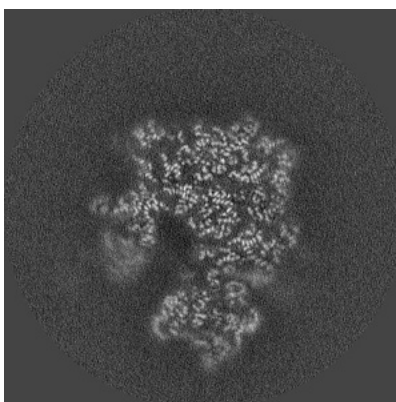


Z Index: 190

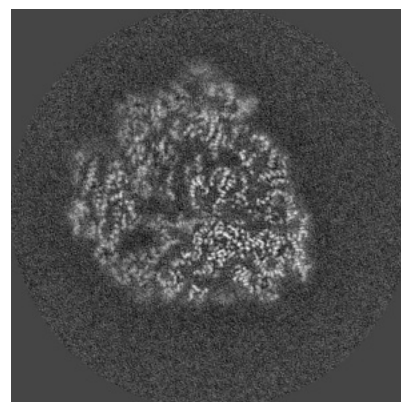
### 6.3.2 Raw map



X Index: 199



Y Index: 207

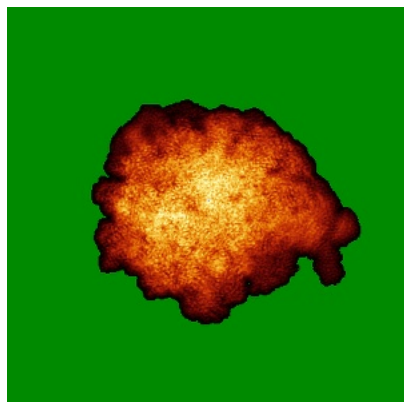


Z Index: 190

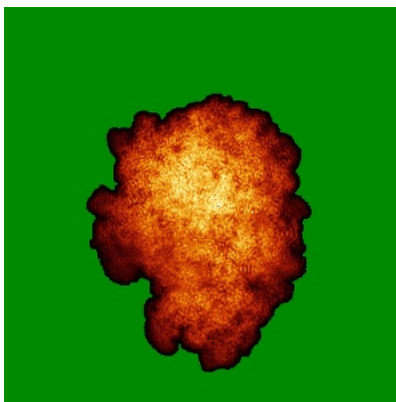
The images above show the largest variance slices of the map in three orthogonal directions.

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

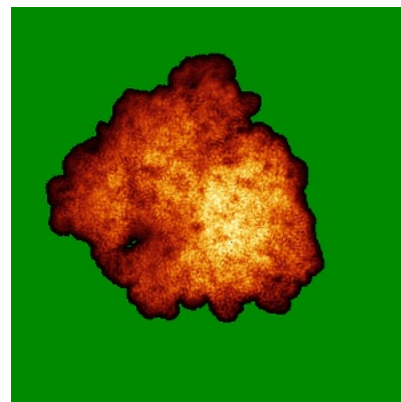
### 6.4.1 Primary map



X

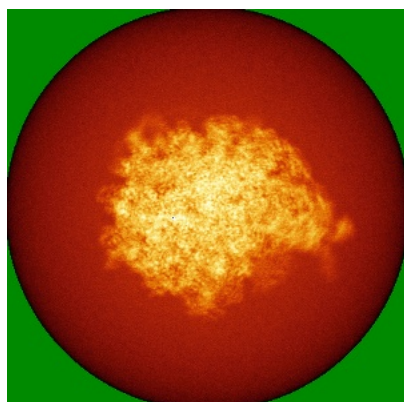


Y

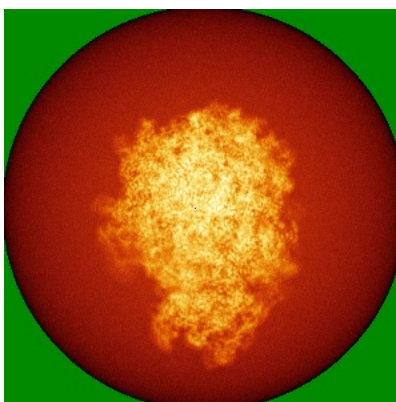


Z

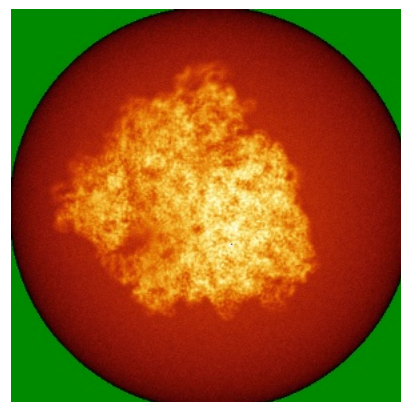
### 6.4.2 Raw map



X



Y

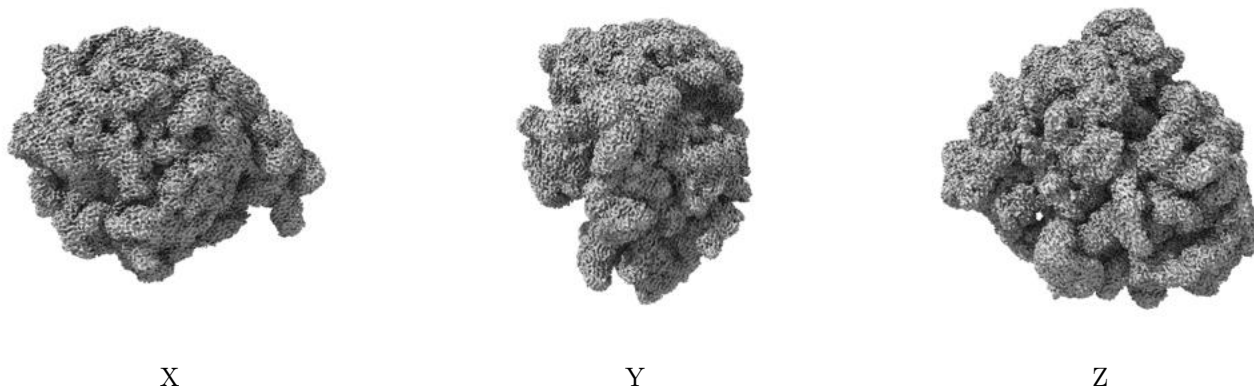


Z

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

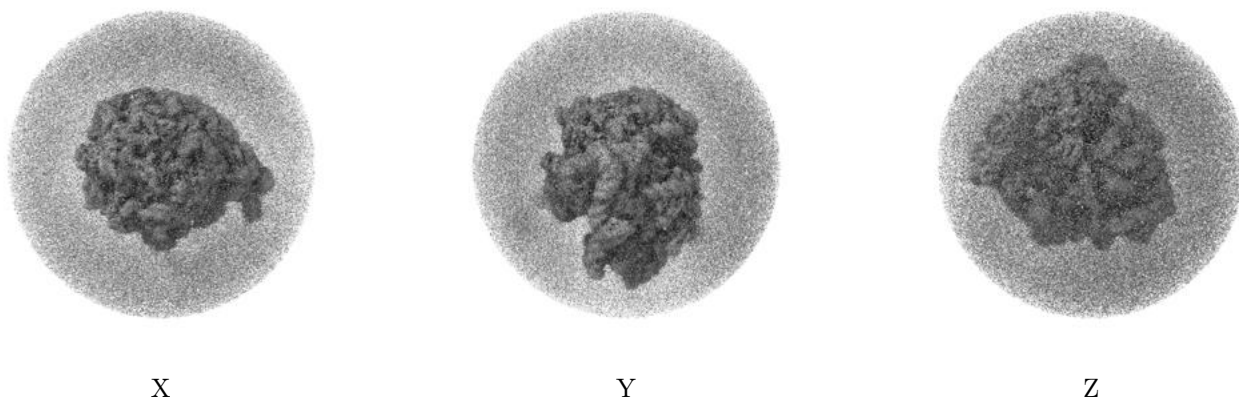
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.00532. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

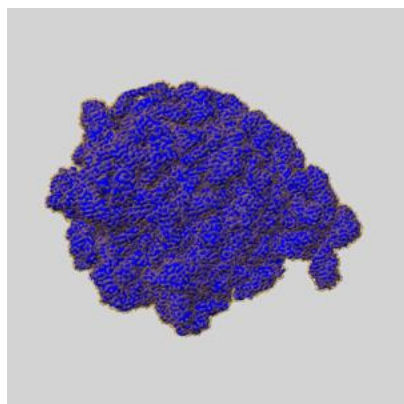
## 6.6 Mask visualisation [i](#)

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

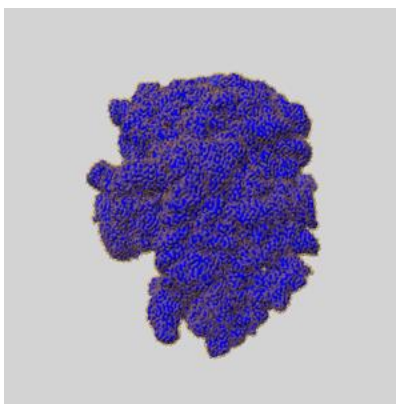
A mask typically either:

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

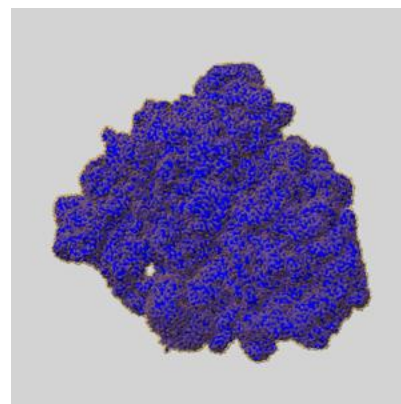
### 6.6.1 emd\_8829\_msk\_1.map [i](#)



X



Y

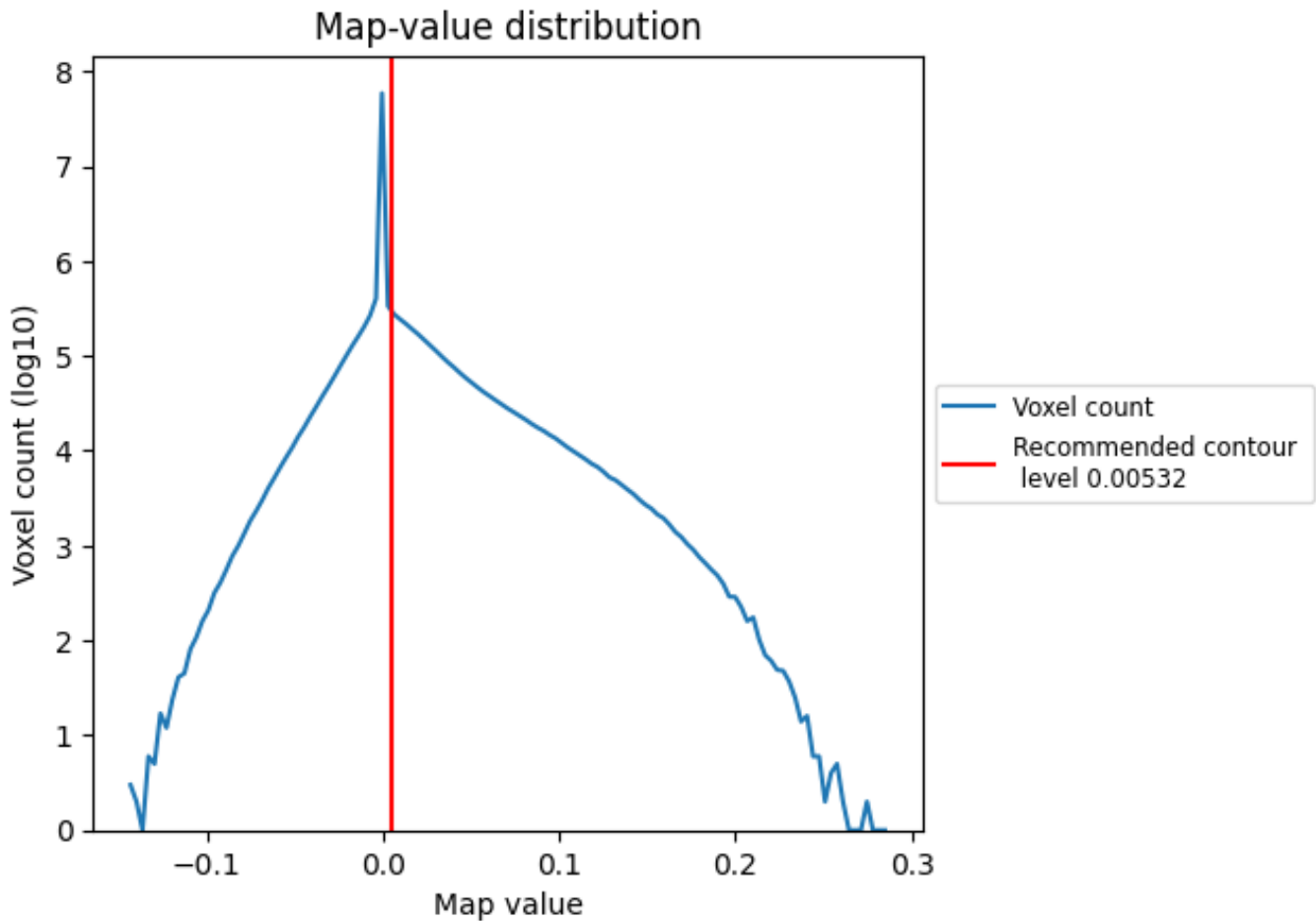


Z

## 7 Map analysis [i](#)

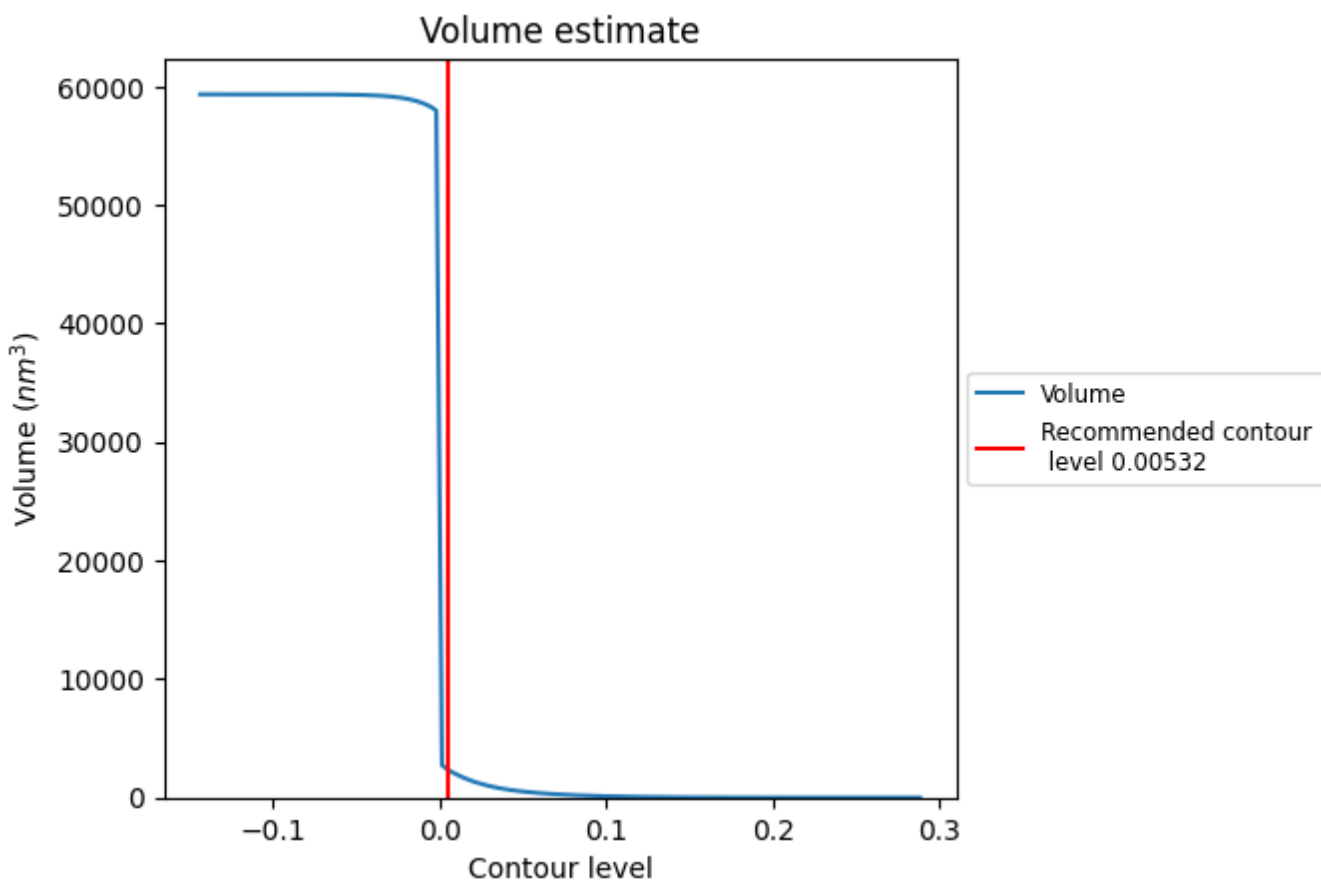
This section contains the results of statistical analysis of the map.

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



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

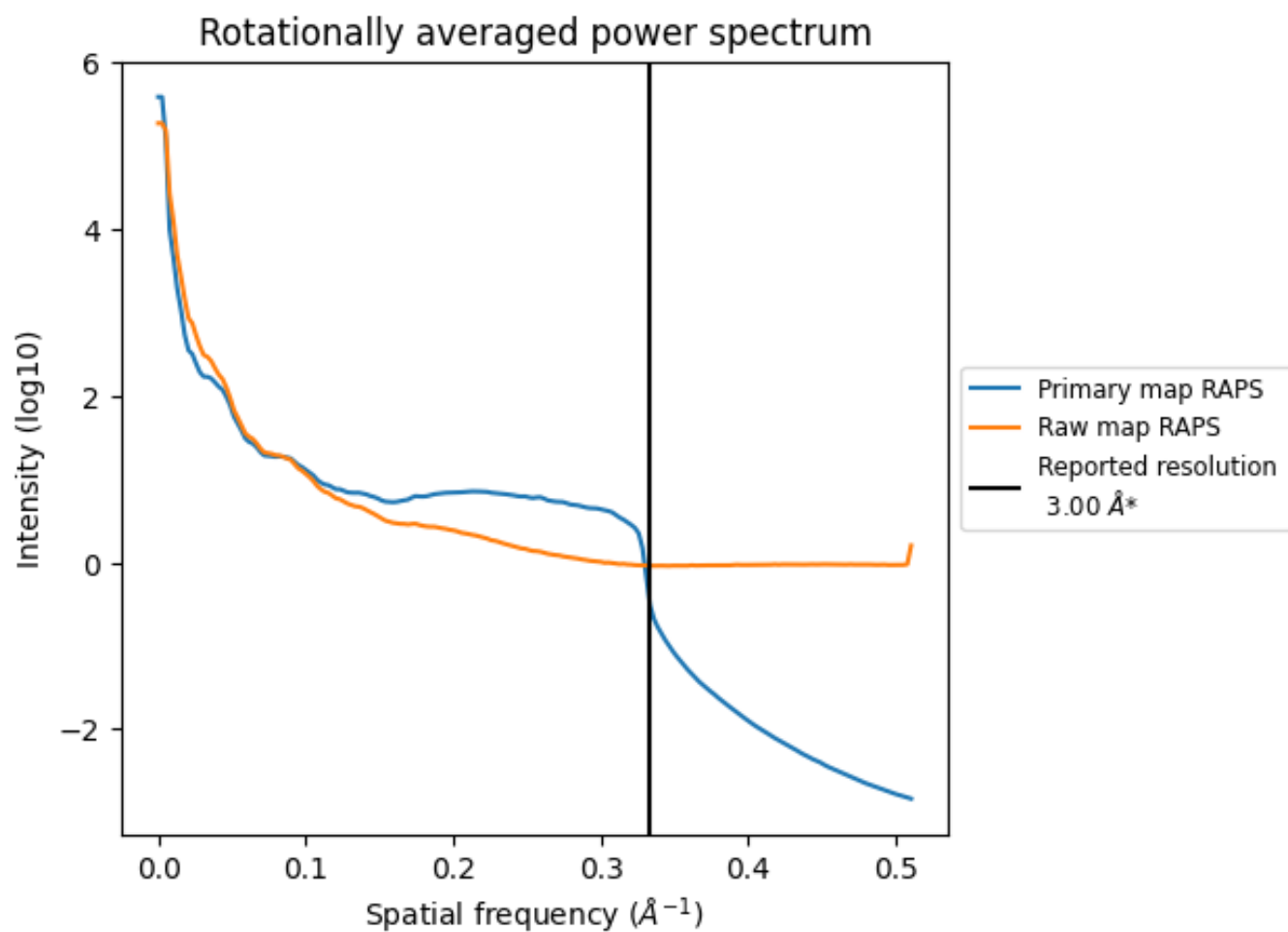
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2339  $\text{nm}^3$ ; this corresponds to an approximate mass of 2113 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 [i](#)

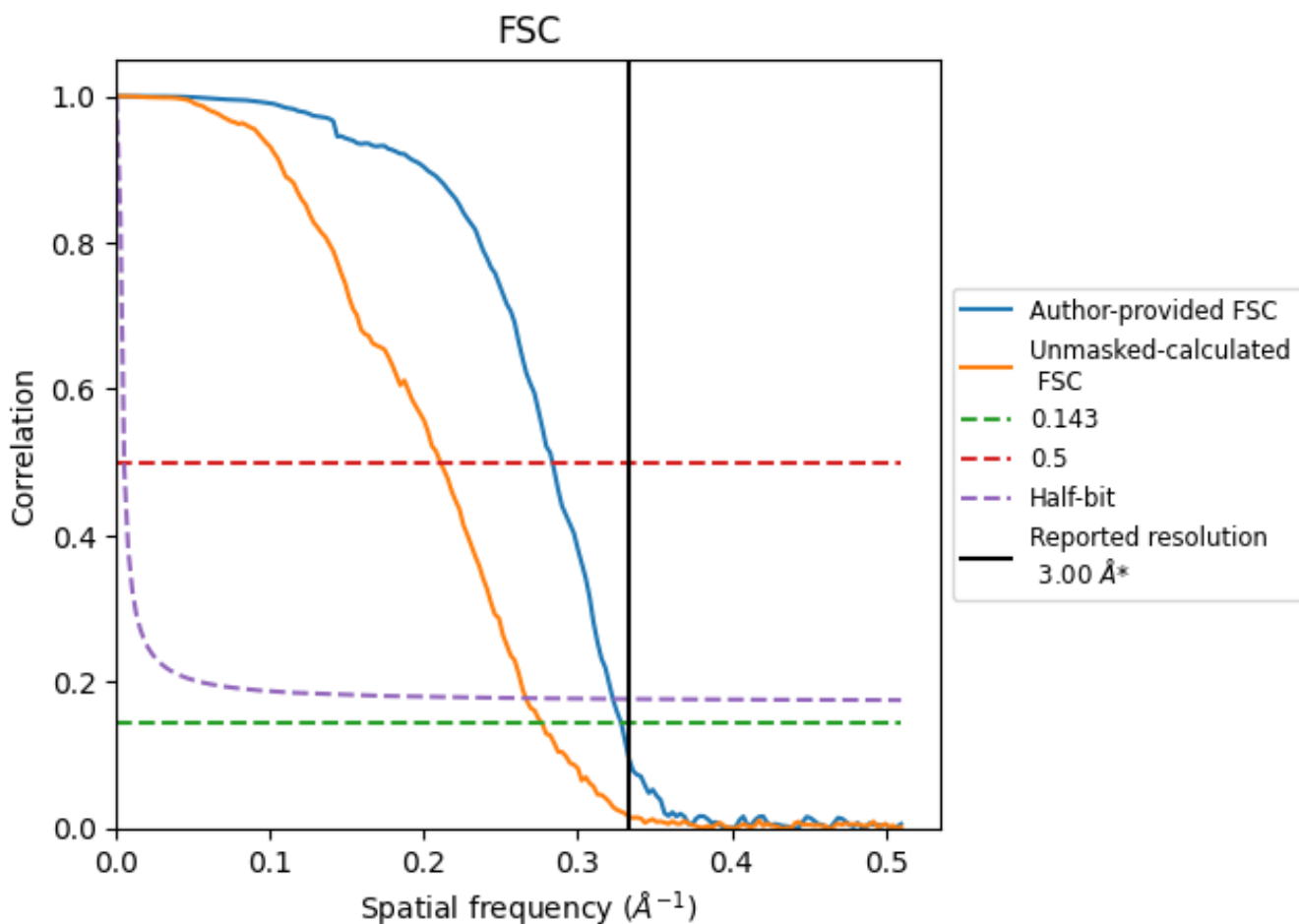


\*Reported resolution corresponds to spatial frequency of 0.333 Å<sup>-1</sup>

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

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

### 8.1 FSC [i](#)



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



## 8.2 Resolution estimates [i](#)

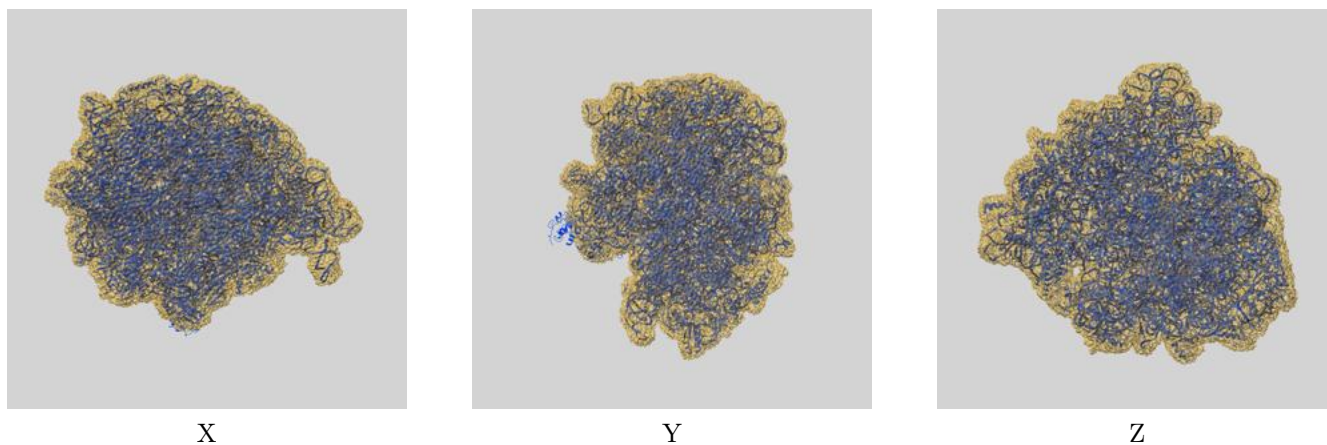
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 3.00                               | -    | -        |
| Author-provided FSC curve | 3.05                               | 3.53 | 3.10     |
| Unmasked-calculated*      | 3.61                               | 4.75 | 3.76     |

\*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 3.61 differs from the reported value 3.0 by more than 10 %

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

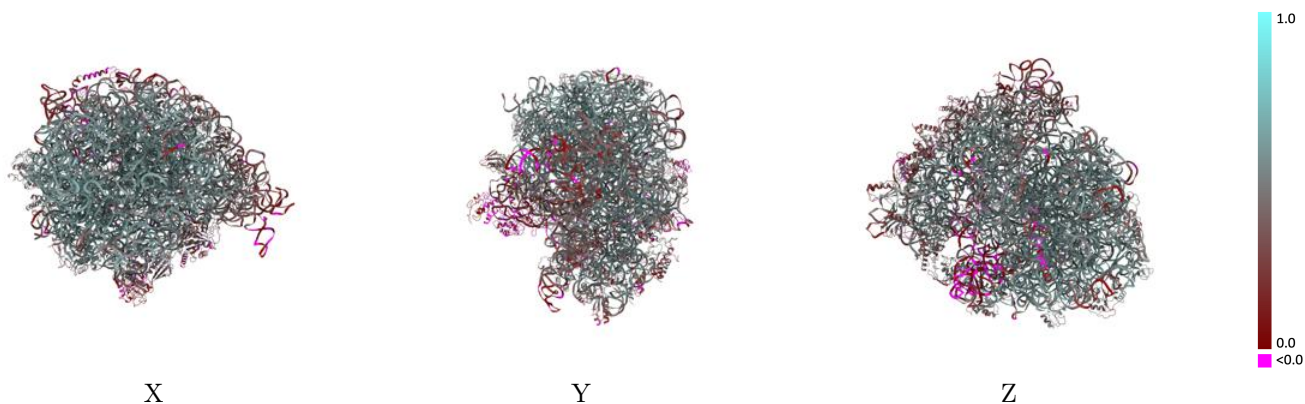
This section contains information regarding the fit between EMDB map EMD-8829 and PDB model 5WFS. Per-residue inclusion information can be found in section 3 on page 20.

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



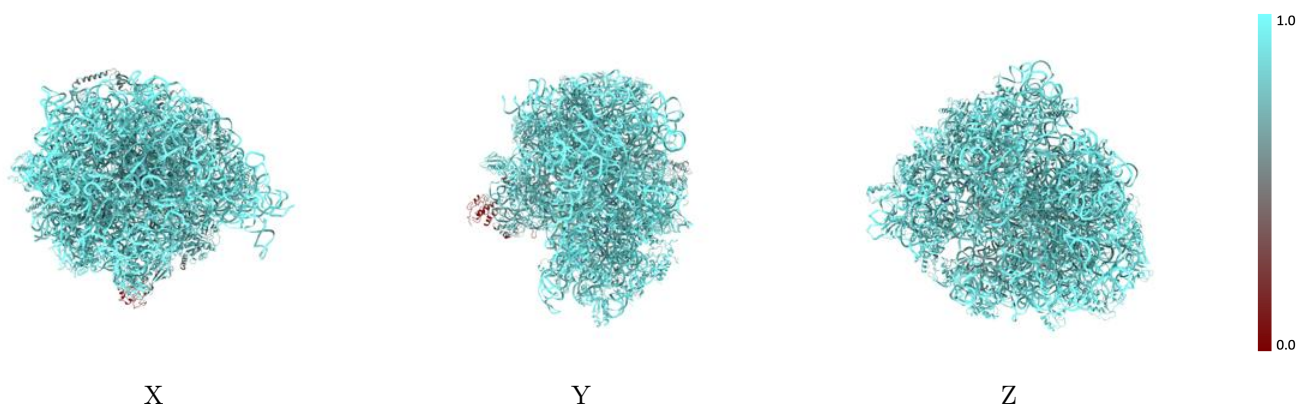
The images above show the 3D surface view of the map at the recommended contour level 0.00532 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



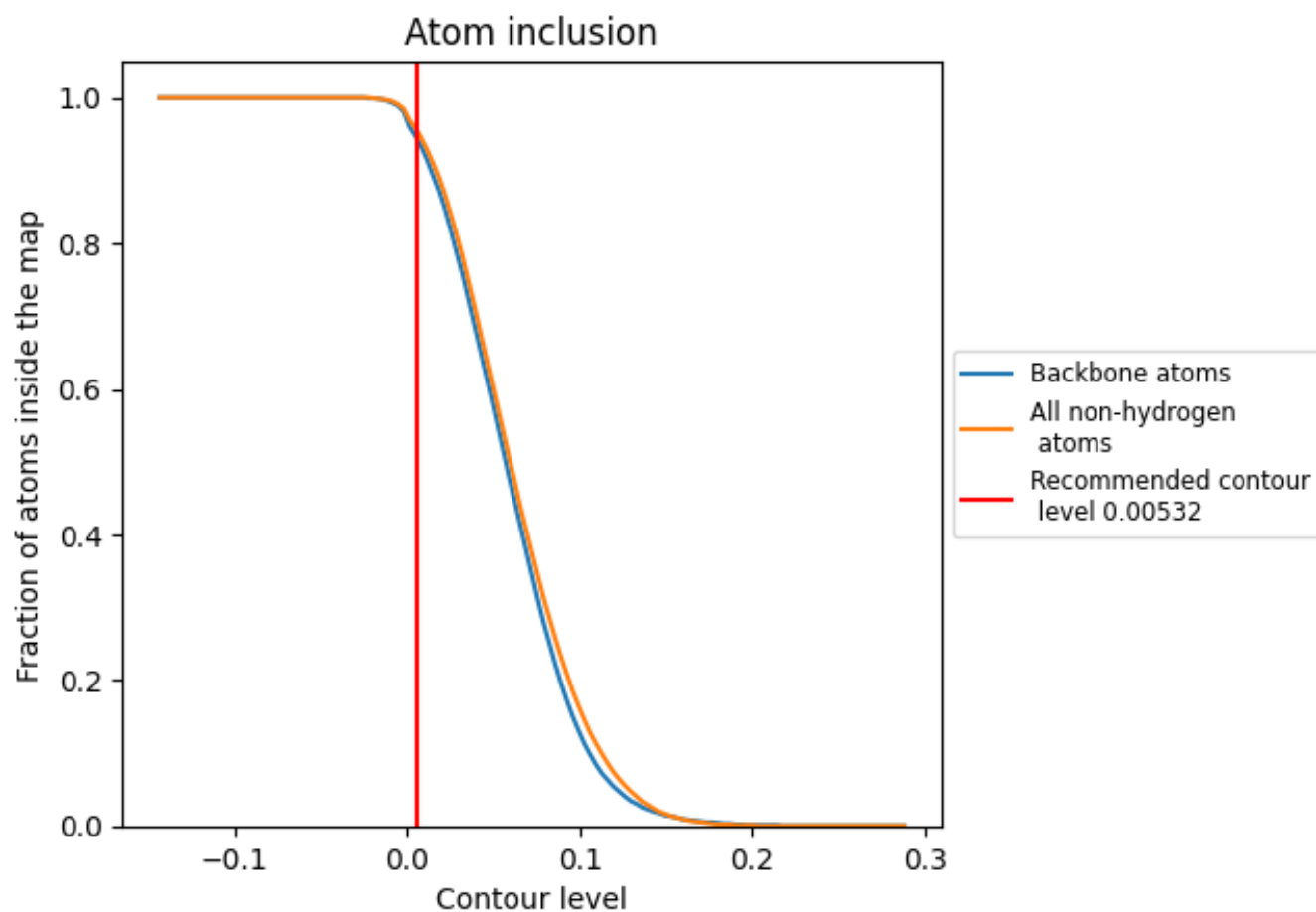
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.00532).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 96% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary



















































The table lists the average atom inclusion at the recommended contour level (0.00532) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion   | Q-score  |
|-------|--|--|
| All   |  0.9570   |  0.4750   |
| 0     |  0.9620   |  0.5080   |
| 1     |  0.9240   |  0.4640   |
| 2     |  0.9880   |  0.5860   |
| 3     |  0.9840   |  0.5760   |
| 4     |  0.9520   |  0.4940   |
| 5     |  0.1120   |  -0.0200  |
| 6     |  0.8880   |  0.3120   |
| A     |  0.9870   |  0.5350   |
| B     |  0.9940   |  0.5140   |
| C     |  0.9740   |  0.5550   |
| D     |  0.9660   |  0.5260   |
| E     |  0.9690   |  0.5080   |
| F     |  0.9360   |  0.4310   |
| G     |  0.9370  |  0.3790  |
| H     |  0.7350 |  0.2180 |
| I     |  0.6190 |  0.0210 |
| J     |  0.9650 |  0.5270 |
| K     |  0.9520 |  0.5180 |
| L     |  0.9650 |  0.5170 |
| M     |  0.9690 |  0.5180 |
| N     |  0.9860 |  0.5530 |
| O     |  0.9680 |  0.4480 |
| P     |  0.9570 |  0.5080 |
| Q     |  0.9560 |  0.5500 |
| R     |  0.9390 |  0.4830 |
| S     |  0.9520 |  0.5230 |
| T     |  0.9340 |  0.4560 |
| U     |  0.9450 |  0.4450 |
| V     |  0.9490 |  0.4600 |
| W     |  0.9640 |  0.5480 |
| X     |  0.9550 |  0.5170 |
| Y     |  0.9380 |  0.4430 |
| Z     |  0.9650 |  0.5020 |
| a     |  0.9870 |  0.4800 |



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| Chain | Atom inclusion   | Q-score  |
|-------|--|--|
| b     |  0.8950   |  0.3360   |
| c     |  0.9420   |  0.4360   |
| d     |  0.8990   |  0.2860   |
| e     |  0.9530   |  0.4820   |
| f     |  0.9230   |  0.4070   |
| g     |  0.9160   |  0.3700   |
| h     |  0.9490   |  0.4840   |
| i     |  0.9220   |  0.3850   |
| j     |  0.8960   |  0.3370   |
| k     |  0.9460   |  0.4300   |
| l     |  0.9080   |  0.4010   |
| m     |  0.9440   |  0.4280   |
| n     |  0.9500   |  0.4390   |
| o     |  0.9410   |  0.4440   |
| p     |  0.8930   |  0.2610   |
| q     |  0.9150   |  0.3710   |
| r     |  0.8970   |  0.4030   |
| s     |  0.9520  |  0.4260  |
| t     |  0.9200 |  0.3290 |
| u     |  0.8210 |  0.2580 |
| v     |  0.9720 |  0.4880 |
| w     |  0.7450 |  0.0740 |
| x     |  0.9840 |  0.4960 |
| y     |  0.9160 |  0.2870 |
| z     |  0.8290 |  0.2520 |