



## Full wwPDB EM Validation Report ⓘ

Dec 12, 2022 – 08:00 PM EST

PDB ID : 3JBV  
EMDB ID : EMD-6486  
Title : Mechanisms of Ribosome Stalling by SecM at Multiple Elongation Steps  
Authors : Zhang, J.; Pan, X.J.; Yan, K.G.; Sun, S.; Gao, N.; Sui, S.F.  
Deposited on : 2015-10-16  
Resolution : 3.32 Å(reported)  
Based on initial model : 4V7T

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:

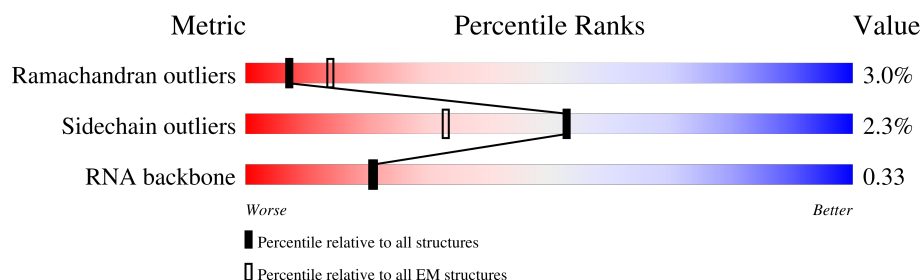
EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

# 1 Overall quality at a glance

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

The reported resolution of this entry is 3.32 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     | 1542   |                  |
| 2   | B     | 241    |                  |
| 3   | C     | 233    |                  |
| 4   | D     | 206    |                  |
| 5   | E     | 167    |                  |
| 6   | F     | 131    |                  |
| 7   | G     | 156    |                  |
| 8   | H     | 130    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 9   | I     | 130    |                  |
| 10  | J     | 103    |                  |
| 11  | K     | 129    |                  |
| 12  | L     | 124    |                  |
| 13  | M     | 118    |                  |
| 14  | N     | 101    |                  |
| 15  | O     | 89     |                  |
| 16  | P     | 82     |                  |
| 17  | Q     | 84     |                  |
| 18  | R     | 75     |                  |
| 19  | S     | 92     |                  |
| 20  | T     | 87     |                  |
| 21  | U     | 71     |                  |
| 22  | V     | 76     |                  |
| 23  | W     | 75     |                  |
| 24  | X     | 11     |                  |
| 25  | 0     | 78     |                  |
| 26  | 1     | 63     |                  |
| 27  | 2     | 59     |                  |
| 28  | 3     | 57     |                  |
| 29  | 4     | 55     |                  |
| 30  | 6     | 46     |                  |
| 31  | 7     | 65     |                  |
| 32  | 8     | 38     |                  |
| 33  | a     | 120    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 34  | b     | 2904   |                  |
| 35  | c     | 273    |                  |
| 36  | i     | 142    |                  |
| 37  | d     | 209    |                  |
| 38  | e     | 201    |                  |
| 39  | f     | 179    |                  |
| 40  | g     | 177    |                  |
| 41  | h     | 149    |                  |
| 42  | j     | 142    |                  |
| 43  | k     | 123    |                  |
| 44  | l     | 144    |                  |
| 45  | m     | 136    |                  |
| 46  | n     | 127    |                  |
| 47  | o     | 117    |                  |
| 48  | p     | 115    |                  |
| 49  | q     | 118    |                  |
| 50  | r     | 103    |                  |
| 51  | s     | 110    |                  |
| 52  | t     | 100    |                  |
| 53  | u     | 104    |                  |
| 54  | w     | 94     |                  |
| 55  | y     | 85     |                  |
| 56  | z     | 27     |                  |

## 2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 145911 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 RNA (1530-MER).

| Mol | Chain | Residues | Atoms |       |      |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|-------|
| 1   | A     | 1530     | Total | C     | N    | O     | P    | 0       | 0     |
|     |       |          | 32831 | 14642 | 6024 | 10635 | 1530 |         |       |

- Molecule 2 is a protein called 30S ribosomal protein S2.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 2   | B     | 218      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1704  | 1081 | 305 | 311 | 7 |         |       |

- Molecule 3 is a protein called 30S ribosomal protein S3.

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

- Molecule 4 is a protein called 30S ribosomal protein S4.

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

- Molecule 5 is a protein called 30S ribosomal protein S5.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 5   | E     | 150      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1105  | 687 | 211 | 201 | 6 |         |       |

- Molecule 6 is a protein called 30S ribosomal protein S6.

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

- Molecule 7 is a protein called 30S ribosomal protein S7.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 7   | G     | 150      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1174  | 730 | 226 | 214 | 4 |         |       |

- Molecule 8 is a protein called 30S ribosomal protein S8.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 8   | H     | 129      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 979   | 616 | 173 | 184 | 6 |         |       |

- Molecule 9 is a protein called 30S ribosomal protein S9.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 9   | I     | 127      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1022  | 634 | 206 | 179 | 3 |         |       |

- Molecule 10 is a protein called 30S ribosomal protein S10.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 10  | J     | 98       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 786   | 493 | 150 | 142 | 1 |         |       |

- Molecule 11 is a protein called 30S ribosomal protein S11.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 11  | K     | 117      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 877   | 540 | 174 | 160 | 3 |         |       |

- Molecule 12 is a protein called 30S ribosomal protein S12.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 12  | L     | 123      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 955   | 590 | 196 | 165 | 4 |         |       |

- Molecule 13 is a protein called 30S ribosomal protein S13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 13  | M     | 113      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 876   | 541 | 177 | 155 | 3 |         |       |

- Molecule 14 is a protein called 30S ribosomal protein S14.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 14  | N     | 96       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 774   | 483 | 160 | 128 | 3 |         |       |

- Molecule 15 is a protein called 30S ribosomal protein S15.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 15  | O     | 88       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 716   | 440 | 146 | 129 | 1 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| O     | 79      | ARG      | GLN    | conflict | UNP P0ADZ4 |

- Molecule 16 is a protein called 30S ribosomal protein S16.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 16  | P     | 82       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 649   | 406 | 128 | 114 | 1 |         |       |

- Molecule 17 is a protein called 30S ribosomal protein S17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 17  | Q     | 80       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 648   | 411 | 121 | 113 | 3 |         |       |

- Molecule 18 is a protein called 30S ribosomal protein S18.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 18  | R     | 55       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 455   | 288 | 86 | 81 |         |       |

- Molecule 19 is a protein called 30S ribosomal protein S19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 19  | S     | 79       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 637   | 408 | 120 | 107 | 2 |         |       |

- Molecule 20 is a protein called 30S ribosomal protein S20.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 20  | T     | 85       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 665   | 411 | 137 | 114 | 3 |         |       |

- Molecule 21 is a protein called 30S ribosomal protein S21.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 21  | U     | 51       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 425   | 265 | 86 | 73 | 1 |         |       |

- Molecule 22 is a RNA chain called RNA (76-MER).

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 22  | V     | 76       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 1620  | 723 | 290 | 532 | 75 |         |       |

- Molecule 23 is a RNA chain called RNA (75-MER).

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 23  | W     | 75       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 1599  | 713 | 287 | 525 | 74 |         |       |

- Molecule 24 is a RNA chain called RNA (5'-R(P\*CP\*UP\*GP\*GP\*CP\*CP\*CP\*UP\*CP\*A P\*A)-3').

| Mol | Chain | Residues | Atoms |     |    |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|----|---------|-------|
| 24  | X     | 11       | Total | C   | N  | O  | P  | 0       | 0     |
|     |       |          | 231   | 103 | 39 | 78 | 11 |         |       |

- Molecule 25 is a protein called 50S ribosomal protein L28.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 25  | 0     | 77       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 625   | 388 | 129 | 106 | 2 |         |       |

- Molecule 26 is a protein called 50S ribosomal protein L29.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 26  | 1     | 62       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 501   | 308 | 98 | 94 | 1 |         |       |

- Molecule 27 is a protein called 50S ribosomal protein L30.



| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 27  | 2     | 58       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 449   | 281 | 87 | 79 | 2 |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 28  | 3     | 56       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 444   | 269 | 94 | 80 | 1 |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 29  | 4     | 50       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 409   | 263 | 75 | 71 |   |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 30  | 6     | 46       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 377   | 228 | 90 | 57 | 2 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 31  | 7     | 64       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 504   | 323 | 105 | 74 | 2 |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 32  | 8     | 38       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 302   | 185 | 65 | 48 | 4 |         |       |

- Molecule 33 is a RNA chain called RNA (118-MER).

| Mol | Chain | Residues | Atoms |      |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|-------|
| 33  | a     | 117      | Total | C    | N   | O   | P   | 0       | 0     |
|     |       |          | 2506  | 1116 | 459 | 814 | 117 |         |       |

- Molecule 34 is a RNA chain called RNA (2903-MER).

| Mol | Chain | Residues | Atoms |       |       |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|-------|
| 34  | b     | 2903     | Total | C     | N     | O     | P    | 0       | 0     |
|     |       |          | 62321 | 27801 | 11467 | 20150 | 2903 |         |       |

- Molecule 35 is a protein called 50S ribosomal protein L2.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 35  | c     | 271      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2082  | 1288 | 423 | 364 | 7 |         |       |

- Molecule 36 is a protein called 50S ribosomal protein L9.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 36  | i     | 134      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 976   | 614 | 169 | 187 | 6 |         |       |

- Molecule 37 is a protein called 50S ribosomal protein L11.

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

- Molecule 38 is a protein called 50S ribosomal protein L3.

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

- Molecule 39 is a protein called 50S ribosomal protein L4.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 39  | f     | 177      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1410  | 899 | 249 | 256 | 6 |         |       |

- Molecule 40 is a protein called 50S ribosomal protein L5.

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

- Molecule 41 is a protein called 50S ribosomal protein L6.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 41  | h     | 149      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1111  | 699 | 197 | 214 | 1 |         |       |

- Molecule 42 is a protein called 50S ribosomal protein L13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 42  | j     | 142      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1129  | 714 | 212 | 199 | 4 |         |       |

- Molecule 43 is a protein called 50S ribosomal protein L14.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 43  | k     | 122      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 938   | 587 | 180 | 165 | 6 |         |       |

- Molecule 44 is a protein called 50S ribosomal protein L15.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 44  | l     | 144      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1053  | 654 | 207 | 190 | 2 |         |       |

- Molecule 45 is a protein called 50S ribosomal protein L16.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 45  | m     | 135      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1063  | 680 | 201 | 176 | 6 |         |       |

- Molecule 46 is a protein called 50S ribosomal protein L17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 46  | n     | 120      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 960   | 593 | 196 | 166 | 5 |         |       |

- Molecule 47 is a protein called 50S ribosomal protein L18.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 47  | o     | 116      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 892   | 552 | 178 | 162 |         |       |

- Molecule 48 is a protein called 50S ribosomal protein L19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 48  | p     | 114      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 917   | 574 | 179 | 163 | 1 |         |       |

- Molecule 49 is a protein called 50S ribosomal protein L20.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 49  | q     | 117      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 947   | 604 | 192 | 151 |   |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 50  | r     | 103      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 816   | 516 | 153 | 145 | 2 |         |       |

- Molecule 51 is a protein called 50S ribosomal protein L22.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 51  | s     | 110      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 857   | 532 | 166 | 156 | 3 |         |       |

- Molecule 52 is a protein called 50S ribosomal protein L23.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 52  | t     | 93       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 738   | 466 | 139 | 131 | 2 |         |       |

- Molecule 53 is a protein called 50S ribosomal protein L24.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 53  | u     | 102      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 779   | 492 | 146 | 141 |   |         |       |

- Molecule 54 is a protein called 50S ribosomal protein L25.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 54  | w     | 94       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 753   | 479 | 137 | 134 | 3 |         |       |

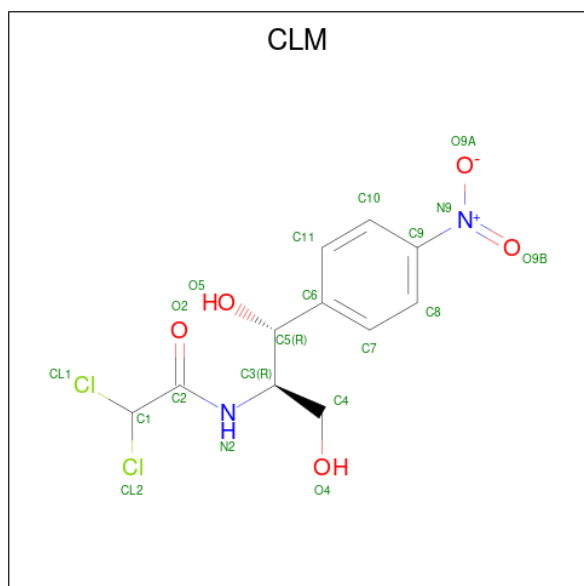
- Molecule 55 is a protein called 50S ribosomal protein L27.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 55  | y     | 75       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 569   | 353 | 113 | 102 | 1 |         |       |

- Molecule 56 is a protein called Secretion monitor.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 56  | z     | 27       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 211   | 134 | 35 | 42 |         |       |

- Molecule 57 is CHLORAMPHENICOL (three-letter code: CLM) (formula:  $C_{11}H_{12}Cl_2N_2O_5$ ).

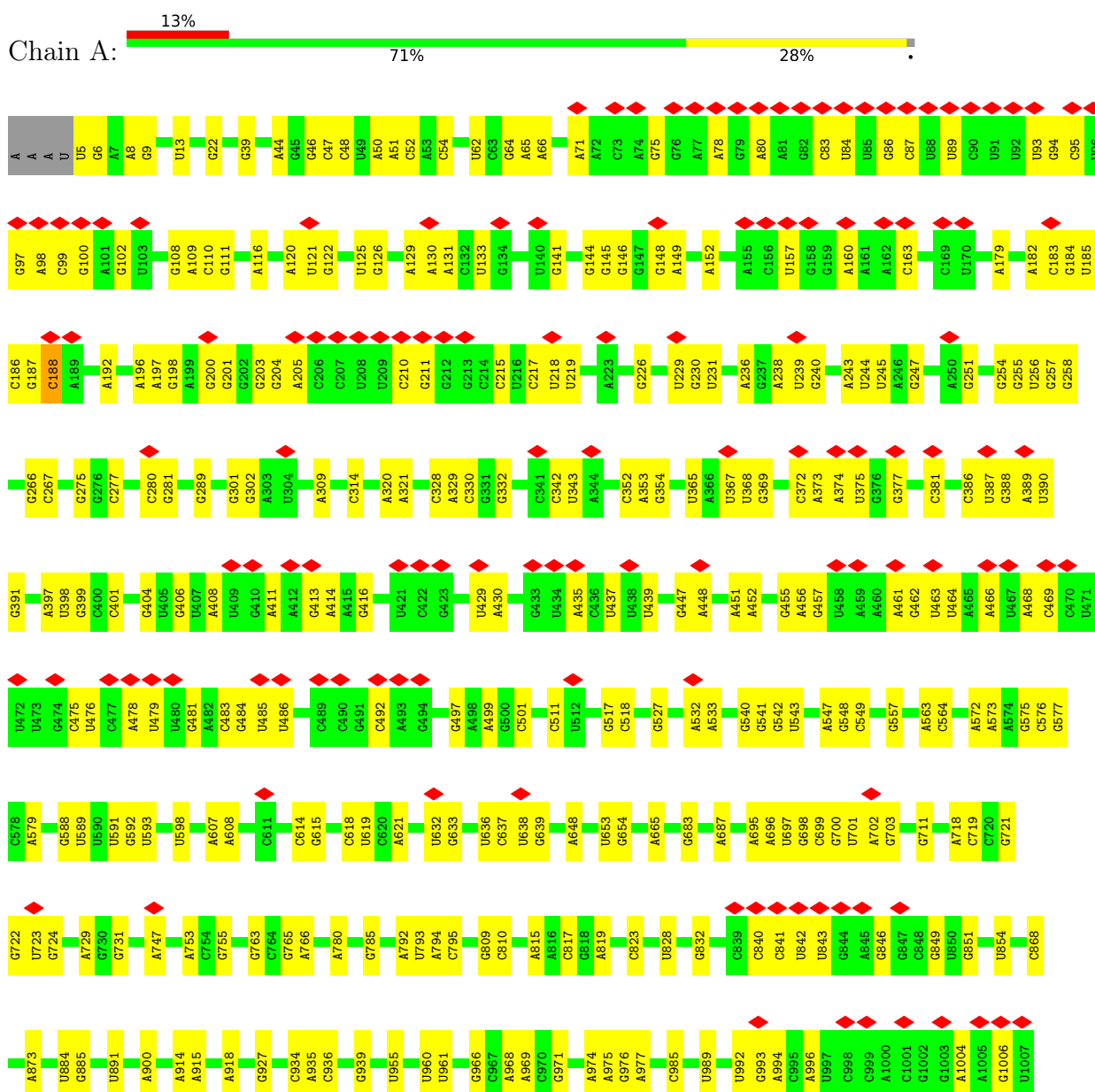


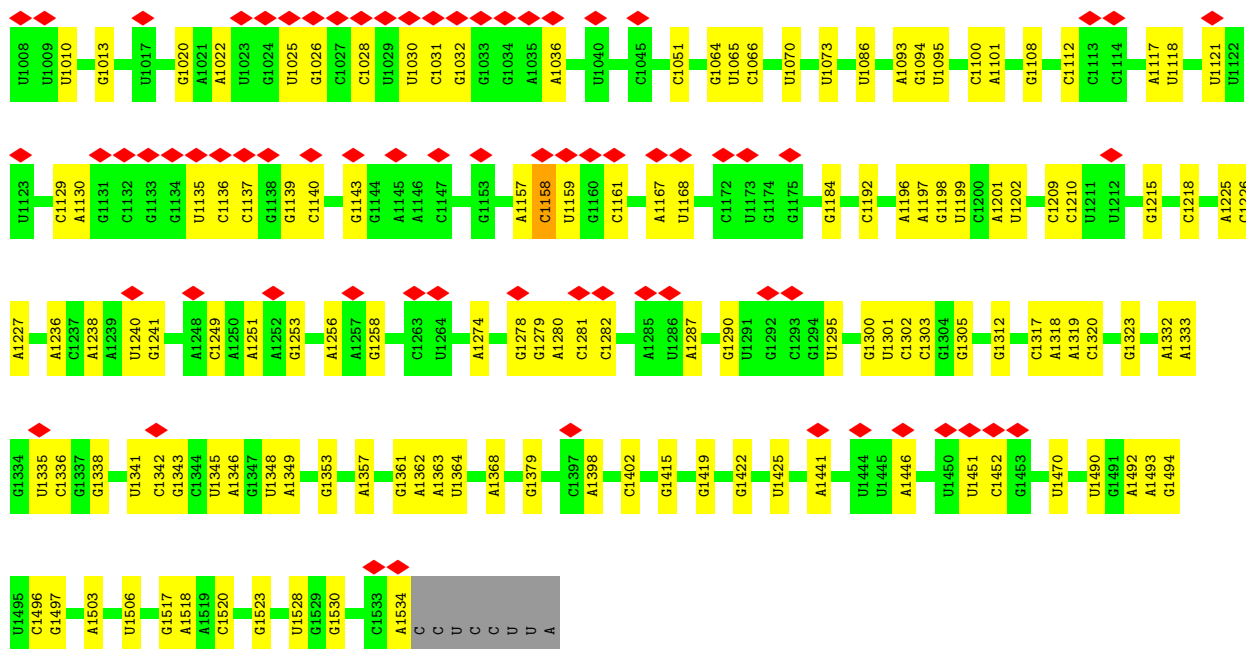
| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 57  | b     | 1        | Total | C  | Cl | N | O | 0       |
|     |       |          | 20    | 11 | 2  | 2 | 5 |         |

### 3 Residue-property plots

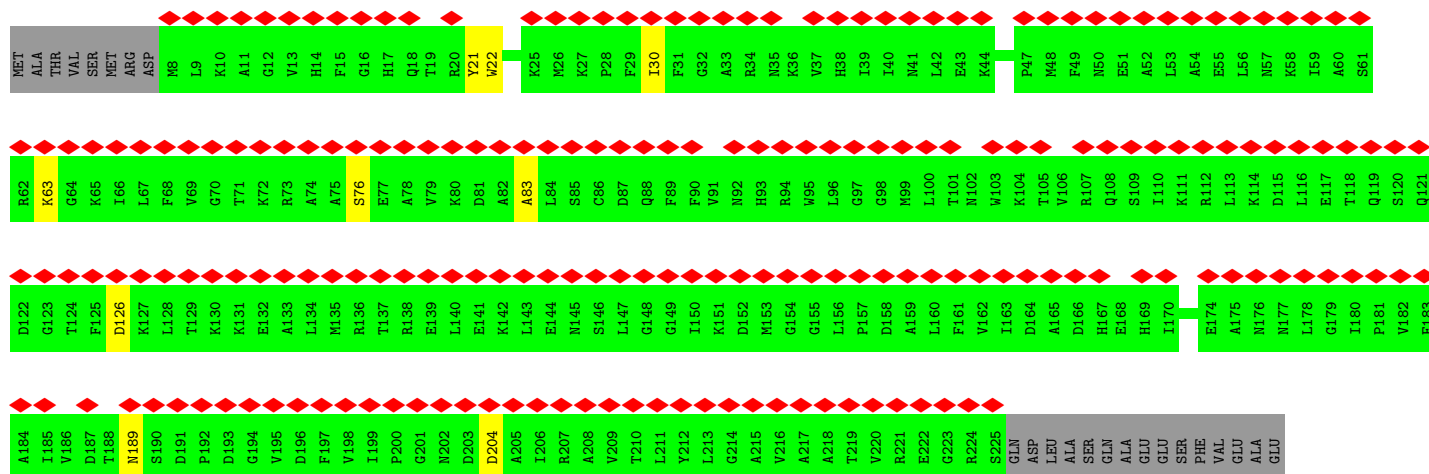
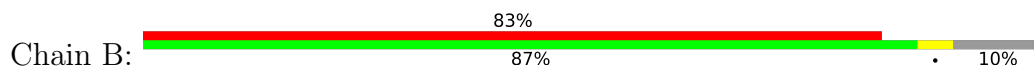
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: RNA (1530-MER)

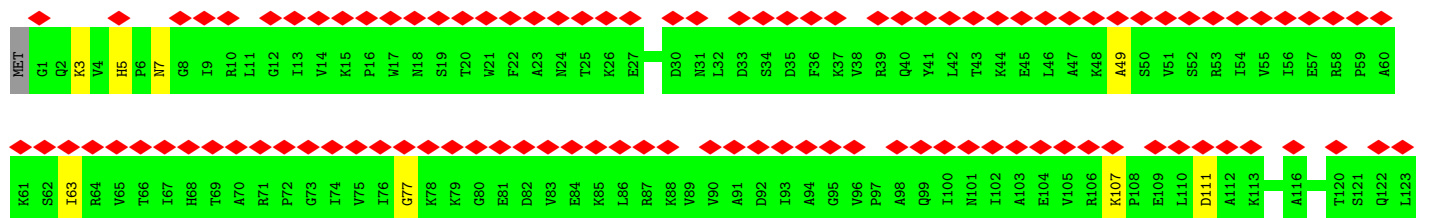
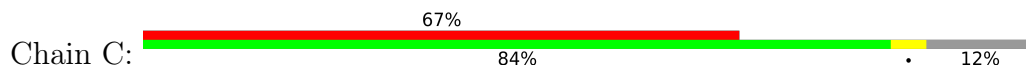


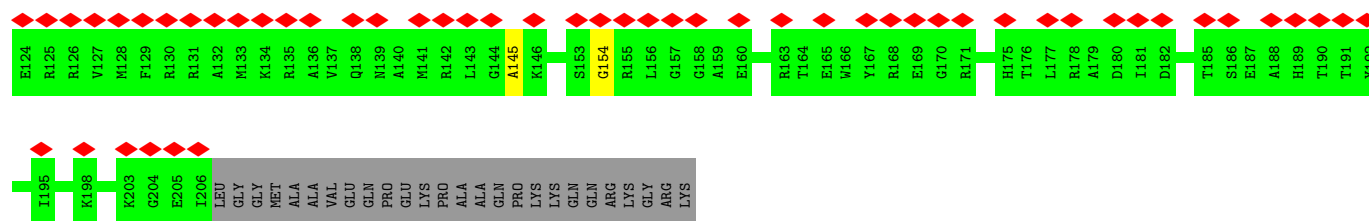


• Molecule 2: 30S ribosomal protein S2

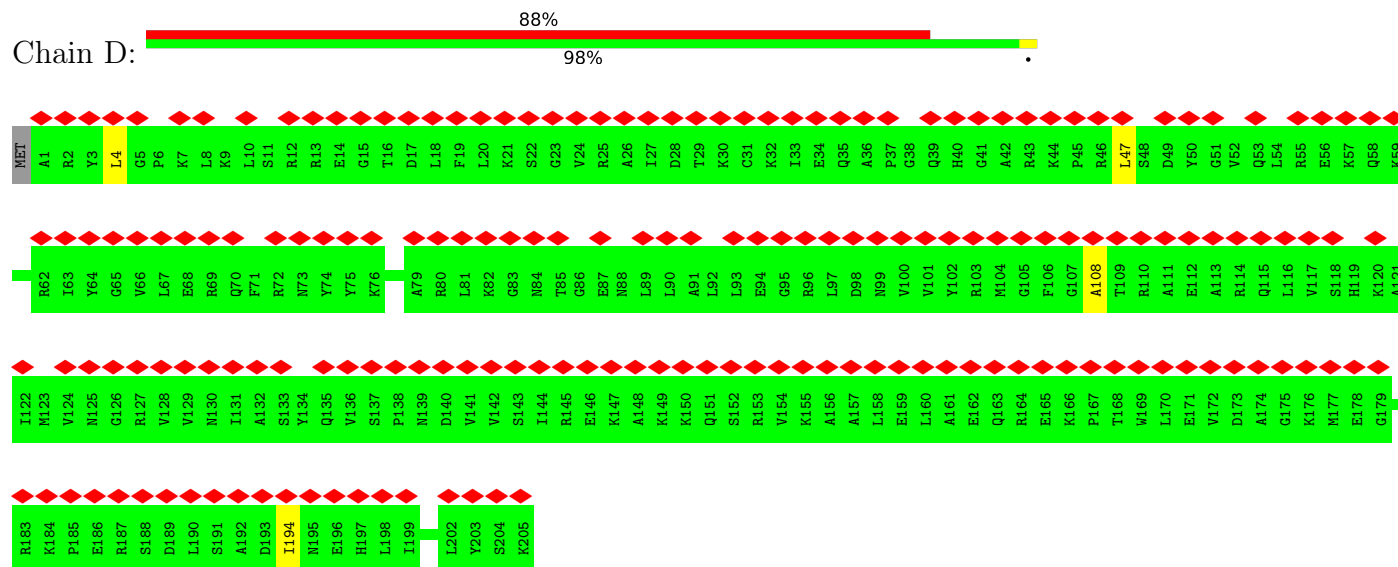


• Molecule 3: 30S ribosomal protein S3

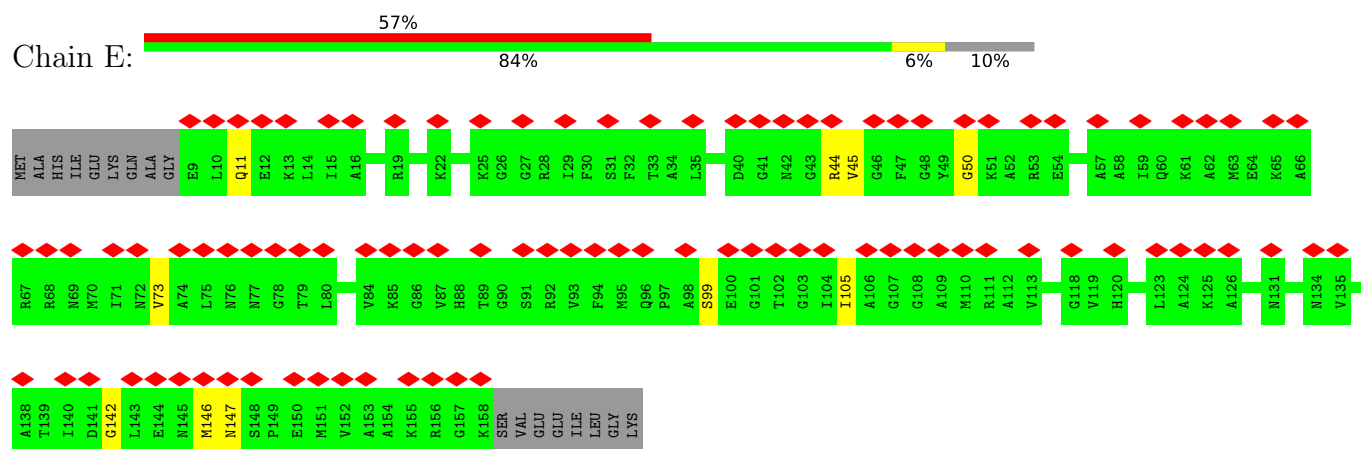




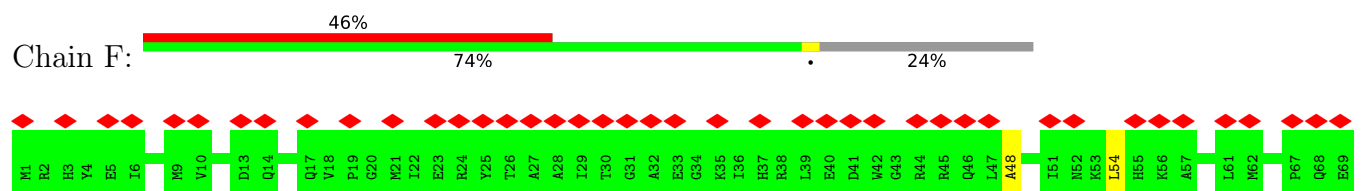
• Molecule 4: 30S ribosomal protein S4



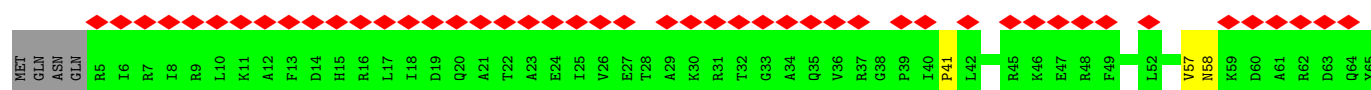
• Molecule 5: 30S ribosomal protein S5

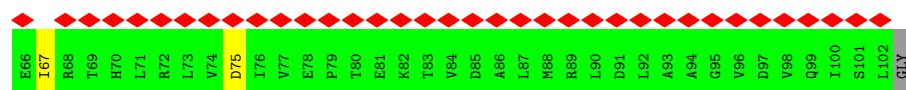


• Molecule 6: 30S ribosomal protein S6

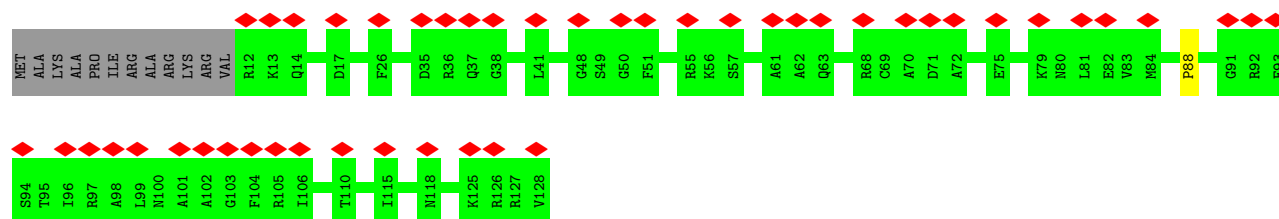
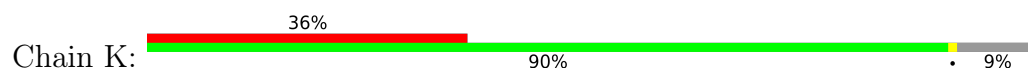




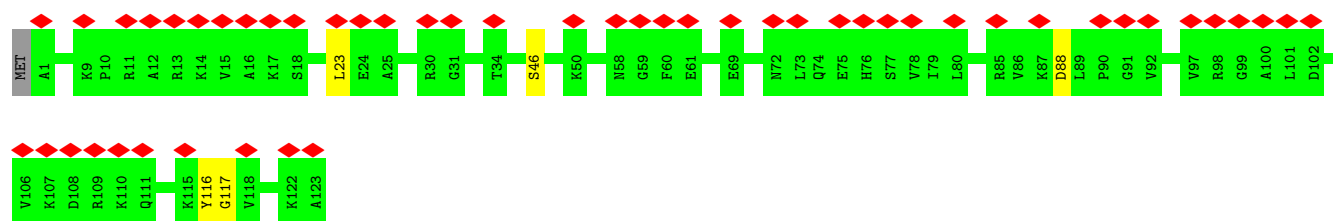
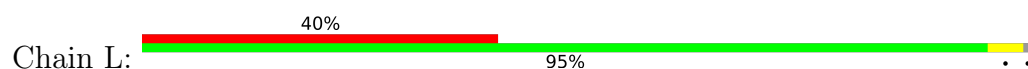




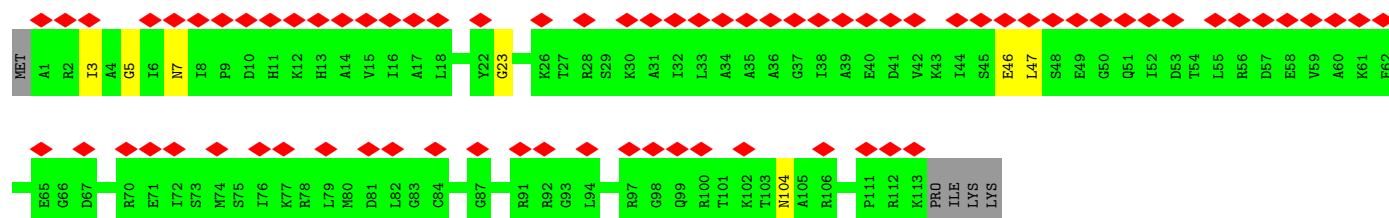
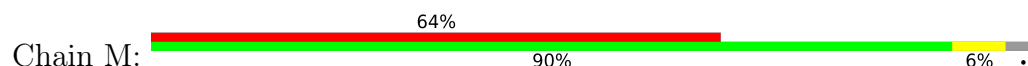
- Molecule 11: 30S ribosomal protein S11



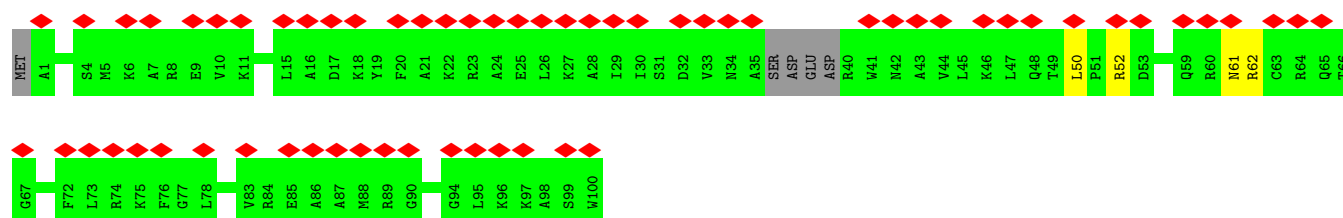
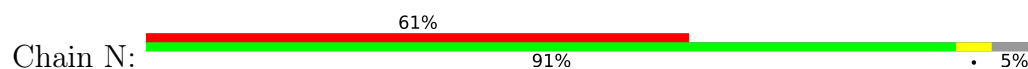
- Molecule 12: 30S ribosomal protein S12



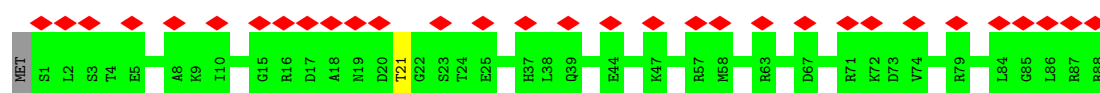
- Molecule 13: 30S ribosomal protein S13



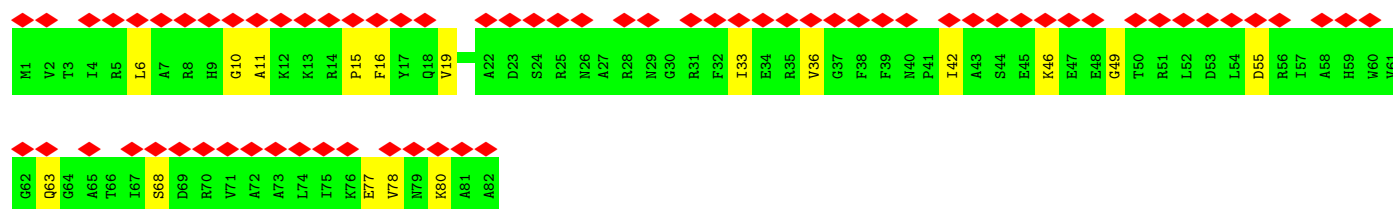
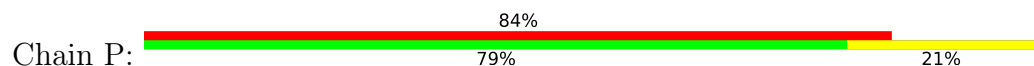
- Molecule 14: 30S ribosomal protein S14



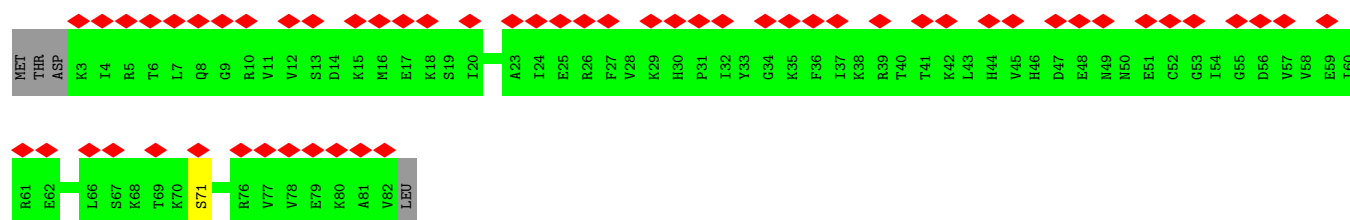
- Molecule 15: 30S ribosomal protein S15



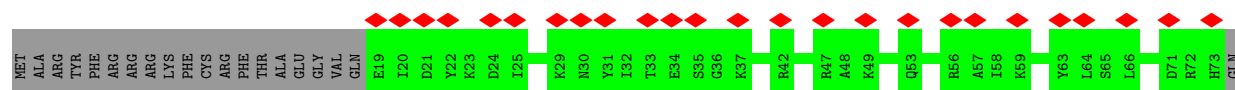
- Molecule 16: 30S ribosomal protein S16



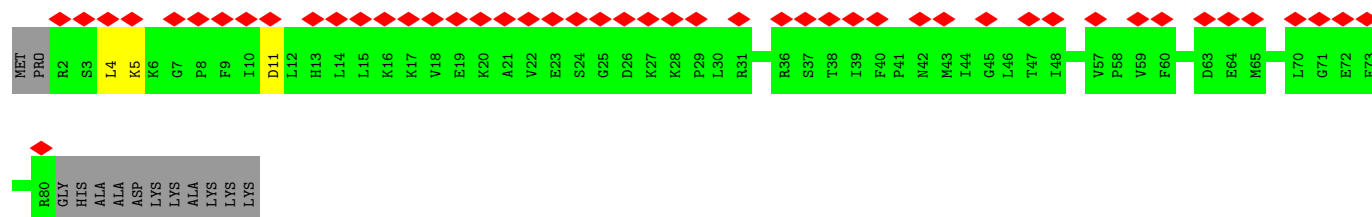
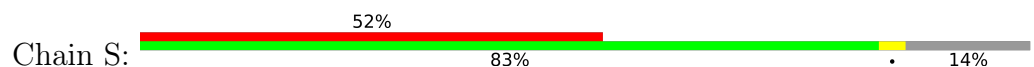
- Molecule 17: 30S ribosomal protein S17



- Molecule 18: 30S ribosomal protein S18

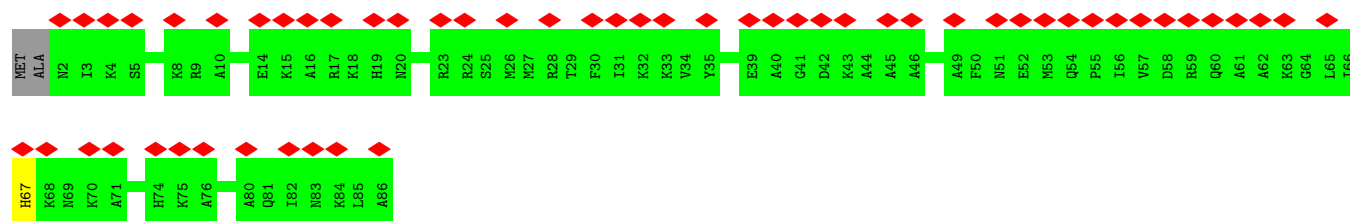


- Molecule 19: 30S ribosomal protein S19

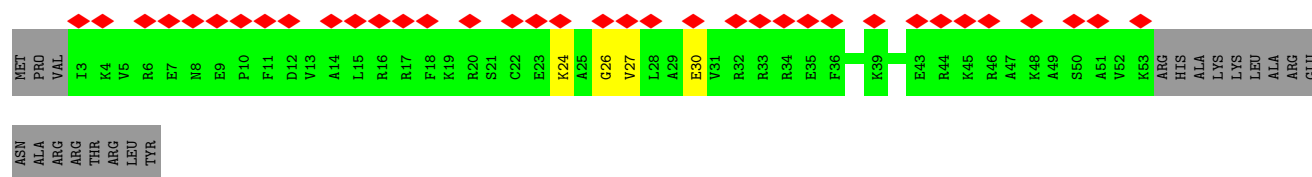


- Molecule 20: 30S ribosomal protein S20

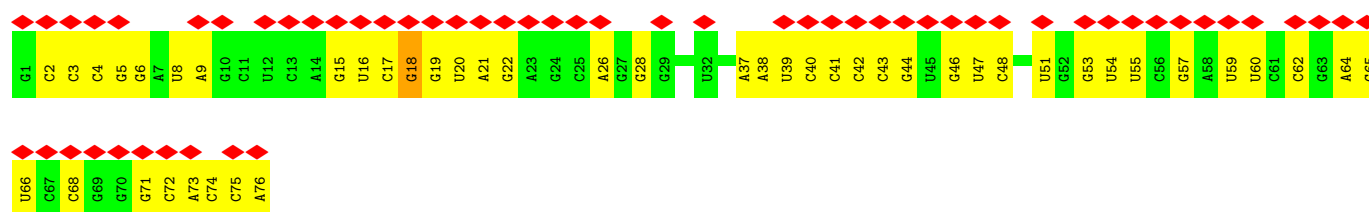
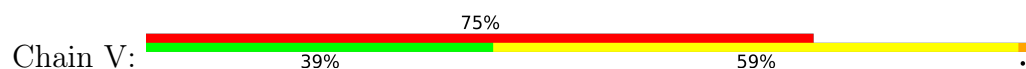




- Molecule 21: 30S ribosomal protein S21



- Molecule 22: RNA (76-MER)



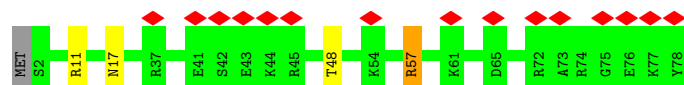
- Molecule 23: RNA (75-MER)



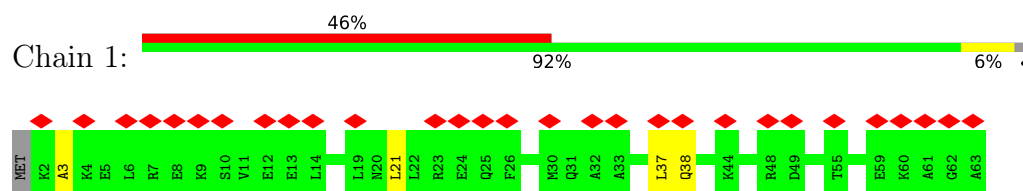
- Molecule 24: RNA (5'-R(P\*CP\*UP\*GP\*GP\*CP\*CP\*UP\*CP\*AP\*A)-3')



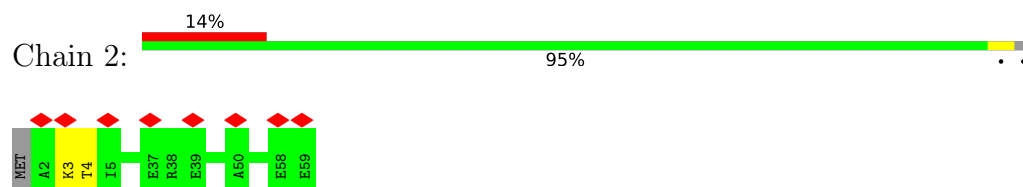
- Molecule 25: 50S ribosomal protein L28



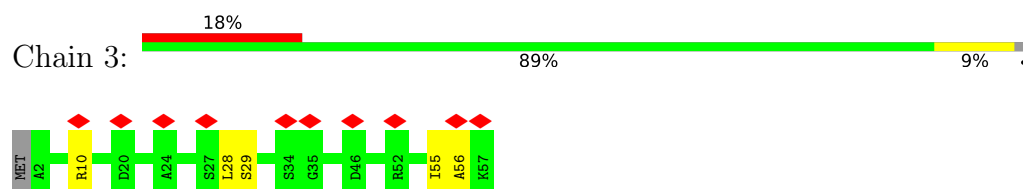
## • Molecule 26: 50S ribosomal protein L29



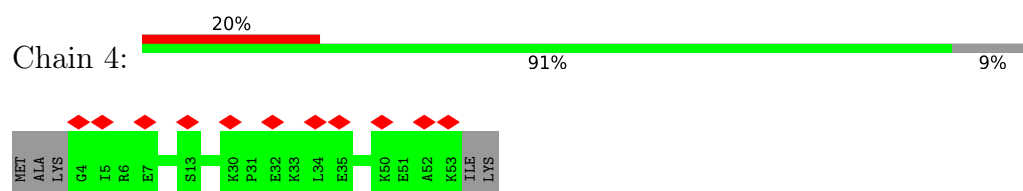
## • Molecule 27: 50S ribosomal protein L30



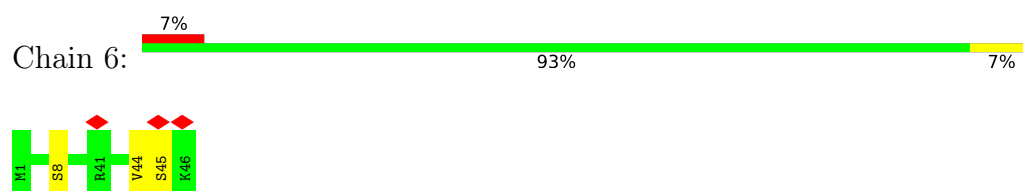
## • Molecule 28: 50S ribosomal protein L32



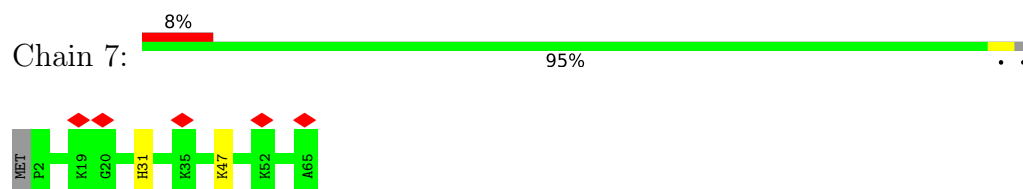
## • Molecule 29: 50S ribosomal protein L33



## • Molecule 30: 50S ribosomal protein L34

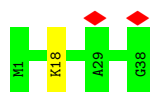


## • Molecule 31: 50S ribosomal protein L35



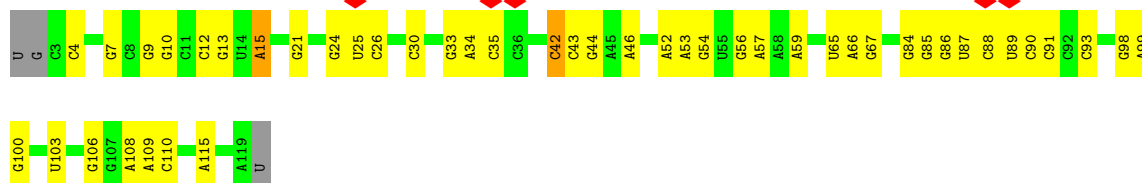
## • Molecule 32: 50S ribosomal protein L36





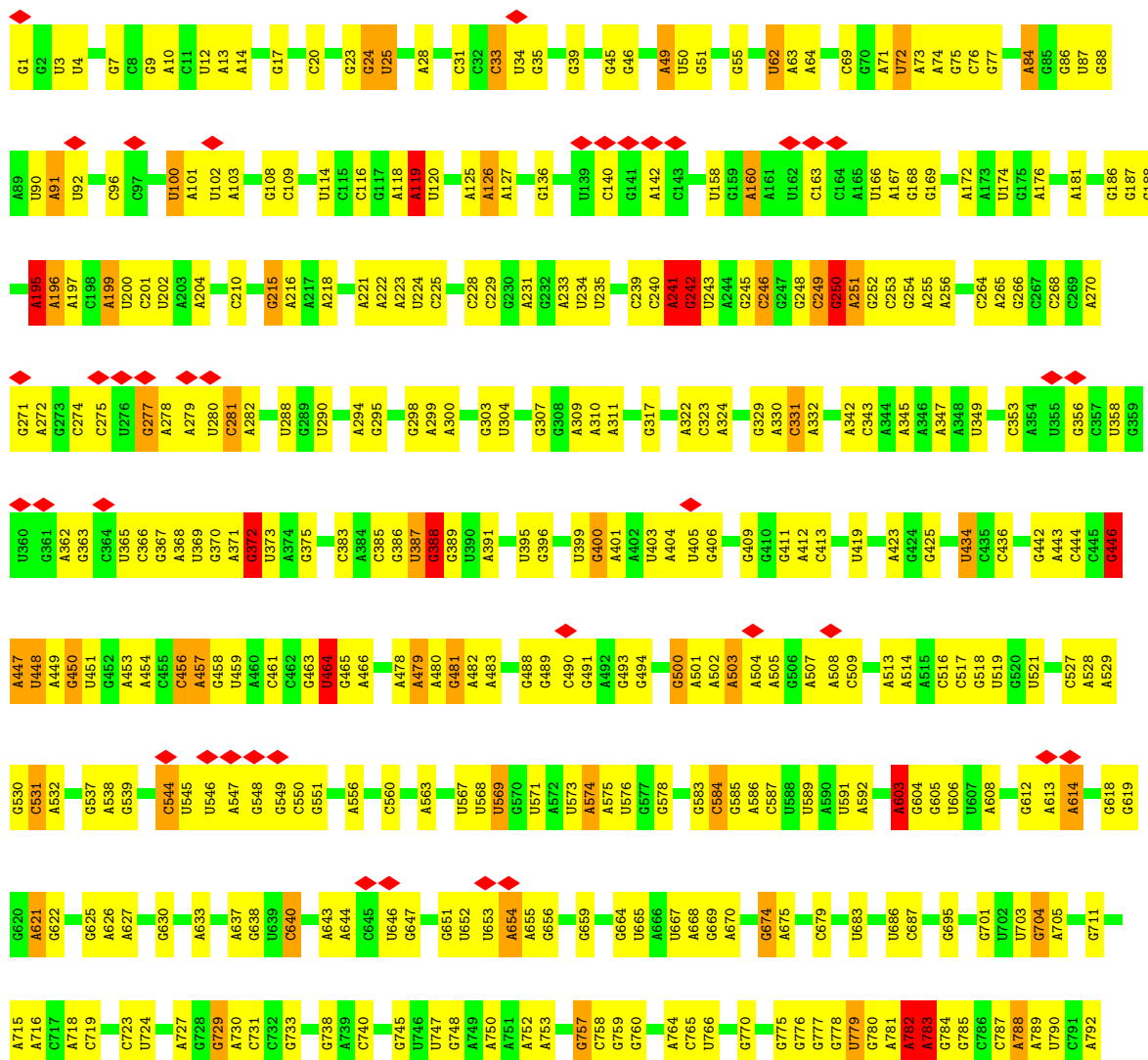
• Molecule 33: RNA (118-MER)

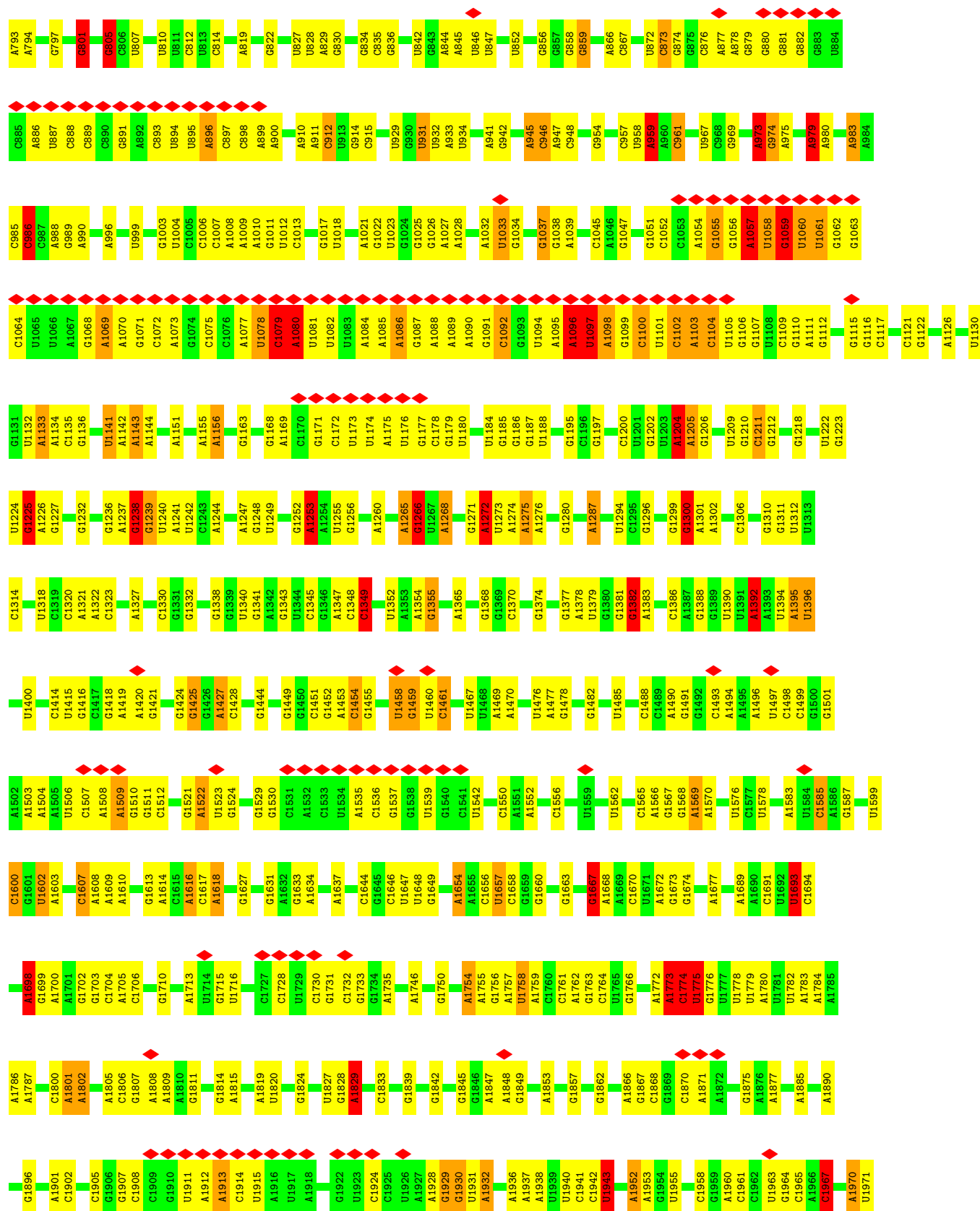
Chain a: 59% 37%

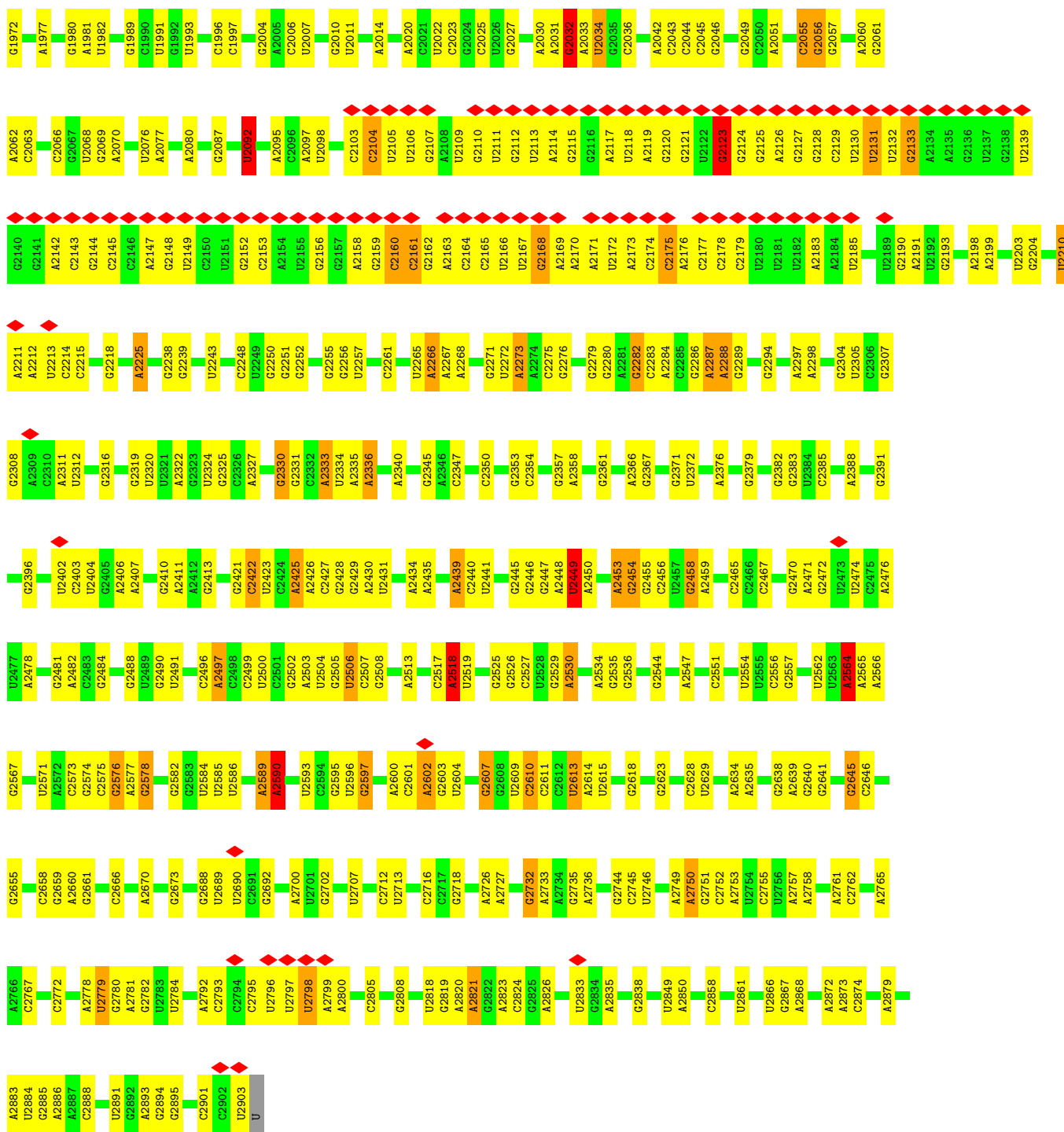


• Molecule 34: RNA (2903-MER)

Chain b: 9% 55% 38% 5%





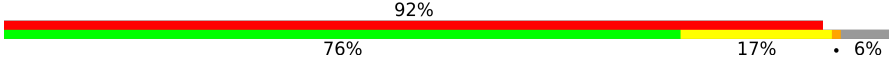


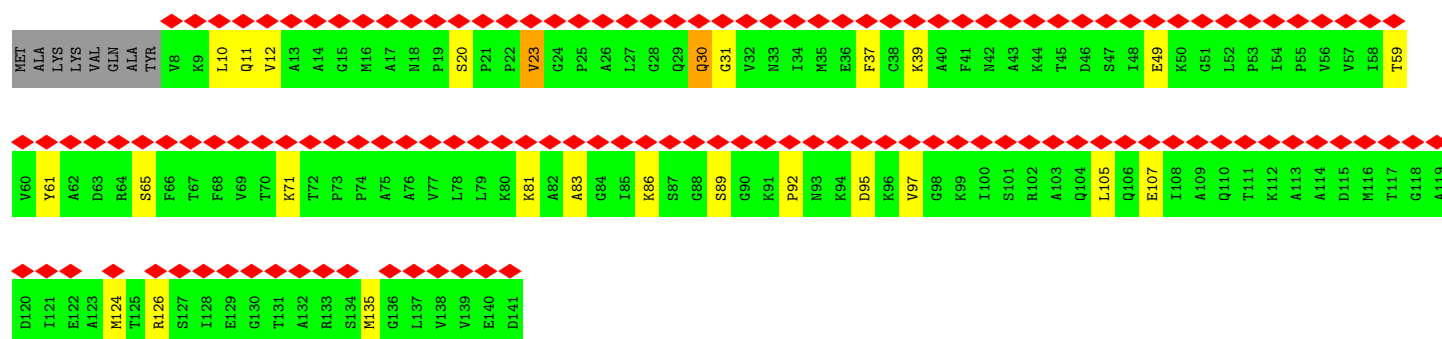
- Molecule 35: 50S ribosomal protein L2



- Molecule 36: 50S ribosomal protein L9

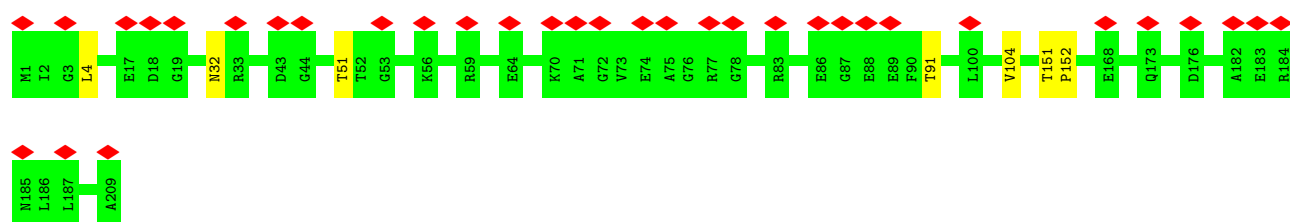


Chain i: 

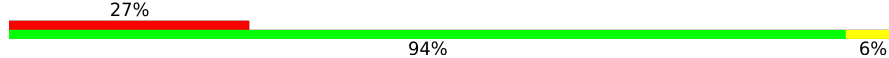


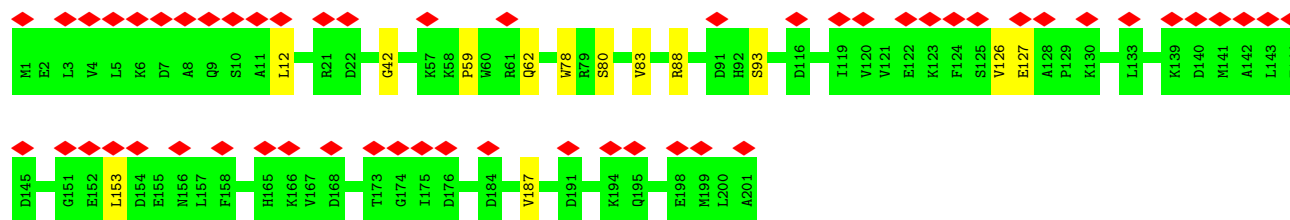
• Molecule 37: 50S ribosomal protein L11

Chain d: 

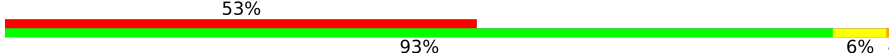


• Molecule 38: 50S ribosomal protein L3

Chain e: 

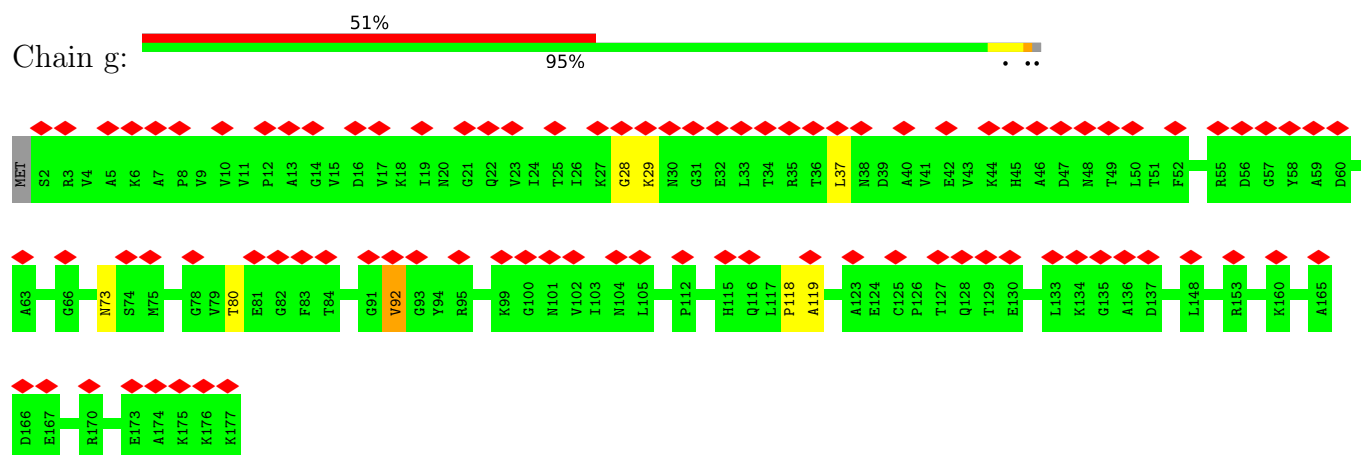


• Molecule 39: 50S ribosomal protein L4

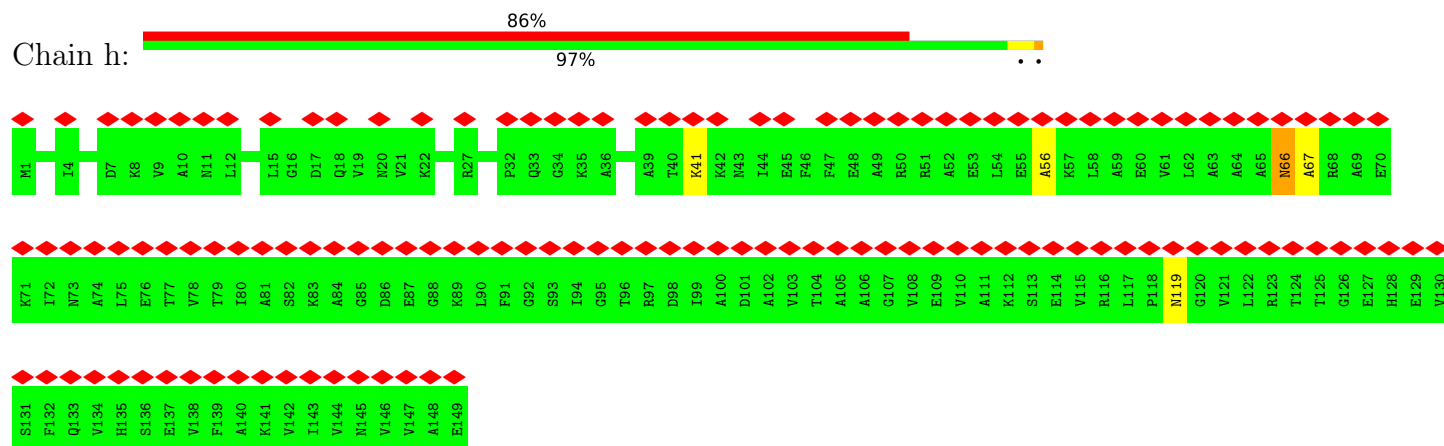
Chain f: 



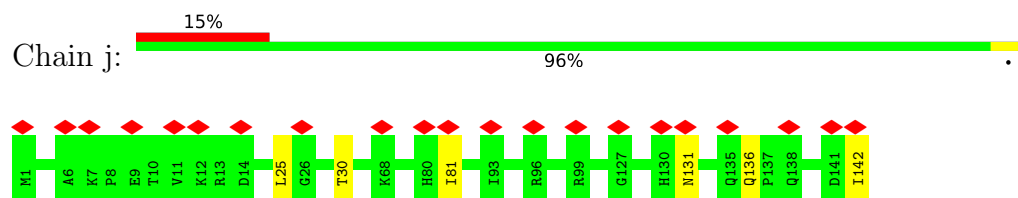
- Molecule 40: 50S ribosomal protein L5



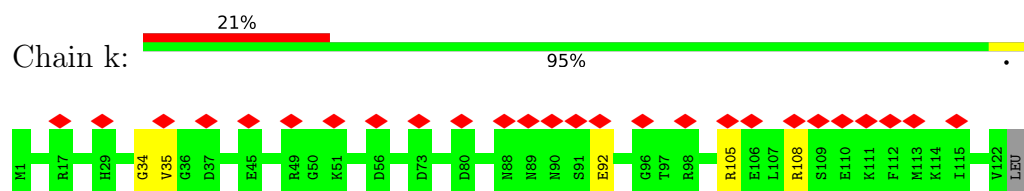
- Molecule 41: 50S ribosomal protein L6



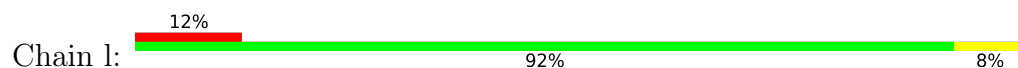
- Molecule 42: 50S ribosomal protein L13

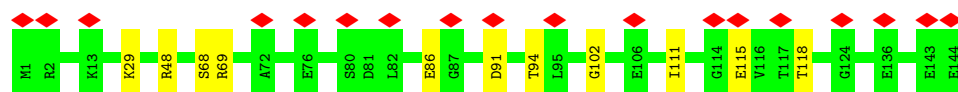


- Molecule 43: 50S ribosomal protein L14

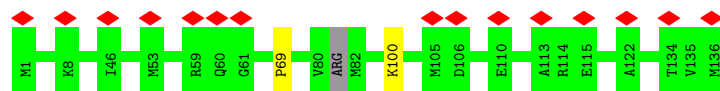


- Molecule 44: 50S ribosomal protein L15

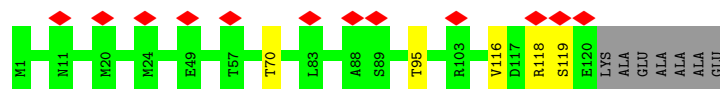
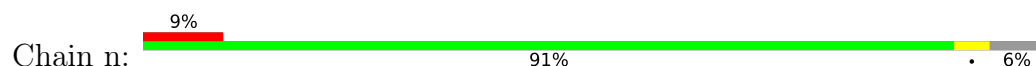




- Molecule 45: 50S ribosomal protein L16



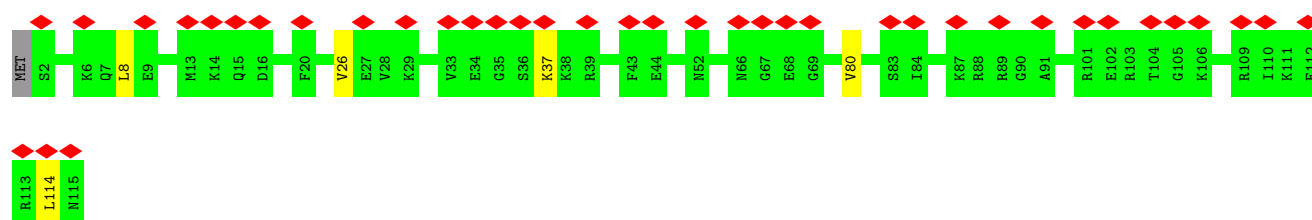
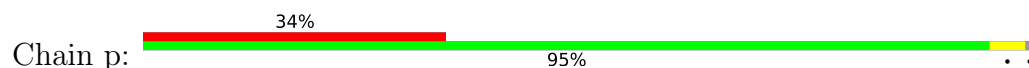
- Molecule 46: 50S ribosomal protein L17



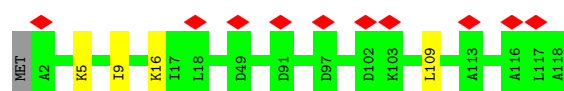
- Molecule 47: 50S ribosomal protein L18



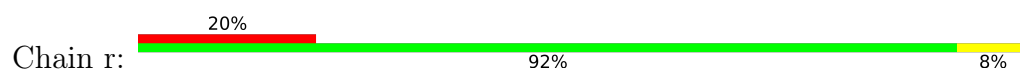
- Molecule 48: 50S ribosomal protein L19

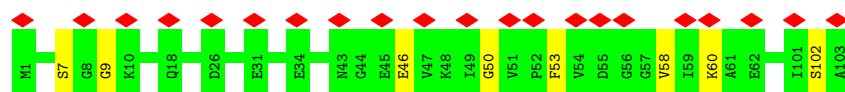


- Molecule 49: 50S ribosomal protein L20

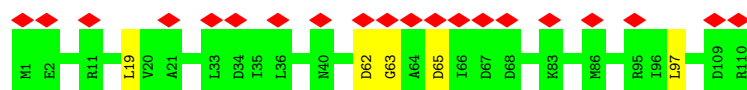
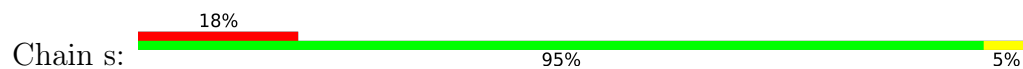


- Molecule 50: 50S ribosomal protein L21

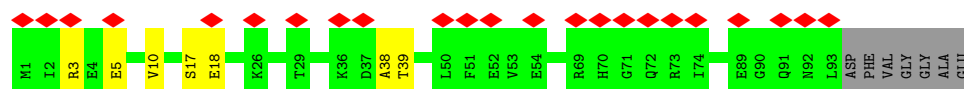
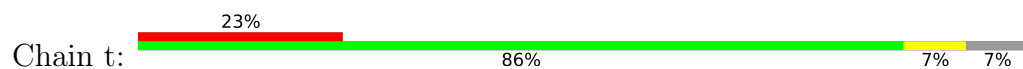




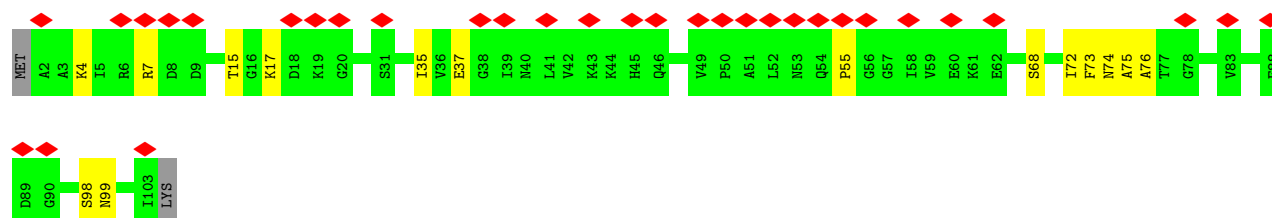
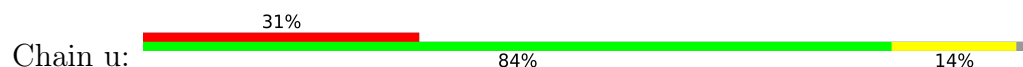
- Molecule 51: 50S ribosomal protein L22



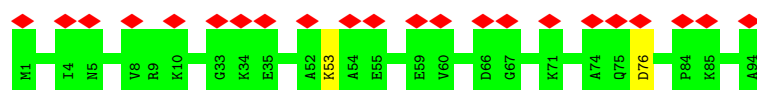
- Molecule 52: 50S ribosomal protein L23



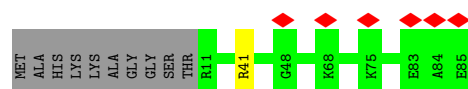
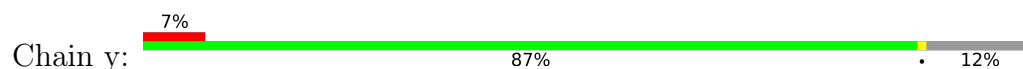
- Molecule 53: 50S ribosomal protein L24



- Molecule 54: 50S ribosomal protein L25



- Molecule 55: 50S ribosomal protein L27



- Molecule 56: Secretion monitor



|    |    |    |    |    |    |    |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
|----|----|----|----|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| E3 | Q4 | R5 | L6 | I7 | S8 | E9 | E10 | D11 | L12 | F13 | S14 | T15 | P16 | V17 | W18 | I19 | S20 | Q21 | A22 | Q23 | G24 | T25 | R26 | A27 | G28 | P29 |
|----|----|----|----|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

## 4 Experimental information

| Property                             | Value                           | Source    |
|--------------------------------------|---------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                 | Depositor |
| Imposed symmetry                     | POINT, C1                       | Depositor |
| Number of particles used             | 60354                           | Depositor |
| Resolution determination method      | Not provided                    |           |
| CTF correction method                | CTFFIND                         | Depositor |
| Microscope                           | FEI TITAN KRIOS                 | Depositor |
| Voltage (kV)                         | 300                             | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 16                              | Depositor |
| Minimum defocus (nm)                 | 3500                            | Depositor |
| Maximum defocus (nm)                 | 1000                            | Depositor |
| Magnification                        | 37878                           | Depositor |
| Image detector                       | GATAN K2 SUMMIT (4k x 4k)       | Depositor |
| Maximum map value                    | 0.187                           | Depositor |
| Minimum map value                    | -0.107                          | Depositor |
| Average map value                    | 0.000                           | Depositor |
| Map value standard deviation         | 0.009                           | Depositor |
| Recommended contour level            | 0.03                            | Depositor |
| Map size ( $\text{\AA}$ )            | 422.40002, 422.40002, 422.40002 | wwPDB     |
| Map dimensions                       | 320, 320, 320                   | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0                | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 1.32, 1.32, 1.32                | Depositor |

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CLM

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     | 0.47         | 0/36762       | 0.79        | 8/57350 (0.0%) |
| 2   | B     | 0.28         | 0/1735        | 0.50        | 0/2338         |
| 3   | C     | 0.32         | 0/1651        | 0.53        | 0/2225         |
| 4   | D     | 0.31         | 0/1665        | 0.52        | 0/2227         |
| 5   | E     | 0.34         | 0/1118        | 0.56        | 0/1504         |
| 6   | F     | 0.28         | 0/835         | 0.53        | 0/1128         |
| 7   | G     | 0.28         | 0/1187        | 0.51        | 0/1591         |
| 8   | H     | 0.32         | 0/989         | 0.52        | 0/1326         |
| 9   | I     | 0.31         | 0/1034        | 0.58        | 0/1375         |
| 10  | J     | 0.29         | 0/796         | 0.56        | 0/1077         |
| 11  | K     | 0.28         | 0/893         | 0.52        | 0/1205         |
| 12  | L     | 0.32         | 0/969         | 0.56        | 0/1300         |
| 13  | M     | 0.27         | 0/884         | 0.49        | 0/1181         |
| 14  | N     | 0.30         | 0/785         | 0.50        | 0/1043         |
| 15  | O     | 0.30         | 0/724         | 0.48        | 0/966          |
| 16  | P     | 0.29         | 0/659         | 0.49        | 0/884          |
| 17  | Q     | 0.31         | 0/657         | 0.49        | 0/881          |
| 18  | R     | 0.29         | 0/462         | 0.50        | 0/621          |
| 19  | S     | 0.30         | 0/652         | 0.51        | 0/877          |
| 20  | T     | 0.31         | 0/671         | 0.49        | 0/888          |
| 21  | U     | 0.29         | 0/430         | 0.60        | 0/570          |
| 22  | V     | 0.33         | 0/1810        | 0.80        | 3/2821 (0.1%)  |
| 23  | W     | 0.35         | 1/1786 (0.1%) | 0.92        | 6/2784 (0.2%)  |
| 24  | X     | 0.87         | 1/256 (0.4%)  | 0.81        | 0/394          |
| 25  | 0     | 0.41         | 0/635         | 0.76        | 1/848 (0.1%)   |
| 26  | 1     | 0.35         | 0/502         | 0.63        | 0/667          |
| 27  | 2     | 0.39         | 0/453         | 0.64        | 0/605          |
| 28  | 3     | 0.42         | 0/450         | 0.80        | 1/599 (0.2%)   |
| 29  | 4     | 0.38         | 0/416         | 0.61        | 0/554          |
| 30  | 6     | 0.48         | 0/380         | 0.86        | 0/498          |
| 31  | 7     | 0.40         | 0/513         | 0.65        | 0/676          |
| 32  | 8     | 0.40         | 0/303         | 0.77        | 0/397          |

| Mol | Chain | Bond lengths |                  | Bond angles |                   |
|-----|-------|--------------|------------------|-------------|-------------------|
|     |       | RMSZ         | # Z  >5          | RMSZ        | # Z  >5           |
| 33  | a     | 0.45         | 1/2802 (0.0%)    | 0.89        | 4/4369 (0.1%)     |
| 34  | b     | 0.59         | 84/69800 (0.1%)  | 1.02        | 432/108892 (0.4%) |
| 35  | c     | 0.42         | 0/2121           | 0.76        | 2/2852 (0.1%)     |
| 36  | i     | 0.24         | 0/989            | 0.48        | 0/1334            |
| 37  | d     | 0.39         | 0/1586           | 0.67        | 2/2134 (0.1%)     |
| 38  | e     | 0.39         | 0/1571           | 0.64        | 1/2113 (0.0%)     |
| 39  | f     | 0.39         | 0/1434           | 0.66        | 0/1926            |
| 40  | g     | 0.36         | 0/1343           | 0.59        | 1/1816 (0.1%)     |
| 41  | h     | 0.27         | 0/1122           | 0.60        | 1/1515 (0.1%)     |
| 42  | j     | 0.39         | 0/1152           | 0.63        | 0/1551            |
| 43  | k     | 0.41         | 0/947            | 0.71        | 0/1268            |
| 44  | l     | 0.41         | 0/1062           | 0.71        | 0/1413            |
| 45  | m     | 0.41         | 0/1081           | 0.67        | 0/1443            |
| 46  | n     | 0.42         | 0/973            | 0.71        | 0/1301            |
| 47  | o     | 0.38         | 0/902            | 0.73        | 2/1209 (0.2%)     |
| 48  | p     | 0.38         | 0/929            | 0.67        | 0/1242            |
| 49  | q     | 0.45         | 0/960            | 0.74        | 0/1278            |
| 50  | r     | 0.43         | 0/829            | 0.65        | 0/1107            |
| 51  | s     | 0.39         | 0/864            | 0.70        | 0/1156            |
| 52  | t     | 0.41         | 0/744            | 0.67        | 1/994 (0.1%)      |
| 53  | u     | 0.39         | 0/787            | 0.68        | 0/1051            |
| 54  | w     | 0.36         | 0/766            | 0.59        | 0/1025            |
| 55  | y     | 0.38         | 0/576            | 0.64        | 0/762             |
| 56  | z     | 0.46         | 1/215 (0.5%)     | 0.91        | 1/291 (0.3%)      |
| All | All   | 0.50         | 88/158617 (0.1%) | 0.87        | 466/237442 (0.2%) |

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 |
|-----|-------|---------------------|---------------------|
| 9   | I     | 0                   | 1                   |
| 27  | 2     | 0                   | 1                   |
| 34  | b     | 0                   | 64                  |
| 35  | c     | 0                   | 1                   |
| 37  | d     | 0                   | 1                   |
| 43  | k     | 0                   | 1                   |
| 44  | l     | 0                   | 1                   |
| 50  | r     | 0                   | 1                   |
| All | All   | 0                   | 71                  |

All (88) bond length outliers are listed below:



| Mol | Chain | Res  | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|--------|-------------|----------|
| 34  | b     | 2610 | C    | O3'-P   | 18.27  | 1.83        | 1.61     |
| 34  | b     | 2123 | G    | C6-N1   | 17.59  | 1.51        | 1.39     |
| 34  | b     | 2504 | U    | O3'-P   | 16.95  | 1.81        | 1.61     |
| 34  | b     | 2123 | G    | N3-C4   | 16.78  | 1.47        | 1.35     |
| 34  | b     | 2123 | G    | N9-C8   | 14.57  | 1.48        | 1.37     |
| 34  | b     | 2248 | C    | O3'-P   | 14.30  | 1.78        | 1.61     |
| 34  | b     | 399  | U    | C5'-C4' | 13.61  | 1.67        | 1.51     |
| 34  | b     | 1323 | C    | O3'-P   | 13.24  | 1.77        | 1.61     |
| 34  | b     | 2131 | U    | N1-C6   | 13.03  | 1.49        | 1.38     |
| 34  | b     | 2131 | U    | N3-C4   | 12.28  | 1.49        | 1.38     |
| 34  | b     | 1585 | C    | N1-C6   | 11.40  | 1.44        | 1.37     |
| 34  | b     | 2123 | G    | C5-C4   | 11.24  | 1.46        | 1.38     |
| 34  | b     | 1096 | A    | O3'-P   | 10.45  | 1.73        | 1.61     |
| 34  | b     | 1382 | G    | C2-N2   | -10.45 | 1.24        | 1.34     |
| 34  | b     | 1079 | C    | C2-O2   | -10.30 | 1.15        | 1.24     |
| 24  | X     | 12   | C    | OP3-P   | -10.25 | 1.48        | 1.61     |
| 34  | b     | 1    | G    | OP3-P   | -9.96  | 1.49        | 1.61     |
| 34  | b     | 1349 | C    | C4-N4   | -9.60  | 1.25        | 1.33     |
| 34  | b     | 1585 | C    | N3-C4   | 9.25   | 1.40        | 1.33     |
| 34  | b     | 979  | A    | O3'-P   | 9.15   | 1.72        | 1.61     |
| 34  | b     | 1059 | G    | C6-O6   | -9.06  | 1.16        | 1.24     |
| 34  | b     | 1654 | A    | N3-C4   | 8.92   | 1.40        | 1.34     |
| 34  | b     | 2506 | U    | O3'-P   | -8.90  | 1.50        | 1.61     |
| 34  | b     | 1654 | A    | C6-N1   | 8.25   | 1.41        | 1.35     |
| 34  | b     | 2602 | A    | O3'-P   | -8.24  | 1.51        | 1.61     |
| 34  | b     | 1057 | A    | O3'-P   | 8.21   | 1.71        | 1.61     |
| 34  | b     | 514  | A    | N3-C4   | 8.18   | 1.39        | 1.34     |
| 34  | b     | 1059 | G    | N9-C4   | 7.99   | 1.44        | 1.38     |
| 34  | b     | 674  | G    | O3'-P   | 7.92   | 1.70        | 1.61     |
| 34  | b     | 1059 | G    | C2-N3   | 7.79   | 1.39        | 1.32     |
| 34  | b     | 2123 | G    | N1-C2   | 7.78   | 1.44        | 1.37     |
| 34  | b     | 1349 | C    | N1-C2   | 7.74   | 1.47        | 1.40     |
| 34  | b     | 1654 | A    | N7-C5   | 7.71   | 1.43        | 1.39     |
| 34  | b     | 1654 | A    | N9-C8   | 7.68   | 1.43        | 1.37     |
| 34  | b     | 514  | A    | N7-C5   | 7.67   | 1.43        | 1.39     |
| 34  | b     | 2131 | U    | C2-O2   | 7.47   | 1.29        | 1.22     |
| 34  | b     | 2446 | G    | O3'-P   | 7.33   | 1.70        | 1.61     |
| 34  | b     | 1382 | G    | N1-C2   | -7.25  | 1.31        | 1.37     |
| 34  | b     | 2575 | C    | O3'-P   | 7.22   | 1.69        | 1.61     |
| 34  | b     | 1079 | C    | O3'-P   | 7.12   | 1.69        | 1.61     |
| 34  | b     | 1382 | G    | C5-C6   | 7.10   | 1.49        | 1.42     |
| 34  | b     | 778  | G    | O3'-P   | 7.05   | 1.69        | 1.61     |
| 34  | b     | 514  | A    | C6-N1   | 6.91   | 1.40        | 1.35     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 34  | b     | 2161 | C    | O3'-P   | 6.90  | 1.69        | 1.61     |
| 34  | b     | 1585 | C    | C2-O2   | 6.83  | 1.30        | 1.24     |
| 34  | b     | 1079 | C    | C2-N3   | -6.78 | 1.30        | 1.35     |
| 34  | b     | 1059 | G    | N1-C2   | -6.68 | 1.32        | 1.37     |
| 34  | b     | 779  | U    | O3'-P   | 6.66  | 1.69        | 1.61     |
| 34  | b     | 1079 | C    | N3-C4   | -6.62 | 1.29        | 1.33     |
| 34  | b     | 1349 | C    | C2-N3   | -6.61 | 1.30        | 1.35     |
| 34  | b     | 1382 | G    | C6-N1   | -6.59 | 1.34        | 1.39     |
| 34  | b     | 1058 | U    | O3'-P   | 6.46  | 1.69        | 1.61     |
| 34  | b     | 1266 | G    | O3'-P   | 6.44  | 1.68        | 1.61     |
| 34  | b     | 1773 | A    | O3'-P   | 6.43  | 1.68        | 1.61     |
| 34  | b     | 1061 | U    | O3'-P   | 6.38  | 1.68        | 1.61     |
| 34  | b     | 583  | G    | O3'-P   | 6.36  | 1.68        | 1.61     |
| 34  | b     | 2453 | A    | O3'-P   | 6.34  | 1.68        | 1.61     |
| 33  | a     | 25   | U    | C2-N3   | 6.31  | 1.42        | 1.37     |
| 34  | b     | 1349 | C    | N3-C4   | -6.21 | 1.29        | 1.33     |
| 34  | b     | 1059 | G    | N3-C4   | 6.12  | 1.39        | 1.35     |
| 34  | b     | 1585 | C    | C4-C5   | 6.06  | 1.47        | 1.43     |
| 34  | b     | 1059 | G    | C6-N1   | -6.00 | 1.35        | 1.39     |
| 34  | b     | 1186 | G    | O3'-P   | 5.98  | 1.68        | 1.61     |
| 34  | b     | 1058 | U    | N3-C4   | -5.86 | 1.33        | 1.38     |
| 34  | b     | 2449 | U    | O3'-P   | 5.69  | 1.68        | 1.61     |
| 34  | b     | 1097 | U    | O5'-C5' | 5.67  | 1.53        | 1.44     |
| 34  | b     | 514  | A    | N9-C8   | 5.46  | 1.42        | 1.37     |
| 34  | b     | 1268 | A    | O3'-P   | 5.45  | 1.67        | 1.61     |
| 34  | b     | 757  | G    | O3'-P   | 5.43  | 1.67        | 1.61     |
| 34  | b     | 2004 | G    | O3'-P   | 5.40  | 1.67        | 1.61     |
| 23  | W     | 36   | C    | O3'-P   | -5.40 | 1.54        | 1.61     |
| 34  | b     | 2518 | A    | O3'-P   | 5.37  | 1.67        | 1.61     |
| 34  | b     | 2123 | G    | C6-O6   | 5.36  | 1.28        | 1.24     |
| 34  | b     | 760  | G    | O3'-P   | 5.34  | 1.67        | 1.61     |
| 56  | z     | 29   | PRO  | N-CD    | 5.34  | 1.55        | 1.47     |
| 34  | b     | 2578 | G    | O3'-P   | 5.30  | 1.67        | 1.61     |
| 34  | b     | 780  | G    | O3'-P   | 5.29  | 1.67        | 1.61     |
| 34  | b     | 942  | G    | O3'-P   | 5.28  | 1.67        | 1.61     |
| 34  | b     | 331  | C    | N1-C2   | 5.25  | 1.45        | 1.40     |
| 34  | b     | 1096 | A    | C3'-O3' | 5.23  | 1.49        | 1.42     |
| 34  | b     | 2574 | G    | O3'-P   | 5.14  | 1.67        | 1.61     |
| 34  | b     | 87   | U    | O3'-P   | 5.11  | 1.67        | 1.61     |
| 34  | b     | 17   | G    | O3'-P   | 5.10  | 1.67        | 1.61     |
| 34  | b     | 948  | C    | O3'-P   | 5.06  | 1.67        | 1.61     |
| 34  | b     | 1310 | G    | O3'-P   | 5.05  | 1.67        | 1.61     |

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| Mol | Chain | Res  | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 34  | b     | 331  | C    | C4-C5 | 5.04 | 1.47        | 1.43     |
| 34  | b     | 395  | U    | O3'-P | 5.04 | 1.67        | 1.61     |
| 34  | b     | 2551 | C    | O3'-P | 5.01 | 1.67        | 1.61     |

All (466) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 23  | W     | 36   | C    | O3'-P-O5'   | 22.33  | 146.43      | 104.00   |
| 34  | b     | 2602 | A    | P-O3'-C3'   | 15.43  | 138.22      | 119.70   |
| 34  | b     | 1275 | A    | N9-C1'-C2'  | 15.08  | 133.61      | 114.00   |
| 34  | b     | 1096 | A    | N9-C1'-C2'  | -14.60 | 95.02       | 114.00   |
| 34  | b     | 400  | G    | N9-C1'-C2'  | 14.53  | 132.89      | 114.00   |
| 34  | b     | 1079 | C    | O4'-C1'-N1  | 14.09  | 119.47      | 108.20   |
| 34  | b     | 1058 | U    | O4'-C1'-N1  | 13.73  | 119.19      | 108.20   |
| 34  | b     | 2123 | G    | N9-C1'-C2'  | 13.68  | 131.78      | 114.00   |
| 34  | b     | 1300 | G    | N9-C1'-C2'  | 13.56  | 131.63      | 114.00   |
| 35  | c     | 156  | ARG  | NE-CZ-NH2   | -12.28 | 114.16      | 120.30   |
| 34  | b     | 2597 | G    | N9-C1'-C2'  | 11.95  | 129.53      | 114.00   |
| 56  | z     | 28   | GLY  | C-N-CD      | -11.54 | 95.21       | 120.60   |
| 34  | b     | 1059 | G    | N3-C2-N2    | 11.51  | 127.96      | 119.90   |
| 34  | b     | 2504 | U    | P-O3'-C3'   | 11.35  | 133.31      | 119.70   |
| 34  | b     | 1204 | A    | N9-C1'-C2'  | 10.77  | 128.00      | 114.00   |
| 34  | b     | 959  | A    | N9-C1'-C2'  | 10.71  | 127.92      | 114.00   |
| 34  | b     | 1059 | G    | C4-N9-C1'   | 10.71  | 140.42      | 126.50   |
| 34  | b     | 1349 | C    | C2-N1-C1'   | 10.60  | 130.46      | 118.80   |
| 34  | b     | 979  | A    | N9-C1'-C2'  | -10.57 | 100.26      | 114.00   |
| 34  | b     | 782  | A    | N9-C1'-C2'  | 10.51  | 127.66      | 114.00   |
| 34  | b     | 2161 | C    | C2'-C3'-O3' | 10.47  | 132.53      | 109.50   |
| 35  | c     | 156  | ARG  | NE-CZ-NH1   | 10.43  | 125.51      | 120.30   |
| 34  | b     | 2449 | U    | N1-C1'-C2'  | -10.36 | 100.53      | 114.00   |
| 34  | b     | 1349 | C    | N1-C2-O2    | 10.24  | 125.04      | 118.90   |
| 34  | b     | 2160 | C    | C2'-C3'-O3' | 10.20  | 131.94      | 109.50   |
| 34  | b     | 1205 | A    | N9-C1'-C2'  | 10.14  | 127.18      | 114.00   |
| 34  | b     | 1667 | G    | N9-C1'-C2'  | -10.04 | 100.95      | 114.00   |
| 34  | b     | 2454 | G    | N9-C1'-C2'  | -9.94  | 101.07      | 112.00   |
| 34  | b     | 1059 | G    | C8-N9-C1'   | -9.93  | 114.09      | 127.00   |
| 23  | W     | 36   | C    | P-O3'-C3'   | 9.77   | 131.42      | 119.70   |
| 23  | W     | 36   | C    | OP2-P-O3'   | -9.72  | 83.82       | 105.20   |
| 34  | b     | 973  | A    | N9-C1'-C2'  | 9.66   | 126.56      | 114.00   |
| 34  | b     | 2123 | G    | N9-C4-C5    | -9.66  | 101.54      | 105.40   |
| 34  | b     | 372  | G    | O4'-C1'-N9  | 9.62   | 115.90      | 108.20   |
| 34  | b     | 49   | A    | N9-C1'-C2'  | 9.56   | 126.43      | 114.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 34  | b     | 2123 | G    | C4-C5-N7    | 9.38  | 114.55      | 110.80   |
| 33  | a     | 33   | G    | N9-C1'-C2'  | -9.34 | 101.72      | 112.00   |
| 34  | b     | 1266 | G    | O4'-C1'-N9  | 9.33  | 115.67      | 108.20   |
| 34  | b     | 1057 | A    | N9-C1'-C2'  | -9.20 | 101.88      | 112.00   |
| 34  | b     | 986  | C    | N1-C1'-C2'  | 9.19  | 125.95      | 114.00   |
| 34  | b     | 983  | A    | N9-C1'-C2'  | 9.13  | 125.87      | 114.00   |
| 34  | b     | 2779 | U    | N1-C1'-C2'  | 8.96  | 125.65      | 114.00   |
| 34  | b     | 2161 | C    | O4'-C4'-C3' | -8.95 | 95.05       | 104.00   |
| 34  | b     | 1349 | C    | C6-N1-C1'   | -8.89 | 110.13      | 120.80   |
| 34  | b     | 873  | C    | C2'-C3'-O3' | 8.77  | 128.78      | 109.50   |
| 34  | b     | 1943 | U    | N1-C1'-C2'  | 8.75  | 125.37      | 114.00   |
| 34  | b     | 242  | G    | N9-C1'-C2'  | -8.69 | 102.44      | 112.00   |
| 34  | b     | 1930 | G    | C2'-C3'-O3' | 8.67  | 128.57      | 109.50   |
| 34  | b     | 399  | U    | N1-C1'-C2'  | 8.66  | 125.25      | 114.00   |
| 34  | b     | 1037 | G    | N9-C1'-C2'  | -8.64 | 102.50      | 112.00   |
| 34  | b     | 246  | C    | N1-C1'-C2'  | 8.54  | 125.10      | 114.00   |
| 34  | b     | 1059 | G    | N1-C2-N2    | -8.33 | 108.70      | 116.20   |
| 34  | b     | 788  | A    | N9-C1'-C2'  | -8.31 | 102.85      | 112.00   |
| 34  | b     | 1657 | U    | C5'-C4'-C3' | 8.29  | 129.27      | 116.00   |
| 34  | b     | 1225 | G    | N9-C1'-C2'  | 8.27  | 124.75      | 114.00   |
| 34  | b     | 2175 | C    | N1-C1'-C2'  | -8.26 | 102.92      | 112.00   |
| 34  | b     | 2248 | C    | O3'-P-O5'   | -8.22 | 88.39       | 104.00   |
| 34  | b     | 748  | G    | O3'-P-O5'   | -8.20 | 88.42       | 104.00   |
| 34  | b     | 614  | A    | N9-C1'-C2'  | 8.18  | 124.63      | 114.00   |
| 34  | b     | 1454 | C    | N1-C1'-C2'  | -8.13 | 103.06      | 112.00   |
| 34  | b     | 2304 | G    | C2'-C3'-O3' | 8.13  | 127.39      | 109.50   |
| 34  | b     | 241  | A    | N9-C1'-C2'  | 8.12  | 124.55      | 114.00   |
| 34  | b     | 1069 | A    | N9-C1'-C2'  | -8.12 | 103.07      | 112.00   |
| 34  | b     | 2266 | A    | N9-C1'-C2'  | 8.05  | 124.46      | 114.00   |
| 34  | b     | 1970 | A    | N9-C1'-C2'  | 8.04  | 124.46      | 114.00   |
| 34  | b     | 1059 | G    | N1-C6-O6    | -8.02 | 115.09      | 119.90   |
| 34  | b     | 2161 | C    | C5'-C4'-O4' | 8.02  | 118.73      | 109.10   |
| 34  | b     | 544  | C    | N1-C1'-C2'  | 8.02  | 124.42      | 114.00   |
| 34  | b     | 1657 | U    | C5'-C4'-O4' | 8.01  | 118.71      | 109.10   |
| 34  | b     | 1943 | U    | O4'-C1'-N1  | -8.00 | 101.80      | 108.20   |
| 34  | b     | 1967 | C    | N1-C1'-C2'  | 7.92  | 124.30      | 114.00   |
| 34  | b     | 2467 | C    | N1-C1'-C2'  | -7.92 | 103.29      | 112.00   |
| 34  | b     | 1079 | C    | N3-C4-N4    | -7.91 | 112.46      | 118.00   |
| 34  | b     | 446  | G    | N9-C1'-C2'  | -7.84 | 103.38      | 112.00   |
| 34  | b     | 1952 | A    | N9-C1'-C2'  | 7.83  | 124.18      | 114.00   |
| 34  | b     | 974  | G    | O4'-C1'-N9  | 7.82  | 114.46      | 108.20   |
| 34  | b     | 2092 | U    | N1-C1'-C2'  | 7.82  | 124.16      | 114.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 34  | b     | 1079 | C    | N3-C2-O2    | -7.80 | 116.44      | 121.90   |
| 34  | b     | 753  | A    | P-O3'-C3'   | -7.79 | 110.35      | 119.70   |
| 34  | b     | 1392 | A    | O4'-C1'-N9  | 7.79  | 114.43      | 108.20   |
| 34  | b     | 100  | U    | O4'-C1'-N1  | 7.78  | 114.43      | 108.20   |
| 34  | b     | 537  | G    | N9-C1'-C2'  | -7.75 | 103.47      | 112.00   |
| 34  | b     | 748  | G    | OP2-P-O3'   | 7.71  | 122.17      | 105.20   |
| 34  | b     | 1058 | U    | N1-C1'-C2'  | 7.68  | 123.99      | 114.00   |
| 34  | b     | 1382 | G    | N1-C6-O6    | -7.67 | 115.30      | 119.90   |
| 34  | b     | 2506 | U    | OP2-P-O3'   | -7.67 | 88.33       | 105.20   |
| 1   | A     | 1158 | C    | C2-N1-C1'   | 7.63  | 127.19      | 118.80   |
| 34  | b     | 2645 | G    | N9-C1'-C2'  | -7.60 | 103.64      | 112.00   |
| 34  | b     | 395  | U    | N1-C1'-C2'  | -7.60 | 103.64      | 112.00   |
| 34  | b     | 2092 | U    | O4'-C1'-N1  | -7.58 | 102.13      | 108.20   |
| 34  | b     | 25   | U    | N1-C1'-C2'  | 7.54  | 123.81      | 114.00   |
| 34  | b     | 1097 | U    | O4'-C4'-C3' | -7.52 | 96.48       | 104.00   |
| 34  | b     | 2032 | G    | N9-C1'-C2'  | 7.52  | 123.77      | 114.00   |
| 34  | b     | 1057 | A    | C2'-C3'-O3' | 7.51  | 126.02      | 109.50   |
| 34  | b     | 2602 | A    | OP2-P-O3'   | 7.49  | 121.68      | 105.20   |
| 34  | b     | 946  | C    | C2'-C3'-O3' | 7.49  | 125.97      | 109.50   |
| 34  | b     | 450  | G    | N9-C1'-C2'  | -7.47 | 103.78      | 112.00   |
| 34  | b     | 464  | U    | N1-C1'-C2'  | 7.47  | 123.72      | 114.00   |
| 34  | b     | 1704 | C    | C2'-C3'-O3' | 7.47  | 125.94      | 109.50   |
| 34  | b     | 2613 | U    | N1-C1'-C2'  | 7.45  | 123.69      | 114.00   |
| 34  | b     | 2518 | A    | C2'-C3'-O3' | 7.43  | 125.85      | 109.50   |
| 34  | b     | 1773 | A    | N9-C1'-C2'  | -7.43 | 103.83      | 112.00   |
| 34  | b     | 1395 | A    | O4'-C1'-N9  | 7.41  | 114.12      | 108.20   |
| 34  | b     | 2449 | U    | O4'-C1'-N1  | 7.38  | 114.10      | 108.20   |
| 34  | b     | 1829 | A    | N9-C1'-C2'  | -7.38 | 103.89      | 112.00   |
| 34  | b     | 423  | A    | N9-C1'-C2'  | 7.37  | 123.59      | 114.00   |
| 34  | b     | 388  | G    | O4'-C1'-N9  | 7.36  | 114.09      | 108.20   |
| 34  | b     | 167  | A    | N9-C1'-C2'  | 7.36  | 123.57      | 114.00   |
| 34  | b     | 1096 | A    | C4'-C3'-O3' | 7.33  | 127.67      | 113.00   |
| 34  | b     | 1098 | A    | O4'-C4'-C3' | -7.33 | 96.67       | 104.00   |
| 34  | b     | 801  | G    | O4'-C1'-N9  | -7.31 | 102.35      | 108.20   |
| 34  | b     | 2161 | C    | C4'-C3'-C2' | -7.29 | 95.31       | 102.60   |
| 34  | b     | 1932 | A    | N9-C1'-C2'  | 7.28  | 123.47      | 114.00   |
| 34  | b     | 1126 | A    | N9-C1'-C2'  | 7.24  | 123.41      | 114.00   |
| 34  | b     | 2867 | G    | O4'-C1'-N9  | 7.24  | 113.99      | 108.20   |
| 34  | b     | 2123 | G    | O4'-C1'-N9  | 7.24  | 113.99      | 108.20   |
| 34  | b     | 1779 | U    | O4'-C1'-N1  | 7.21  | 113.97      | 108.20   |
| 34  | b     | 479  | A    | C2'-C3'-O3' | 7.21  | 125.37      | 109.50   |
| 34  | b     | 1382 | G    | C5-C6-O6    | 7.21  | 132.92      | 128.60   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | A     | 1158 | C    | N1-C2-O2    | 7.20  | 123.22      | 118.90   |
| 34  | b     | 783  | A    | O5'-P-OP1   | -7.19 | 99.23       | 105.70   |
| 34  | b     | 2518 | A    | O4'-C1'-N9  | -7.15 | 102.48      | 108.20   |
| 34  | b     | 2051 | A    | N9-C1'-C2'  | -7.13 | 104.15      | 112.00   |
| 34  | b     | 2439 | A    | N9-C1'-C2'  | -7.13 | 104.15      | 112.00   |
| 34  | b     | 1698 | A    | N9-C1'-C2'  | 7.13  | 123.27      | 114.00   |
| 34  | b     | 1392 | A    | C1'-O4'-C4' | -7.12 | 104.20      | 109.90   |
| 34  | b     | 1395 | A    | C1'-O4'-C4' | -7.12 | 104.21      | 109.90   |
| 34  | b     | 729  | G    | O5'-P-OP1   | -7.11 | 99.30       | 105.70   |
| 34  | b     | 1275 | A    | O4'-C1'-N9  | 7.10  | 113.88      | 108.20   |
| 34  | b     | 783  | A    | O4'-C1'-N9  | 7.09  | 113.88      | 108.20   |
| 34  | b     | 479  | A    | C4'-C3'-O3' | -7.09 | 94.52       | 109.40   |
| 34  | b     | 1773 | A    | C2'-C3'-O3' | 7.04  | 124.98      | 109.50   |
| 34  | b     | 1929 | G    | N9-C1'-C2'  | -7.04 | 104.26      | 112.00   |
| 34  | b     | 576  | U    | N1-C1'-C2'  | 7.03  | 123.14      | 114.00   |
| 34  | b     | 1037 | G    | C5'-C4'-O4' | 7.02  | 117.53      | 109.10   |
| 34  | b     | 1272 | A    | N9-C1'-C2'  | 7.02  | 123.12      | 114.00   |
| 34  | b     | 1392 | A    | N9-C1'-C2'  | 7.01  | 123.12      | 114.00   |
| 34  | b     | 2282 | G    | N9-C1'-C2'  | -7.01 | 104.29      | 112.00   |
| 34  | b     | 2504 | U    | O3'-P-O5'   | -7.01 | 90.69       | 104.00   |
| 23  | W     | 33   | U    | O3'-P-O5'   | 7.00  | 117.30      | 104.00   |
| 34  | b     | 2530 | A    | N9-C1'-C2'  | 6.98  | 123.08      | 114.00   |
| 34  | b     | 2589 | A    | N9-C1'-C2'  | -6.95 | 104.36      | 112.00   |
| 34  | b     | 1396 | U    | C5'-C4'-O4' | 6.94  | 117.43      | 109.10   |
| 34  | b     | 2210 | U    | N1-C1'-C2'  | 6.93  | 123.00      | 114.00   |
| 34  | b     | 1774 | C    | N1-C1'-C2'  | -6.87 | 104.44      | 112.00   |
| 34  | b     | 531  | C    | N1-C1'-C2'  | 6.87  | 122.93      | 114.00   |
| 34  | b     | 1103 | A    | O4'-C4'-C3' | -6.86 | 97.14       | 104.00   |
| 34  | b     | 1103 | A    | O4'-C1'-N9  | 6.84  | 113.67      | 108.20   |
| 34  | b     | 1096 | A    | C3'-C2'-C1' | 6.84  | 106.97      | 101.50   |
| 34  | b     | 1499 | C    | N1-C1'-C2'  | -6.83 | 104.49      | 112.00   |
| 34  | b     | 1079 | C    | C5-C4-N4    | 6.82  | 124.98      | 120.20   |
| 34  | b     | 2272 | U    | N1-C1'-C2'  | 6.80  | 122.84      | 114.00   |
| 37  | d     | 4    | LEU  | CB-CG-CD2   | -6.79 | 99.45       | 111.00   |
| 34  | b     | 1311 | G    | N9-C1'-C2'  | -6.78 | 104.54      | 112.00   |
| 34  | b     | 388  | G    | C1'-O4'-C4' | -6.75 | 104.50      | 109.90   |
| 34  | b     | 199  | A    | O4'-C1'-N9  | 6.73  | 113.59      | 108.20   |
| 1   | A     | 188  | C    | N1-C2-O2    | 6.73  | 122.94      | 118.90   |
| 34  | b     | 2504 | U    | OP1-P-O3'   | 6.72  | 119.98      | 105.20   |
| 34  | b     | 931  | U    | N1-C1'-C2'  | 6.71  | 122.73      | 114.00   |
| 34  | b     | 704  | G    | C4'-C3'-O3' | 6.70  | 126.39      | 113.00   |
| 34  | b     | 912  | C    | N1-C1'-C2'  | 6.68  | 122.69      | 114.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 34  | b     | 1168 | G    | C2'-C3'-O3' | 6.68  | 124.39      | 113.70   |
| 34  | b     | 202  | U    | N1-C1'-C2'  | 6.66  | 122.66      | 114.00   |
| 34  | b     | 2340 | A    | N9-C1'-C2'  | 6.66  | 122.66      | 114.00   |
| 34  | b     | 1754 | A    | N9-C1'-C2'  | 6.66  | 122.66      | 114.00   |
| 34  | b     | 1775 | U    | N1-C1'-C2'  | -6.65 | 104.68      | 112.00   |
| 34  | b     | 989  | G    | N9-C1'-C2'  | -6.63 | 104.70      | 112.00   |
| 34  | b     | 674  | G    | N9-C1'-C2'  | -6.63 | 104.71      | 112.00   |
| 34  | b     | 1996 | C    | N1-C1'-C2'  | 6.63  | 122.61      | 114.00   |
| 34  | b     | 748  | G    | P-O3'-C3'   | 6.61  | 127.63      | 119.70   |
| 34  | b     | 2499 | C    | C4'-C3'-O3' | 6.61  | 126.21      | 113.00   |
| 34  | b     | 9    | G    | C2'-C3'-O3' | 6.59  | 124.25      | 113.70   |
| 34  | b     | 481  | G    | O4'-C1'-N9  | 6.58  | 113.47      | 108.20   |
| 34  | b     | 1569 | A    | N9-C1'-C2'  | 6.58  | 122.56      | 114.00   |
| 34  | b     | 1567 | G    | N9-C1'-C2'  | 6.55  | 122.52      | 114.00   |
| 34  | b     | 2123 | G    | N3-C4-C5    | 6.55  | 131.88      | 128.60   |
| 34  | b     | 2336 | A    | N9-C1'-C2'  | 6.54  | 122.50      | 114.00   |
| 34  | b     | 2879 | A    | N9-C1'-C2'  | 6.54  | 122.50      | 114.00   |
| 34  | b     | 2526 | G    | N9-C1'-C2'  | -6.53 | 104.82      | 112.00   |
| 34  | b     | 1092 | C    | N1-C1'-C2'  | 6.52  | 122.48      | 114.00   |
| 34  | b     | 1058 | U    | C1'-O4'-C4' | -6.51 | 104.69      | 109.90   |
| 34  | b     | 2097 | A    | C2'-C3'-O3' | 6.50  | 124.11      | 113.70   |
| 34  | b     | 1779 | U    | C1'-O4'-C4' | -6.50 | 104.70      | 109.90   |
| 34  | b     | 1133 | A    | O4'-C1'-N9  | 6.50  | 113.40      | 108.20   |
| 34  | b     | 1349 | C    | N3-C2-O2    | -6.49 | 117.36      | 121.90   |
| 34  | b     | 2161 | C    | C4'-C3'-O3' | 6.47  | 125.94      | 113.00   |
| 34  | b     | 1396 | U    | C5'-C4'-C3' | 6.46  | 126.34      | 116.00   |
| 34  | b     | 1057 | A    | C4'-C3'-C2' | -6.46 | 96.14       | 102.60   |
| 34  | b     | 603  | A    | O4'-C1'-N9  | -6.44 | 103.05      | 108.20   |
| 34  | b     | 168  | G    | C2'-C3'-O3' | 6.43  | 124.00      | 113.70   |
| 1   | A     | 188  | C    | C2-N1-C1'   | 6.42  | 125.86      | 118.80   |
| 34  | b     | 2248 | C    | OP2-P-O3'   | 6.42  | 119.32      | 105.20   |
| 34  | b     | 1097 | U    | C5'-C4'-C3' | 6.42  | 126.27      | 116.00   |
| 34  | b     | 805  | G    | N9-C1'-C2'  | 6.41  | 122.34      | 114.00   |
| 34  | b     | 1616 | A    | C5'-C4'-O4' | 6.41  | 116.80      | 109.10   |
| 34  | b     | 1458 | U    | N1-C1'-C2'  | 6.41  | 122.33      | 114.00   |
| 34  | b     | 608  | A    | N9-C1'-C2'  | 6.41  | 122.33      | 114.00   |
| 34  | b     | 630  | G    | N9-C1'-C2'  | -6.41 | 104.95      | 112.00   |
| 34  | b     | 1238 | G    | N9-C1'-C2'  | -6.41 | 104.95      | 112.00   |
| 34  | b     | 49   | A    | C8-N9-C1'   | -6.40 | 116.18      | 127.70   |
| 34  | b     | 503  | A    | C5'-C4'-O4' | 6.39  | 116.77      | 109.10   |
| 34  | b     | 961  | C    | O5'-P-OP2   | -6.37 | 99.96       | 105.70   |
| 34  | b     | 448  | U    | N1-C1'-C2'  | -6.37 | 104.99      | 112.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 34  | b     | 1693 | U    | N1-C1'-C2'  | 6.34  | 122.25      | 114.00   |
| 34  | b     | 1323 | C    | OP2-P-O3'   | 6.34  | 119.16      | 105.20   |
| 34  | b     | 2129 | C    | N1-C1'-C2'  | 6.31  | 122.20      | 114.00   |
| 34  | b     | 2750 | A    | O4'-C1'-N9  | -6.30 | 103.16      | 108.20   |
| 34  | b     | 254  | G    | N9-C1'-C2'  | -6.29 | 105.08      | 112.00   |
| 34  | b     | 2175 | C    | C4'-C3'-O3' | 6.29  | 125.59      | 113.00   |
| 34  | b     | 2607 | G    | P-O3'-C3'   | 6.28  | 127.24      | 119.70   |
| 23  | W     | 36   | C    | OP1-P-O3'   | -6.28 | 91.39       | 105.20   |
| 34  | b     | 409  | G    | C2'-C3'-O3' | 6.27  | 123.73      | 113.70   |
| 34  | b     | 2066 | C    | N1-C1'-C2'  | 6.27  | 122.15      | 114.00   |
| 34  | b     | 2593 | U    | N1-C1'-C2'  | 6.26  | 122.14      | 114.00   |
| 34  | b     | 1272 | A    | O4'-C1'-N9  | -6.25 | 103.20      | 108.20   |
| 34  | b     | 1058 | U    | N3-C4-O4    | -6.25 | 115.02      | 119.40   |
| 34  | b     | 488  | G    | N9-C1'-C2'  | -6.23 | 105.14      | 112.00   |
| 34  | b     | 787  | C    | N1-C1'-C2'  | 6.22  | 122.09      | 114.00   |
| 34  | b     | 1253 | A    | N9-C1'-C2'  | 6.20  | 122.06      | 114.00   |
| 34  | b     | 2425 | A    | N9-C1'-C2'  | 6.18  | 122.04      | 114.00   |
| 34  | b     | 2160 | C    | O4'-C1'-N1  | 6.17  | 113.14      | 108.20   |
| 34  | b     | 72   | U    | N1-C1'-C2'  | 6.17  | 122.02      | 114.00   |
| 34  | b     | 2496 | C    | O5'-P-OP2   | -6.17 | 100.15      | 105.70   |
| 34  | b     | 2324 | U    | C4'-C3'-O3' | 6.17  | 125.33      | 113.00   |
| 34  | b     | 2821 | A    | N9-C1'-C2'  | 6.15  | 121.99      | 114.00   |
| 34  | b     | 2123 | G    | C1'-O4'-C4' | -6.14 | 104.98      | 109.90   |
| 34  | b     | 250  | G    | N9-C1'-C2'  | 6.14  | 121.98      | 114.00   |
| 34  | b     | 1758 | U    | N1-C1'-C2'  | 6.12  | 121.95      | 114.00   |
| 34  | b     | 703  | U    | C2'-C3'-O3' | 6.12  | 123.48      | 113.70   |
| 34  | b     | 215  | G    | N9-C1'-C2'  | 6.11  | 121.94      | 114.00   |
| 34  | b     | 618  | G    | N9-C1'-C2'  | 6.11  | 121.94      | 114.00   |
| 34  | b     | 1801 | A    | N9-C1'-C2'  | 6.11  | 121.94      | 114.00   |
| 34  | b     | 753  | A    | O3'-P-O5'   | 6.11  | 115.60      | 104.00   |
| 34  | b     | 1055 | G    | C8-N9-C1'   | -6.09 | 119.08      | 127.00   |
| 34  | b     | 1323 | C    | O3'-P-O5'   | -6.07 | 92.47       | 104.00   |
| 34  | b     | 500  | G    | N9-C1'-C2'  | -6.05 | 105.34      | 112.00   |
| 40  | g     | 37   | LEU  | CB-CG-CD1   | -6.05 | 100.72      | 111.00   |
| 34  | b     | 1078 | U    | C2'-C3'-O3' | 6.05  | 123.38      | 113.70   |
| 34  | b     | 1349 | C    | C5'-C4'-O4' | 6.05  | 116.36      | 109.10   |
| 34  | b     | 91   | A    | N9-C1'-C2'  | 6.04  | 121.85      | 114.00   |
| 34  | b     | 1059 | G    | N3-C4-N9    | 6.01  | 129.61      | 126.00   |
| 34  | b     | 2225 | A    | N9-C1'-C2'  | -6.01 | 105.39      | 112.00   |
| 34  | b     | 450  | G    | C2'-C3'-O3' | 5.99  | 123.29      | 113.70   |
| 34  | b     | 1239 | G    | N9-C1'-C2'  | -5.99 | 105.41      | 112.00   |
| 34  | b     | 1824 | G    | N9-C1'-C2'  | -5.98 | 105.42      | 112.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 34  | b     | 196  | A    | O4'-C1'-N9  | 5.98  | 112.98      | 108.20   |
| 34  | b     | 1055 | G    | C4-N9-C1'   | 5.97  | 134.27      | 126.50   |
| 34  | b     | 1616 | A    | C5'-C4'-C3' | 5.97  | 125.55      | 116.00   |
| 34  | b     | 945  | A    | O5'-P-OP1   | -5.96 | 100.34      | 105.70   |
| 34  | b     | 1098 | A    | C4'-C3'-O3' | 5.96  | 124.91      | 113.00   |
| 34  | b     | 84   | A    | N9-C1'-C2'  | -5.96 | 105.45      | 112.00   |
| 34  | b     | 2131 | U    | N1-C2-N3    | -5.94 | 111.33      | 114.90   |
| 34  | b     | 126  | A    | N9-C1'-C2'  | 5.94  | 121.72      | 114.00   |
| 34  | b     | 603  | A    | C2'-C3'-O3' | 5.93  | 123.18      | 113.70   |
| 34  | b     | 457  | A    | N9-C1'-C2'  | 5.91  | 121.68      | 114.00   |
| 34  | b     | 1057 | A    | C4'-C3'-O3' | 5.90  | 124.81      | 113.00   |
| 34  | b     | 158  | U    | N1-C1'-C2'  | 5.89  | 121.66      | 114.00   |
| 34  | b     | 372  | G    | C1'-O4'-C4' | -5.89 | 105.19      | 109.90   |
| 34  | b     | 1779 | U    | C5'-C4'-O4' | 5.89  | 116.17      | 109.10   |
| 34  | b     | 729  | G    | O4'-C1'-N9  | 5.88  | 112.91      | 108.20   |
| 33  | a     | 42   | C    | N1-C1'-C2'  | 5.87  | 121.63      | 114.00   |
| 34  | b     | 2658 | C    | C2'-C3'-O3' | 5.87  | 123.09      | 113.70   |
| 34  | b     | 456  | C    | N1-C1'-C2'  | 5.86  | 121.62      | 114.00   |
| 34  | b     | 1275 | A    | C1'-O4'-C4' | -5.86 | 105.21      | 109.90   |
| 34  | b     | 1097 | U    | N1-C1'-C2'  | -5.86 | 105.55      | 112.00   |
| 34  | b     | 1211 | C    | O4'-C1'-N1  | -5.86 | 103.51      | 108.20   |
| 34  | b     | 1327 | A    | N9-C1'-C2'  | 5.86  | 121.61      | 114.00   |
| 34  | b     | 574  | A    | O4'-C1'-N9  | -5.85 | 103.52      | 108.20   |
| 34  | b     | 1096 | A    | O4'-C1'-N9  | 5.85  | 112.88      | 108.20   |
| 34  | b     | 2453 | A    | N9-C1'-C2'  | -5.85 | 105.57      | 112.00   |
| 28  | 3     | 10   | ARG  | NE-CZ-NH2   | 5.84  | 123.22      | 120.30   |
| 34  | b     | 2518 | A    | N9-C1'-C2'  | 5.84  | 121.59      | 114.00   |
| 34  | b     | 2104 | C    | C2'-C3'-O3' | 5.83  | 123.04      | 113.70   |
| 34  | b     | 2576 | G    | P-O5'-C5'   | 5.83  | 130.23      | 120.90   |
| 34  | b     | 458  | G    | O4'-C1'-N9  | 5.82  | 112.86      | 108.20   |
| 34  | b     | 603  | A    | N9-C1'-C2'  | 5.82  | 121.57      | 114.00   |
| 34  | b     | 1102 | C    | N1-C1'-C2'  | 5.81  | 121.56      | 114.00   |
| 34  | b     | 2330 | G    | N9-C1'-C2'  | -5.81 | 105.61      | 112.00   |
| 34  | b     | 2133 | G    | N9-C1'-C2'  | 5.80  | 121.54      | 114.00   |
| 34  | b     | 2056 | G    | N9-C1'-C2'  | 5.79  | 121.53      | 114.00   |
| 34  | b     | 2273 | A    | N9-C1'-C2'  | 5.79  | 121.53      | 114.00   |
| 34  | b     | 434  | U    | N1-C1'-C2'  | -5.78 | 105.64      | 112.00   |
| 34  | b     | 2340 | A    | C8-N9-C1'   | -5.78 | 117.29      | 127.70   |
| 34  | b     | 49   | A    | C4-N9-C1'   | 5.78  | 136.71      | 126.30   |
| 34  | b     | 1618 | A    | N9-C1'-C2'  | 5.78  | 121.51      | 114.00   |
| 34  | b     | 1060 | U    | C4'-C3'-O3' | 5.77  | 124.55      | 113.00   |
| 34  | b     | 2160 | C    | C1'-O4'-C4' | -5.77 | 105.28      | 109.90   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 34  | b     | 2210 | U    | O4'-C1'-N1  | -5.77 | 103.58      | 108.20   |
| 34  | b     | 1522 | A    | N9-C1'-C2'  | 5.76  | 121.49      | 114.00   |
| 34  | b     | 1349 | C    | N3-C4-N4    | -5.76 | 113.97      | 118.00   |
| 34  | b     | 1266 | G    | C1'-O4'-C4' | -5.76 | 105.30      | 109.90   |
| 34  | b     | 1079 | C    | C3'-C2'-C1' | -5.75 | 96.90       | 101.50   |
| 34  | b     | 2454 | G    | C4-N9-C1'   | -5.75 | 119.03      | 126.50   |
| 34  | b     | 1266 | G    | O4'-C1'-C2' | -5.74 | 100.06      | 105.80   |
| 34  | b     | 2160 | C    | N1-C1'-C2'  | -5.74 | 105.69      | 112.00   |
| 34  | b     | 1509 | A    | N9-C1'-C2'  | 5.72  | 121.44      | 114.00   |
| 34  | b     | 896  | A    | O4'-C1'-N9  | 5.72  | 112.77      | 108.20   |
| 34  | b     | 979  | A    | C4'-C3'-C2' | -5.71 | 96.89       | 102.60   |
| 34  | b     | 1382 | G    | N1-C2-N2    | -5.71 | 111.06      | 116.20   |
| 34  | b     | 1103 | A    | C2'-C3'-O3' | 5.71  | 122.83      | 113.70   |
| 34  | b     | 640  | C    | N1-C1'-C2'  | 5.70  | 121.41      | 114.00   |
| 34  | b     | 2271 | G    | N9-C1'-C2'  | 5.69  | 121.39      | 114.00   |
| 34  | b     | 24   | G    | N9-C1'-C2'  | 5.68  | 121.39      | 114.00   |
| 34  | b     | 1211 | C    | C4'-C3'-O3' | -5.68 | 97.47       | 109.40   |
| 34  | b     | 2333 | A    | N9-C1'-C2'  | -5.68 | 105.75      | 112.00   |
| 34  | b     | 1080 | A    | N1-C6-N6    | -5.68 | 115.19      | 118.60   |
| 34  | b     | 2161 | C    | C3'-C2'-C1' | -5.68 | 96.96       | 101.50   |
| 34  | b     | 2160 | C    | C4'-C3'-C2' | -5.67 | 96.93       | 102.60   |
| 34  | b     | 2732 | G    | O4'-C1'-N9  | 5.67  | 112.73      | 108.20   |
| 34  | b     | 249  | C    | N1-C1'-C2'  | -5.66 | 105.77      | 112.00   |
| 34  | b     | 1693 | U    | O4'-C1'-N1  | -5.65 | 103.68      | 108.20   |
| 34  | b     | 1459 | G    | N9-C1'-C2'  | 5.64  | 121.34      | 114.00   |
| 34  | b     | 31   | C    | N1-C1'-C2'  | -5.63 | 105.80      | 112.00   |
| 1   | A     | 1158 | C    | N3-C2-O2    | -5.63 | 117.96      | 121.90   |
| 22  | V     | 18   | G    | N9-C1'-C2'  | 5.62  | 121.31      | 114.00   |
| 34  | b     | 160  | A    | N9-C1'-C2'  | 5.62  | 121.31      | 114.00   |
| 34  | b     | 2045 | C    | N1-C1'-C2'  | -5.62 | 105.82      | 112.00   |
| 34  | b     | 251  | A    | N9-C1'-C2'  | 5.61  | 121.30      | 114.00   |
| 34  | b     | 516  | C    | C2'-C3'-O3' | 5.61  | 122.67      | 113.70   |
| 34  | b     | 569  | U    | N1-C1'-C2'  | 5.61  | 121.29      | 114.00   |
| 1   | A     | 365  | U    | C2-N1-C1'   | 5.60  | 124.42      | 117.70   |
| 34  | b     | 447  | A    | N9-C1'-C2'  | -5.60 | 105.84      | 112.00   |
| 34  | b     | 1226 | A    | N9-C1'-C2'  | 5.60  | 121.28      | 114.00   |
| 34  | b     | 834  | G    | C2'-C3'-O3' | 5.59  | 122.65      | 113.70   |
| 34  | b     | 801  | G    | C2'-C3'-O3' | 5.58  | 122.62      | 113.70   |
| 34  | b     | 2287 | A    | O4'-C1'-N9  | 5.57  | 112.65      | 108.20   |
| 34  | b     | 2508 | G    | N9-C1'-C2'  | -5.57 | 105.88      | 112.00   |
| 34  | b     | 1349 | C    | O4'-C1'-C2' | -5.56 | 100.24      | 105.80   |
| 34  | b     | 1265 | A    | N9-C1'-C2'  | 5.55  | 121.22      | 114.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 34  | b     | 1069 | A    | O4'-C1'-N9  | 5.55  | 112.64      | 108.20   |
| 34  | b     | 2282 | G    | O4'-C1'-N9  | 5.54  | 112.63      | 108.20   |
| 33  | a     | 15   | A    | N9-C1'-C2'  | 5.54  | 121.20      | 114.00   |
| 47  | o     | 25   | ARG  | NE-CZ-NH2   | 5.54  | 123.07      | 120.30   |
| 34  | b     | 1585 | C    | N3-C4-C5    | 5.54  | 124.11      | 121.90   |
| 34  | b     | 108  | G    | N9-C1'-C2'  | -5.54 | 105.91      | 112.00   |
| 34  | b     | 2330 | G    | C5'-C4'-O4' | 5.53  | 115.74      | 109.10   |
| 34  | b     | 783  | A    | O4'-C4'-C3' | -5.52 | 98.48       | 104.00   |
| 47  | o     | 18   | LEU  | CB-CA-C     | 5.51  | 120.68      | 110.20   |
| 34  | b     | 974  | G    | C1'-O4'-C4' | -5.51 | 105.49      | 109.90   |
| 34  | b     | 1055 | G    | C5'-C4'-O4' | 5.51  | 115.72      | 109.10   |
| 34  | b     | 2055 | C    | C2'-C3'-O3' | 5.51  | 122.52      | 113.70   |
| 34  | b     | 2458 | G    | N9-C1'-C2'  | -5.51 | 105.94      | 112.00   |
| 22  | V     | 18   | G    | O4'-C1'-N9  | -5.51 | 103.80      | 108.20   |
| 34  | b     | 119  | A    | N9-C1'-C2'  | 5.50  | 121.15      | 114.00   |
| 34  | b     | 1343 | G    | N9-C1'-C2'  | 5.50  | 121.15      | 114.00   |
| 34  | b     | 2051 | A    | O5'-P-OP1   | -5.50 | 100.75      | 105.70   |
| 34  | b     | 62   | U    | O4'-C1'-N1  | 5.49  | 112.59      | 108.20   |
| 34  | b     | 1607 | C    | O4'-C1'-N1  | -5.49 | 103.81      | 108.20   |
| 34  | b     | 241  | A    | O4'-C1'-N9  | -5.49 | 103.81      | 108.20   |
| 34  | b     | 1815 | A    | N9-C1'-C2'  | 5.48  | 121.12      | 114.00   |
| 34  | b     | 835  | C    | N1-C1'-C2'  | -5.48 | 105.97      | 112.00   |
| 34  | b     | 2506 | U    | O3'-P-O5'   | 5.47  | 114.39      | 104.00   |
| 34  | b     | 1156 | A    | N9-C1'-C2'  | 5.46  | 121.10      | 114.00   |
| 34  | b     | 2750 | A    | N9-C1'-C2'  | 5.46  | 121.10      | 114.00   |
| 34  | b     | 753  | A    | OP1-P-O3'   | -5.46 | 93.19       | 105.20   |
| 34  | b     | 1600 | C    | N1-C1'-C2'  | 5.46  | 121.09      | 114.00   |
| 34  | b     | 1104 | C    | C5'-C4'-O4' | 5.45  | 115.64      | 109.10   |
| 34  | b     | 1755 | A    | N9-C1'-C2'  | 5.45  | 121.08      | 114.00   |
| 34  | b     | 87   | U    | C2'-C3'-O3' | 5.44  | 122.41      | 113.70   |
| 34  | b     | 2057 | G    | N9-C1'-C2'  | 5.42  | 121.05      | 114.00   |
| 34  | b     | 277  | G    | O4'-C1'-C2' | -5.41 | 100.39      | 105.80   |
| 34  | b     | 1602 | U    | N1-C1'-C2'  | -5.41 | 106.05      | 112.00   |
| 34  | b     | 1667 | G    | O4'-C1'-C2' | -5.41 | 100.39      | 105.80   |
| 34  | b     | 1761 | C    | N1-C1'-C2'  | 5.41  | 121.03      | 114.00   |
| 34  | b     | 2034 | U    | N1-C1'-C2'  | 5.41  | 121.03      | 114.00   |
| 34  | b     | 463  | G    | N9-C1'-C2'  | -5.40 | 106.06      | 112.00   |
| 34  | b     | 2471 | A    | N9-C1'-C2'  | -5.40 | 106.06      | 112.00   |
| 1   | A     | 1158 | C    | C6-N1-C1'   | -5.38 | 114.34      | 120.80   |
| 34  | b     | 2266 | A    | O4'-C1'-N9  | -5.38 | 103.89      | 108.20   |
| 34  | b     | 1079 | C    | C1'-O4'-C4' | -5.38 | 105.60      | 109.90   |
| 34  | b     | 2340 | A    | C4-N9-C1'   | 5.37  | 135.96      | 126.30   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 34  | b     | 399  | U    | C5'-C4'-C3' | 5.37  | 124.59      | 116.00   |
| 34  | b     | 621  | A    | N9-C1'-C2'  | 5.37  | 120.98      | 114.00   |
| 34  | b     | 1762 | A    | C2'-C3'-O3' | 5.36  | 122.28      | 113.70   |
| 34  | b     | 1103 | A    | C5'-C4'-O4' | 5.35  | 115.52      | 109.10   |
| 34  | b     | 1667 | G    | C1'-C2'-O2' | 5.34  | 126.63      | 110.60   |
| 34  | b     | 465  | G    | N9-C1'-C2'  | 5.34  | 120.94      | 114.00   |
| 34  | b     | 503  | A    | C5'-C4'-C3' | 5.34  | 124.54      | 116.00   |
| 34  | b     | 1425 | G    | N9-C1'-C2'  | 5.34  | 120.94      | 114.00   |
| 34  | b     | 2288 | A    | C4'-C3'-O3' | 5.34  | 123.68      | 113.00   |
| 34  | b     | 1069 | A    | O4'-C4'-C3' | -5.34 | 98.66       | 104.00   |
| 34  | b     | 1033 | U    | C3'-C2'-C1' | 5.33  | 105.76      | 101.50   |
| 34  | b     | 2010 | G    | N9-C1'-C2'  | -5.32 | 106.14      | 112.00   |
| 34  | b     | 2161 | C    | P-O5'-C5'   | 5.32  | 129.41      | 120.90   |
| 34  | b     | 387  | U    | N1-C1'-C2'  | 5.32  | 120.91      | 114.00   |
| 34  | b     | 1814 | G    | N9-C1'-C2'  | 5.32  | 120.91      | 114.00   |
| 34  | b     | 1100 | C    | C4'-C3'-O3' | 5.31  | 123.62      | 113.00   |
| 34  | b     | 49   | A    | C3'-C2'-C1' | -5.31 | 97.25       | 101.50   |
| 34  | b     | 2175 | C    | C4'-C3'-C2' | -5.31 | 97.29       | 102.60   |
| 34  | b     | 33   | C    | N1-C1'-C2'  | -5.31 | 106.16      | 112.00   |
| 34  | b     | 571  | U    | O4'-C1'-N1  | 5.30  | 112.44      | 108.20   |
| 34  | b     | 1585 | C    | C6-N1-C2    | 5.30  | 122.42      | 120.30   |
| 34  | b     | 859  | G    | O4'-C1'-N9  | 5.29  | 112.44      | 108.20   |
| 34  | b     | 2564 | A    | N9-C1'-C2'  | 5.29  | 120.88      | 114.00   |
| 34  | b     | 281  | C    | N1-C1'-C2'  | 5.29  | 120.88      | 114.00   |
| 34  | b     | 1427 | A    | N9-C1'-C2'  | 5.28  | 120.86      | 114.00   |
| 34  | b     | 1461 | C    | N1-C1'-C2'  | 5.27  | 120.85      | 114.00   |
| 34  | b     | 2732 | G    | O4'-C1'-C2' | -5.27 | 100.53      | 105.80   |
| 34  | b     | 2422 | C    | O4'-C1'-N1  | 5.26  | 112.41      | 108.20   |
| 34  | b     | 1133 | A    | C1'-O4'-C4' | -5.26 | 105.69      | 109.90   |
| 34  | b     | 1086 | A    | N9-C1'-C2'  | 5.25  | 120.83      | 114.00   |
| 34  | b     | 896  | A    | C1'-O4'-C4' | -5.25 | 105.70      | 109.90   |
| 34  | b     | 896  | A    | O4'-C4'-C3' | -5.24 | 98.76       | 104.00   |
| 34  | b     | 446  | G    | C3'-C2'-C1' | 5.23  | 105.68      | 101.50   |
| 52  | t     | 3    | ARG  | NE-CZ-NH1   | 5.23  | 122.91      | 120.30   |
| 25  | 0     | 57   | ARG  | NE-CZ-NH2   | 5.22  | 122.91      | 120.30   |
| 34  | b     | 1616 | A    | N9-C1'-C2'  | 5.21  | 120.77      | 114.00   |
| 34  | b     | 783  | A    | C2'-C3'-O3' | 5.21  | 122.03      | 113.70   |
| 34  | b     | 2168 | G    | C4'-C3'-O3' | 5.21  | 123.41      | 113.00   |
| 34  | b     | 1055 | G    | C3'-C2'-C1' | 5.20  | 105.66      | 101.50   |
| 34  | b     | 1388 | G    | C2'-C3'-O3' | 5.20  | 122.02      | 113.70   |
| 34  | b     | 2282 | G    | O4'-C1'-C2' | -5.20 | 100.60      | 105.80   |
| 34  | b     | 2590 | A    | N9-C1'-C2'  | -5.20 | 106.28      | 112.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 34  | b     | 2391 | G    | C1'-O4'-C4' | -5.19 | 105.75      | 109.90   |
| 34  | b     | 2518 | A    | C5'-C4'-O4' | 5.19  | 115.33      | 109.10   |
| 34  | b     | 2422 | C    | C1'-O4'-C4' | -5.17 | 105.76      | 109.90   |
| 34  | b     | 1253 | A    | O4'-C1'-N9  | -5.17 | 104.07      | 108.20   |
| 37  | d     | 4    | LEU  | CB-CG-CD1   | 5.17  | 119.78      | 111.00   |
| 34  | b     | 979  | A    | C5'-C4'-O4' | 5.15  | 115.28      | 109.10   |
| 34  | b     | 2798 | U    | N1-C1'-C2'  | 5.14  | 120.69      | 114.00   |
| 34  | b     | 1059 | G    | N3-C4-C5    | -5.14 | 126.03      | 128.60   |
| 34  | b     | 1287 | A    | N9-C1'-C2'  | 5.14  | 120.68      | 114.00   |
| 34  | b     | 1772 | A    | C2'-C3'-O3' | 5.13  | 121.90      | 113.70   |
| 34  | b     | 2471 | A    | C4'-C3'-O3' | 5.13  | 123.25      | 113.00   |
| 34  | b     | 957  | C    | N1-C1'-C2'  | 5.12  | 120.66      | 114.00   |
| 34  | b     | 1377 | G    | N9-C1'-C2'  | 5.12  | 120.66      | 114.00   |
| 34  | b     | 1802 | A    | N9-C1'-C2'  | 5.12  | 120.66      | 114.00   |
| 23  | W     | 49   | G    | C2'-C3'-O3' | 5.12  | 121.89      | 113.70   |
| 34  | b     | 1141 | U    | N1-C1'-C2'  | 5.11  | 120.65      | 114.00   |
| 34  | b     | 242  | G    | O4'-C1'-N9  | 5.11  | 112.29      | 108.20   |
| 34  | b     | 100  | U    | C1'-O4'-C4' | -5.09 | 105.83      | 109.90   |
| 34  | b     | 974  | G    | O4'-C1'-C2' | -5.09 | 100.71      | 105.80   |
| 34  | b     | 253  | C    | N1-C1'-C2'  | -5.08 | 106.42      | 112.00   |
| 33  | a     | 66   | A    | C2'-C3'-O3' | 5.07  | 121.81      | 113.70   |
| 41  | h     | 66   | ASN  | N-CA-C      | 5.07  | 124.69      | 111.00   |
| 34  | b     | 1009 | A    | N9-C1'-C2'  | 5.07  | 120.59      | 114.00   |
| 34  | b     | 2330 | G    | C4'-C3'-C2' | -5.07 | 97.53       | 102.60   |
| 34  | b     | 250  | G    | O4'-C1'-N9  | -5.07 | 104.15      | 108.20   |
| 22  | V     | 18   | G    | O4'-C4'-C3' | -5.06 | 98.94       | 104.00   |
| 34  | b     | 1698 | A    | O4'-C1'-N9  | -5.06 | 104.15      | 108.20   |
| 34  | b     | 2288 | A    | O4'-C1'-N9  | 5.06  | 112.25      | 108.20   |
| 34  | b     | 584  | C    | O4'-C1'-C2' | -5.06 | 100.74      | 105.80   |
| 38  | e     | 59   | PRO  | C-N-CA      | 5.06  | 134.34      | 121.70   |
| 34  | b     | 196  | A    | C1'-O4'-C4' | -5.05 | 105.86      | 109.90   |
| 1   | A     | 188  | C    | N3-C2-O2    | -5.05 | 118.36      | 121.90   |
| 34  | b     | 1204 | A    | O4'-C1'-N9  | -5.05 | 104.16      | 108.20   |
| 34  | b     | 801  | G    | N9-C1'-C2'  | 5.03  | 120.54      | 114.00   |
| 34  | b     | 1266 | G    | N9-C1'-C2'  | -5.03 | 106.47      | 112.00   |
| 34  | b     | 2497 | A    | N9-C1'-C2'  | -5.03 | 106.47      | 112.00   |
| 34  | b     | 779  | U    | C5'-C4'-O4' | 5.03  | 115.14      | 109.10   |
| 34  | b     | 1599 | U    | N1-C1'-C2'  | 5.03  | 120.54      | 114.00   |
| 34  | b     | 783  | A    | C4'-C3'-O3' | 5.03  | 123.06      | 113.00   |
| 34  | b     | 1143 | A    | N9-C1'-C2'  | 5.03  | 120.53      | 114.00   |
| 34  | b     | 2488 | G    | N9-C1'-C2'  | 5.03  | 120.53      | 114.00   |
| 34  | b     | 1037 | G    | C5'-C4'-C3' | 5.03  | 124.04      | 116.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 34  | b     | 1355 | G    | N9-C1'-C2'  | -5.03 | 106.47      | 112.00   |
| 34  | b     | 195  | A    | N9-C1'-C2'  | -5.02 | 106.48      | 112.00   |
| 34  | b     | 759  | G    | C2'-C3'-O3' | 5.02  | 121.73      | 113.70   |
| 34  | b     | 62   | U    | C1'-O4'-C4' | -5.02 | 105.89      | 109.90   |
| 34  | b     | 1913 | A    | C2'-C3'-O3' | 5.02  | 121.73      | 113.70   |
| 34  | b     | 176  | A    | N9-C1'-C2'  | 5.01  | 120.51      | 114.00   |
| 34  | b     | 654  | A    | C2'-C3'-O3' | 5.01  | 121.71      | 113.70   |
| 34  | b     | 1607 | C    | N1-C1'-C2'  | 5.01  | 120.51      | 114.00   |
| 34  | b     | 2175 | C    | O4'-C4'-C3' | -5.01 | 98.99       | 104.00   |
| 34  | b     | 1069 | A    | C4'-C3'-O3' | 5.00  | 123.00      | 113.00   |
| 34  | b     | 1101 | U    | N1-C1'-C2'  | -5.00 | 106.50      | 112.00   |

There are no chirality outliers.

All (71) planarity outliers are listed below:

| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 27  | 2     | 3    | LYS  | Peptide   |
| 9   | I     | 124  | PRO  | Peptide   |
| 34  | b     | 1057 | A    | Sidechain |
| 34  | b     | 1059 | G    | Sidechain |
| 34  | b     | 1079 | C    | Sidechain |
| 34  | b     | 1080 | A    | Sidechain |
| 34  | b     | 1096 | A    | Sidechain |
| 34  | b     | 1097 | U    | Sidechain |
| 34  | b     | 119  | A    | Sidechain |
| 34  | b     | 1204 | A    | Sidechain |
| 34  | b     | 1225 | G    | Sidechain |
| 34  | b     | 1238 | G    | Sidechain |
| 34  | b     | 1253 | A    | Sidechain |
| 34  | b     | 1266 | G    | Sidechain |
| 34  | b     | 1272 | A    | Sidechain |
| 34  | b     | 1275 | A    | Sidechain |
| 34  | b     | 1300 | G    | Sidechain |
| 34  | b     | 1349 | C    | Sidechain |
| 34  | b     | 1382 | G    | Sidechain |
| 34  | b     | 1392 | A    | Sidechain |
| 34  | b     | 1667 | G    | Sidechain |
| 34  | b     | 1693 | U    | Sidechain |
| 34  | b     | 1698 | A    | Sidechain |
| 34  | b     | 1759 | A    | Sidechain |
| 34  | b     | 1773 | A    | Sidechain |
| 34  | b     | 1774 | C    | Sidechain |

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| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 34  | b     | 1775 | U    | Sidechain |
| 34  | b     | 1829 | A    | Sidechain |
| 34  | b     | 1943 | U    | Sidechain |
| 34  | b     | 195  | A    | Sidechain |
| 34  | b     | 1967 | C    | Sidechain |
| 34  | b     | 2032 | G    | Sidechain |
| 34  | b     | 2092 | U    | Sidechain |
| 34  | b     | 2123 | G    | Sidechain |
| 34  | b     | 2266 | A    | Sidechain |
| 34  | b     | 2330 | G    | Sidechain |
| 34  | b     | 241  | A    | Sidechain |
| 34  | b     | 242  | G    | Sidechain |
| 34  | b     | 2449 | U    | Sidechain |
| 34  | b     | 2453 | A    | Sidechain |
| 34  | b     | 2454 | G    | Sidechain |
| 34  | b     | 246  | C    | Sidechain |
| 34  | b     | 25   | U    | Sidechain |
| 34  | b     | 250  | G    | Sidechain |
| 34  | b     | 2518 | A    | Sidechain |
| 34  | b     | 2564 | A    | Sidechain |
| 34  | b     | 2589 | A    | Sidechain |
| 34  | b     | 2590 | A    | Sidechain |
| 34  | b     | 2597 | G    | Sidechain |
| 34  | b     | 372  | G    | Sidechain |
| 34  | b     | 388  | G    | Sidechain |
| 34  | b     | 446  | G    | Sidechain |
| 34  | b     | 450  | G    | Sidechain |
| 34  | b     | 464  | U    | Sidechain |
| 34  | b     | 500  | G    | Sidechain |
| 34  | b     | 603  | A    | Sidechain |
| 34  | b     | 674  | G    | Sidechain |
| 34  | b     | 779  | U    | Sidechain |
| 34  | b     | 782  | A    | Sidechain |
| 34  | b     | 783  | A    | Sidechain |
| 34  | b     | 801  | G    | Sidechain |
| 34  | b     | 805  | G    | Sidechain |
| 34  | b     | 959  | A    | Sidechain |
| 34  | b     | 973  | A    | Sidechain |
| 34  | b     | 979  | A    | Sidechain |
| 34  | b     | 986  | C    | Sidechain |
| 35  | c     | 232  | HIS  | Peptide   |
| 37  | d     | 151  | THR  | Peptide   |

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| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 43  | k     | 34  | GLY  | Peptide |
| 44  | l     | 102 | GLY  | Peptide |
| 50  | r     | 50  | GLY  | Peptide |

## 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 |    |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 2   | B     | 216/241 (90%) | 188 (87%) | 19 (9%)  | 9 (4%)   | 3           | 18 |
| 3   | C     | 204/233 (88%) | 171 (84%) | 23 (11%) | 10 (5%)  | 2           | 15 |
| 4   | D     | 203/206 (98%) | 190 (94%) | 9 (4%)   | 4 (2%)   | 7           | 33 |
| 5   | E     | 148/167 (89%) | 131 (88%) | 7 (5%)   | 10 (7%)  | 1           | 9  |
| 6   | F     | 98/131 (75%)  | 81 (83%)  | 14 (14%) | 3 (3%)   | 4           | 24 |
| 7   | G     | 148/156 (95%) | 135 (91%) | 8 (5%)   | 5 (3%)   | 3           | 23 |
| 8   | H     | 127/130 (98%) | 110 (87%) | 15 (12%) | 2 (2%)   | 9           | 37 |
| 9   | I     | 125/130 (96%) | 106 (85%) | 16 (13%) | 3 (2%)   | 6           | 29 |
| 10  | J     | 96/103 (93%)  | 84 (88%)  | 7 (7%)   | 5 (5%)   | 2           | 14 |
| 11  | K     | 115/129 (89%) | 104 (90%) | 10 (9%)  | 1 (1%)   | 17          | 49 |
| 12  | L     | 121/124 (98%) | 94 (78%)  | 22 (18%) | 5 (4%)   | 3           | 18 |
| 13  | M     | 111/118 (94%) | 99 (89%)  | 5 (4%)   | 7 (6%)   | 1           | 10 |
| 14  | N     | 92/101 (91%)  | 80 (87%)  | 8 (9%)   | 4 (4%)   | 2           | 18 |
| 15  | O     | 86/89 (97%)   | 80 (93%)  | 5 (6%)   | 1 (1%)   | 13          | 43 |
| 16  | P     | 80/82 (98%)   | 56 (70%)  | 15 (19%) | 9 (11%)  | 0           | 3  |
| 17  | Q     | 78/84 (93%)   | 66 (85%)  | 11 (14%) | 1 (1%)   | 12          | 40 |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 18  | R     | 53/75 (71%)   | 51 (96%)  | 2 (4%)   | 0        | 100         | 100 |
| 19  | S     | 77/92 (84%)   | 69 (90%)  | 5 (6%)   | 3 (4%)   | 3           | 20  |
| 20  | T     | 83/87 (95%)   | 77 (93%)  | 5 (6%)   | 1 (1%)   | 13          | 43  |
| 21  | U     | 49/71 (69%)   | 40 (82%)  | 5 (10%)  | 4 (8%)   | 1           | 6   |
| 25  | 0     | 75/78 (96%)   | 74 (99%)  | 1 (1%)   | 0        | 100         | 100 |
| 26  | 1     | 60/63 (95%)   | 53 (88%)  | 5 (8%)   | 2 (3%)   | 4           | 23  |
| 27  | 2     | 56/59 (95%)   | 52 (93%)  | 3 (5%)   | 1 (2%)   | 8           | 35  |
| 28  | 3     | 54/57 (95%)   | 49 (91%)  | 3 (6%)   | 2 (4%)   | 3           | 21  |
| 29  | 4     | 48/55 (87%)   | 39 (81%)  | 9 (19%)  | 0        | 100         | 100 |
| 30  | 6     | 44/46 (96%)   | 40 (91%)  | 2 (4%)   | 2 (4%)   | 2           | 16  |
| 31  | 7     | 62/65 (95%)   | 60 (97%)  | 2 (3%)   | 0        | 100         | 100 |
| 32  | 8     | 36/38 (95%)   | 35 (97%)  | 1 (3%)   | 0        | 100         | 100 |
| 35  | c     | 269/273 (98%) | 251 (93%) | 17 (6%)  | 1 (0%)   | 34          | 66  |
| 36  | i     | 132/142 (93%) | 83 (63%)  | 38 (29%) | 11 (8%)  | 1           | 6   |
| 37  | d     | 207/209 (99%) | 194 (94%) | 11 (5%)  | 2 (1%)   | 15          | 47  |
| 38  | e     | 199/201 (99%) | 186 (94%) | 7 (4%)   | 6 (3%)   | 4           | 25  |
| 39  | f     | 175/179 (98%) | 157 (90%) | 12 (7%)  | 6 (3%)   | 3           | 23  |
| 40  | g     | 174/177 (98%) | 139 (80%) | 31 (18%) | 4 (2%)   | 6           | 30  |
| 41  | h     | 147/149 (99%) | 122 (83%) | 20 (14%) | 5 (3%)   | 3           | 23  |
| 42  | j     | 140/142 (99%) | 128 (91%) | 10 (7%)  | 2 (1%)   | 11          | 39  |
| 43  | k     | 120/123 (98%) | 112 (93%) | 6 (5%)   | 2 (2%)   | 9           | 36  |
| 44  | l     | 142/144 (99%) | 126 (89%) | 10 (7%)  | 6 (4%)   | 3           | 18  |
| 45  | m     | 131/136 (96%) | 123 (94%) | 7 (5%)   | 1 (1%)   | 19          | 51  |
| 46  | n     | 118/127 (93%) | 111 (94%) | 4 (3%)   | 3 (2%)   | 5           | 28  |
| 47  | o     | 114/117 (97%) | 104 (91%) | 5 (4%)   | 5 (4%)   | 2           | 17  |
| 48  | p     | 112/115 (97%) | 106 (95%) | 5 (4%)   | 1 (1%)   | 17          | 49  |
| 49  | q     | 115/118 (98%) | 114 (99%) | 1 (1%)   | 0        | 100         | 100 |
| 50  | r     | 101/103 (98%) | 91 (90%)  | 7 (7%)   | 3 (3%)   | 4           | 25  |
| 51  | s     | 108/110 (98%) | 103 (95%) | 2 (2%)   | 3 (3%)   | 5           | 26  |
| 52  | t     | 91/100 (91%)  | 80 (88%)  | 8 (9%)   | 3 (3%)   | 4           | 23  |
| 53  | u     | 100/104 (96%) | 77 (77%)  | 12 (12%) | 11 (11%) | 0           | 3   |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 54  | w     | 92/94 (98%)     | 91 (99%)   | 1 (1%)   | 0        | 100         | 100 |
| 55  | y     | 73/85 (86%)     | 71 (97%)   | 2 (3%)   | 0        | 100         | 100 |
| 56  | z     | 25/27 (93%)     | 20 (80%)   | 5 (20%)  | 0        | 100         | 100 |
| All | All   | 5630/5985 (94%) | 5003 (89%) | 458 (8%) | 169 (3%) | 7           | 25  |

All (169) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | C     | 7   | ASN  |
| 5   | E     | 99  | SER  |
| 8   | H     | 44  | PHE  |
| 9   | I     | 57  | VAL  |
| 12  | L     | 88  | ASP  |
| 16  | P     | 11  | ALA  |
| 16  | P     | 80  | LYS  |
| 19  | S     | 4   | LEU  |
| 20  | T     | 67  | HIS  |
| 21  | U     | 26  | GLY  |
| 21  | U     | 27  | VAL  |
| 21  | U     | 30  | GLU  |
| 26  | 1     | 3   | ALA  |
| 28  | 3     | 56  | ALA  |
| 30  | 6     | 44  | VAL  |
| 36  | i     | 65  | SER  |
| 36  | i     | 92  | PRO  |
| 37  | d     | 152 | PRO  |
| 38  | e     | 153 | LEU  |
| 39  | f     | 62  | GLY  |
| 39  | f     | 123 | ASP  |
| 40  | g     | 119 | ALA  |
| 41  | h     | 41  | LYS  |
| 41  | h     | 66  | ASN  |
| 41  | h     | 67  | ALA  |
| 42  | j     | 81  | ILE  |
| 44  | l     | 29  | LYS  |
| 44  | l     | 68  | SER  |
| 44  | l     | 111 | ILE  |
| 44  | l     | 115 | GLU  |
| 46  | n     | 70  | THR  |
| 46  | n     | 119 | SER  |
| 48  | p     | 114 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 50  | r     | 7   | SER  |
| 51  | s     | 65  | ASP  |
| 52  | t     | 17  | SER  |
| 53  | u     | 7   | ARG  |
| 53  | u     | 17  | LYS  |
| 53  | u     | 72  | ILE  |
| 53  | u     | 73  | PHE  |
| 53  | u     | 75  | ALA  |
| 2   | B     | 22  | TRP  |
| 2   | B     | 83  | ALA  |
| 3   | C     | 49  | ALA  |
| 3   | C     | 154 | GLY  |
| 5   | E     | 44  | ARG  |
| 5   | E     | 45  | VAL  |
| 5   | E     | 73  | VAL  |
| 6   | F     | 48  | ALA  |
| 6   | F     | 94  | HIS  |
| 7   | G     | 148 | LYS  |
| 9   | I     | 119 | LYS  |
| 10  | J     | 57  | VAL  |
| 10  | J     | 58  | ASN  |
| 10  | J     | 67  | ILE  |
| 12  | L     | 23  | LEU  |
| 13  | M     | 3   | ILE  |
| 13  | M     | 46  | GLU  |
| 13  | M     | 104 | ASN  |
| 14  | N     | 50  | LEU  |
| 15  | O     | 21  | THR  |
| 16  | P     | 10  | GLY  |
| 16  | P     | 16  | PHE  |
| 16  | P     | 36  | VAL  |
| 17  | Q     | 71  | SER  |
| 19  | S     | 5   | LYS  |
| 28  | 3     | 55  | ILE  |
| 36  | i     | 30  | GLN  |
| 36  | i     | 105 | LEU  |
| 40  | g     | 92  | VAL  |
| 41  | h     | 119 | ASN  |
| 43  | k     | 35  | VAL  |
| 44  | l     | 69  | ARG  |
| 47  | o     | 59  | ALA  |
| 47  | o     | 101 | GLY  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 51  | s     | 62  | ASP  |
| 51  | s     | 63  | GLY  |
| 52  | t     | 38  | ALA  |
| 53  | u     | 74  | ASN  |
| 53  | u     | 76  | ALA  |
| 53  | u     | 99  | ASN  |
| 2   | B     | 21  | TYR  |
| 2   | B     | 189 | ASN  |
| 2   | B     | 204 | ASP  |
| 3   | C     | 77  | GLY  |
| 3   | C     | 111 | ASP  |
| 3   | C     | 145 | ALA  |
| 4   | D     | 4   | LEU  |
| 4   | D     | 47  | LEU  |
| 4   | D     | 108 | ALA  |
| 5   | E     | 146 | MET  |
| 6   | F     | 54  | LEU  |
| 7   | G     | 114 | SER  |
| 10  | J     | 41  | PRO  |
| 12  | L     | 46  | SER  |
| 13  | M     | 5   | GLY  |
| 13  | M     | 7   | ASN  |
| 13  | M     | 23  | GLY  |
| 14  | N     | 62  | ARG  |
| 16  | P     | 49  | GLY  |
| 16  | P     | 78  | VAL  |
| 21  | U     | 24  | LYS  |
| 35  | c     | 253 | LYS  |
| 36  | i     | 59  | THR  |
| 39  | f     | 175 | PHE  |
| 42  | j     | 25  | LEU  |
| 43  | k     | 108 | ARG  |
| 44  | l     | 86  | GLU  |
| 45  | m     | 69  | PRO  |
| 47  | o     | 34  | HIS  |
| 47  | o     | 66  | GLY  |
| 53  | u     | 4   | LYS  |
| 3   | C     | 3   | LYS  |
| 3   | C     | 5   | HIS  |
| 5   | E     | 11  | GLN  |
| 7   | G     | 4   | ARG  |
| 9   | I     | 112 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11  | K     | 88  | PRO  |
| 13  | M     | 47  | LEU  |
| 26  | 1     | 37  | LEU  |
| 27  | 2     | 4   | THR  |
| 36  | i     | 83  | ALA  |
| 36  | i     | 89  | SER  |
| 38  | e     | 62  | GLN  |
| 38  | e     | 127 | GLU  |
| 39  | f     | 121 | SER  |
| 39  | f     | 174 | ASP  |
| 46  | n     | 118 | ARG  |
| 47  | o     | 100 | HIS  |
| 53  | u     | 98  | SER  |
| 2   | B     | 63  | LYS  |
| 2   | B     | 76  | SER  |
| 2   | B     | 126 | ASP  |
| 4   | D     | 194 | ILE  |
| 5   | E     | 147 | ASN  |
| 7   | G     | 52  | ARG  |
| 7   | G     | 113 | LYS  |
| 10  | J     | 75  | ASP  |
| 12  | L     | 116 | TYR  |
| 14  | N     | 52  | ARG  |
| 14  | N     | 61  | ASN  |
| 19  | S     | 11  | ASP  |
| 36  | i     | 20  | SER  |
| 38  | e     | 80  | SER  |
| 40  | g     | 118 | PRO  |
| 41  | h     | 56  | ALA  |
| 50  | r     | 53  | PHE  |
| 52  | t     | 18  | GLU  |
| 2   | B     | 30  | ILE  |
| 8   | H     | 52  | GLY  |
| 30  | 6     | 45  | SER  |
| 37  | d     | 104 | VAL  |
| 3   | C     | 63  | ILE  |
| 16  | P     | 42  | ILE  |
| 36  | i     | 97  | VAL  |
| 38  | e     | 42  | GLY  |
| 38  | e     | 83  | VAL  |
| 39  | f     | 149 | VAL  |
| 40  | g     | 28  | GLY  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 53  | u     | 55  | PRO  |
| 5   | E     | 105 | ILE  |
| 12  | L     | 117 | GLY  |
| 5   | E     | 50  | GLY  |
| 36  | i     | 23  | VAL  |
| 3   | C     | 107 | LYS  |
| 5   | E     | 142 | GLY  |
| 16  | P     | 15  | PRO  |
| 36  | i     | 31  | GLY  |
| 50  | r     | 9   | GLY  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed      | Rotameric  | Outliers | Percentiles |     |
|-----|-------|---------------|------------|----------|-------------|-----|
| 2   | B     | 180/199 (90%) | 180 (100%) | 0        | 100         | 100 |
| 3   | C     | 170/190 (90%) | 170 (100%) | 0        | 100         | 100 |
| 4   | D     | 172/173 (99%) | 172 (100%) | 0        | 100         | 100 |
| 5   | E     | 113/126 (90%) | 113 (100%) | 0        | 100         | 100 |
| 6   | F     | 87/112 (78%)  | 87 (100%)  | 0        | 100         | 100 |
| 7   | G     | 123/129 (95%) | 123 (100%) | 0        | 100         | 100 |
| 8   | H     | 104/105 (99%) | 104 (100%) | 0        | 100         | 100 |
| 9   | I     | 105/107 (98%) | 105 (100%) | 0        | 100         | 100 |
| 10  | J     | 86/90 (96%)   | 86 (100%)  | 0        | 100         | 100 |
| 11  | K     | 90/99 (91%)   | 90 (100%)  | 0        | 100         | 100 |
| 12  | L     | 103/104 (99%) | 103 (100%) | 0        | 100         | 100 |
| 13  | M     | 91/96 (95%)   | 91 (100%)  | 0        | 100         | 100 |
| 14  | N     | 79/84 (94%)   | 79 (100%)  | 0        | 100         | 100 |
| 15  | O     | 76/77 (99%)   | 76 (100%)  | 0        | 100         | 100 |
| 16  | P     | 65/65 (100%)  | 57 (88%)   | 8 (12%)  | 4           | 20  |
| 17  | Q     | 74/78 (95%)   | 74 (100%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 18  | R     | 48/65 (74%)    | 48 (100%)  | 0        | 100         | 100 |
| 19  | S     | 70/79 (89%)    | 70 (100%)  | 0        | 100         | 100 |
| 20  | T     | 65/66 (98%)    | 65 (100%)  | 0        | 100         | 100 |
| 21  | U     | 44/61 (72%)    | 44 (100%)  | 0        | 100         | 100 |
| 25  | 0     | 67/68 (98%)    | 63 (94%)   | 4 (6%)   | 19          | 50  |
| 26  | 1     | 54/55 (98%)    | 52 (96%)   | 2 (4%)   | 34          | 64  |
| 27  | 2     | 48/49 (98%)    | 48 (100%)  | 0        | 100         | 100 |
| 28  | 3     | 47/48 (98%)    | 45 (96%)   | 2 (4%)   | 29          | 61  |
| 29  | 4     | 45/49 (92%)    | 45 (100%)  | 0        | 100         | 100 |
| 30  | 6     | 38/38 (100%)   | 37 (97%)   | 1 (3%)   | 46          | 72  |
| 31  | 7     | 51/52 (98%)    | 49 (96%)   | 2 (4%)   | 32          | 63  |
| 32  | 8     | 34/34 (100%)   | 33 (97%)   | 1 (3%)   | 42          | 70  |
| 35  | c     | 216/218 (99%)  | 210 (97%)  | 6 (3%)   | 43          | 71  |
| 36  | i     | 104/110 (94%)  | 87 (84%)   | 17 (16%) | 2           | 10  |
| 37  | d     | 164/164 (100%) | 161 (98%)  | 3 (2%)   | 59          | 79  |
| 38  | e     | 165/165 (100%) | 159 (96%)  | 6 (4%)   | 35          | 65  |
| 39  | f     | 148/150 (99%)  | 142 (96%)  | 6 (4%)   | 30          | 62  |
| 40  | g     | 137/138 (99%)  | 133 (97%)  | 4 (3%)   | 42          | 70  |
| 41  | h     | 114/114 (100%) | 114 (100%) | 0        | 100         | 100 |
| 42  | j     | 116/116 (100%) | 112 (97%)  | 4 (3%)   | 37          | 66  |
| 43  | k     | 103/104 (99%)  | 101 (98%)  | 2 (2%)   | 57          | 78  |
| 44  | l     | 103/103 (100%) | 99 (96%)   | 4 (4%)   | 32          | 63  |
| 45  | m     | 108/109 (99%)  | 107 (99%)  | 1 (1%)   | 78          | 88  |
| 46  | n     | 100/103 (97%)  | 98 (98%)   | 2 (2%)   | 55          | 77  |
| 47  | o     | 86/87 (99%)    | 86 (100%)  | 0        | 100         | 100 |
| 48  | p     | 99/100 (99%)   | 95 (96%)   | 4 (4%)   | 31          | 62  |
| 49  | q     | 89/90 (99%)    | 85 (96%)   | 4 (4%)   | 27          | 60  |
| 50  | r     | 84/84 (100%)   | 80 (95%)   | 4 (5%)   | 25          | 58  |
| 51  | s     | 93/93 (100%)   | 91 (98%)   | 2 (2%)   | 52          | 76  |
| 52  | t     | 80/84 (95%)    | 77 (96%)   | 3 (4%)   | 33          | 63  |
| 53  | u     | 83/85 (98%)    | 79 (95%)   | 4 (5%)   | 25          | 58  |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 54  | w     | 78/78 (100%)    | 76 (97%)   | 2 (3%)   | 46          | 72 |
| 55  | y     | 56/63 (89%)     | 55 (98%)   | 1 (2%)   | 59          | 79 |
| 56  | z     | 23/23 (100%)    | 13 (56%)   | 10 (44%) | 0           | 0  |
| All | All   | 4678/4879 (96%) | 4569 (98%) | 109 (2%) | 53          | 75 |

All (109) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 16  | P     | 6   | LEU  |
| 16  | P     | 19  | VAL  |
| 16  | P     | 33  | ILE  |
| 16  | P     | 46  | LYS  |
| 16  | P     | 55  | ASP  |
| 16  | P     | 63  | GLN  |
| 16  | P     | 68  | SER  |
| 16  | P     | 77  | GLU  |
| 25  | 0     | 11  | ARG  |
| 25  | 0     | 17  | ASN  |
| 25  | 0     | 48  | THR  |
| 25  | 0     | 57  | ARG  |
| 26  | 1     | 21  | LEU  |
| 26  | 1     | 38  | GLN  |
| 28  | 3     | 28  | LEU  |
| 28  | 3     | 29  | SER  |
| 30  | 6     | 8   | SER  |
| 31  | 7     | 31  | HIS  |
| 31  | 7     | 47  | LYS  |
| 32  | 8     | 18  | LYS  |
| 35  | c     | 5   | LYS  |
| 35  | c     | 115 | GLN  |
| 35  | c     | 130 | LEU  |
| 35  | c     | 139 | SER  |
| 35  | c     | 157 | SER  |
| 35  | c     | 267 | ILE  |
| 36  | i     | 10  | LEU  |
| 36  | i     | 11  | GLN  |
| 36  | i     | 12  | VAL  |
| 36  | i     | 23  | VAL  |
| 36  | i     | 30  | GLN  |
| 36  | i     | 37  | PHE  |
| 36  | i     | 39  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 36  | i     | 49  | GLU  |
| 36  | i     | 61  | TYR  |
| 36  | i     | 71  | LYS  |
| 36  | i     | 81  | LYS  |
| 36  | i     | 86  | LYS  |
| 36  | i     | 95  | ASP  |
| 36  | i     | 107 | GLU  |
| 36  | i     | 124 | MET  |
| 36  | i     | 126 | ARG  |
| 36  | i     | 135 | MET  |
| 37  | d     | 32  | ASN  |
| 37  | d     | 51  | THR  |
| 37  | d     | 91  | THR  |
| 38  | e     | 12  | LEU  |
| 38  | e     | 78  | TRP  |
| 38  | e     | 88  | ARG  |
| 38  | e     | 93  | SER  |
| 38  | e     | 126 | VAL  |
| 38  | e     | 187 | VAL  |
| 39  | f     | 5   | HIS  |
| 39  | f     | 7   | TYR  |
| 39  | f     | 19  | GLU  |
| 39  | f     | 83  | TYR  |
| 39  | f     | 117 | LEU  |
| 39  | f     | 174 | ASP  |
| 40  | g     | 29  | LYS  |
| 40  | g     | 73  | ASN  |
| 40  | g     | 80  | THR  |
| 40  | g     | 92  | VAL  |
| 42  | j     | 30  | THR  |
| 42  | j     | 131 | ASN  |
| 42  | j     | 136 | GLN  |
| 42  | j     | 142 | ILE  |
| 43  | k     | 92  | GLU  |
| 43  | k     | 105 | ARG  |
| 44  | l     | 48  | ARG  |
| 44  | l     | 91  | ASP  |
| 44  | l     | 94  | THR  |
| 44  | l     | 118 | THR  |
| 45  | m     | 100 | LYS  |
| 46  | n     | 95  | THR  |
| 46  | n     | 116 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 48  | p     | 8   | LEU  |
| 48  | p     | 26  | VAL  |
| 48  | p     | 37  | LYS  |
| 48  | p     | 80  | VAL  |
| 49  | q     | 5   | LYS  |
| 49  | q     | 9   | ILE  |
| 49  | q     | 16  | LYS  |
| 49  | q     | 109 | LEU  |
| 50  | r     | 46  | GLU  |
| 50  | r     | 58  | VAL  |
| 50  | r     | 60  | LYS  |
| 50  | r     | 102 | SER  |
| 51  | s     | 19  | LEU  |
| 51  | s     | 97  | LEU  |
| 52  | t     | 5   | GLU  |
| 52  | t     | 10  | VAL  |
| 52  | t     | 39  | THR  |
| 53  | u     | 15  | THR  |
| 53  | u     | 35  | ILE  |
| 53  | u     | 37  | GLU  |
| 53  | u     | 68  | SER  |
| 54  | w     | 53  | LYS  |
| 54  | w     | 76  | ASP  |
| 55  | y     | 41  | ARG  |
| 56  | z     | 4   | GLN  |
| 56  | z     | 5   | LYS  |
| 56  | z     | 9   | GLU  |
| 56  | z     | 10  | GLU  |
| 56  | z     | 12  | LEU  |
| 56  | z     | 15  | THR  |
| 56  | z     | 18  | TRP  |
| 56  | z     | 20  | SER  |
| 56  | z     | 21  | GLN  |
| 56  | z     | 26  | ARG  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (67) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 92  | ASN  |
| 2   | B     | 202 | ASN  |
| 3   | C     | 24  | ASN  |
| 3   | C     | 101 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | D     | 84  | ASN  |
| 4   | D     | 115 | GLN  |
| 4   | D     | 119 | HIS  |
| 4   | D     | 125 | ASN  |
| 4   | D     | 130 | ASN  |
| 4   | D     | 139 | ASN  |
| 4   | D     | 151 | GLN  |
| 4   | D     | 195 | ASN  |
| 5   | E     | 11  | GLN  |
| 5   | E     | 82  | HIS  |
| 5   | E     | 88  | HIS  |
| 5   | E     | 134 | ASN  |
| 6   | F     | 11  | HIS  |
| 6   | F     | 37  | HIS  |
| 6   | F     | 68  | GLN  |
| 7   | G     | 129 | ASN  |
| 7   | G     | 141 | HIS  |
| 8   | H     | 3   | GLN  |
| 8   | H     | 15  | ASN  |
| 8   | H     | 37  | ASN  |
| 9   | I     | 3   | ASN  |
| 9   | I     | 30  | ASN  |
| 11  | K     | 23  | HIS  |
| 11  | K     | 39  | ASN  |
| 12  | L     | 4   | ASN  |
| 12  | L     | 19  | ASN  |
| 12  | L     | 45  | ASN  |
| 13  | M     | 99  | GLN  |
| 14  | N     | 34  | ASN  |
| 14  | N     | 65  | GLN  |
| 14  | N     | 70  | HIS  |
| 15  | O     | 34  | GLN  |
| 15  | O     | 37  | HIS  |
| 15  | O     | 41  | HIS  |
| 15  | O     | 49  | HIS  |
| 15  | O     | 50  | HIS  |
| 16  | P     | 29  | ASN  |
| 16  | P     | 59  | HIS  |
| 16  | P     | 63  | GLN  |
| 17  | Q     | 30  | HIS  |
| 17  | Q     | 50  | ASN  |
| 19  | S     | 51  | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 19  | S     | 56  | HIS  |
| 20  | T     | 54  | GLN  |
| 20  | T     | 67  | HIS  |
| 20  | T     | 74  | HIS  |
| 32  | 8     | 37  | GLN  |
| 35  | c     | 46  | ASN  |
| 36  | i     | 30  | GLN  |
| 36  | i     | 110 | GLN  |
| 37  | d     | 150 | GLN  |
| 40  | g     | 22  | GLN  |
| 40  | g     | 38  | ASN  |
| 41  | h     | 28  | ASN  |
| 41  | h     | 73  | ASN  |
| 41  | h     | 119 | ASN  |
| 41  | h     | 128 | HIS  |
| 43  | k     | 3   | GLN  |
| 51  | s     | 61  | ASN  |
| 53  | u     | 74  | ASN  |
| 55  | y     | 57  | HIS  |
| 56  | z     | 4   | GLN  |
| 56  | z     | 21  | GLN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1   | A     | 1530/1542 (99%) | 422 (27%)         | 30 (1%)         |
| 22  | V     | 75/76 (98%)     | 45 (60%)          | 9 (12%)         |
| 23  | W     | 75/75 (100%)    | 40 (53%)          | 10 (13%)        |
| 24  | X     | 11/11 (100%)    | 8 (72%)           | 3 (27%)         |
| 33  | a     | 116/120 (96%)   | 43 (37%)          | 0               |
| 34  | b     | 2902/2904 (99%) | 1204 (41%)        | 0               |
| All | All   | 4709/4728 (99%) | 1762 (37%)        | 52 (1%)         |

All (1762) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 6   | G    |
| 1   | A     | 8   | A    |
| 1   | A     | 9   | G    |
| 1   | A     | 13  | U    |
| 1   | A     | 22  | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 39  | G    |
| 1   | A     | 44  | A    |
| 1   | A     | 46  | G    |
| 1   | A     | 47  | C    |
| 1   | A     | 48  | C    |
| 1   | A     | 50  | A    |
| 1   | A     | 51  | A    |
| 1   | A     | 52  | C    |
| 1   | A     | 54  | C    |
| 1   | A     | 62  | U    |
| 1   | A     | 64  | G    |
| 1   | A     | 65  | A    |
| 1   | A     | 66  | A    |
| 1   | A     | 71  | A    |
| 1   | A     | 75  | G    |
| 1   | A     | 78  | A    |
| 1   | A     | 80  | A    |
| 1   | A     | 83  | C    |
| 1   | A     | 84  | U    |
| 1   | A     | 86  | G    |
| 1   | A     | 87  | C    |
| 1   | A     | 89  | U    |
| 1   | A     | 93  | U    |
| 1   | A     | 94  | G    |
| 1   | A     | 95  | C    |
| 1   | A     | 97  | G    |
| 1   | A     | 98  | A    |
| 1   | A     | 99  | C    |
| 1   | A     | 100 | G    |
| 1   | A     | 102 | G    |
| 1   | A     | 108 | G    |
| 1   | A     | 110 | C    |
| 1   | A     | 111 | G    |
| 1   | A     | 116 | A    |
| 1   | A     | 120 | A    |
| 1   | A     | 121 | U    |
| 1   | A     | 122 | G    |
| 1   | A     | 125 | U    |
| 1   | A     | 126 | G    |
| 1   | A     | 129 | A    |
| 1   | A     | 130 | A    |
| 1   | A     | 131 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 133 | U    |
| 1   | A     | 141 | G    |
| 1   | A     | 144 | G    |
| 1   | A     | 145 | G    |
| 1   | A     | 146 | G    |
| 1   | A     | 149 | A    |
| 1   | A     | 152 | A    |
| 1   | A     | 157 | U    |
| 1   | A     | 160 | A    |
| 1   | A     | 163 | C    |
| 1   | A     | 179 | A    |
| 1   | A     | 182 | A    |
| 1   | A     | 183 | C    |
| 1   | A     | 184 | G    |
| 1   | A     | 185 | U    |
| 1   | A     | 186 | C    |
| 1   | A     | 187 | G    |
| 1   | A     | 188 | C    |
| 1   | A     | 192 | A    |
| 1   | A     | 196 | A    |
| 1   | A     | 197 | A    |
| 1   | A     | 198 | G    |
| 1   | A     | 200 | G    |
| 1   | A     | 201 | G    |
| 1   | A     | 203 | G    |
| 1   | A     | 204 | G    |
| 1   | A     | 205 | A    |
| 1   | A     | 210 | C    |
| 1   | A     | 211 | G    |
| 1   | A     | 215 | C    |
| 1   | A     | 217 | C    |
| 1   | A     | 218 | U    |
| 1   | A     | 219 | U    |
| 1   | A     | 226 | G    |
| 1   | A     | 229 | U    |
| 1   | A     | 230 | G    |
| 1   | A     | 231 | U    |
| 1   | A     | 236 | A    |
| 1   | A     | 238 | A    |
| 1   | A     | 239 | U    |
| 1   | A     | 240 | G    |
| 1   | A     | 244 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 245 | U    |
| 1   | A     | 247 | G    |
| 1   | A     | 251 | G    |
| 1   | A     | 255 | G    |
| 1   | A     | 256 | U    |
| 1   | A     | 257 | G    |
| 1   | A     | 258 | G    |
| 1   | A     | 266 | G    |
| 1   | A     | 267 | C    |
| 1   | A     | 275 | G    |
| 1   | A     | 277 | C    |
| 1   | A     | 280 | C    |
| 1   | A     | 281 | G    |
| 1   | A     | 289 | G    |
| 1   | A     | 302 | G    |
| 1   | A     | 309 | A    |
| 1   | A     | 314 | C    |
| 1   | A     | 320 | A    |
| 1   | A     | 321 | A    |
| 1   | A     | 328 | C    |
| 1   | A     | 329 | A    |
| 1   | A     | 330 | C    |
| 1   | A     | 332 | G    |
| 1   | A     | 342 | C    |
| 1   | A     | 343 | U    |
| 1   | A     | 352 | C    |
| 1   | A     | 353 | A    |
| 1   | A     | 354 | G    |
| 1   | A     | 367 | U    |
| 1   | A     | 368 | U    |
| 1   | A     | 369 | G    |
| 1   | A     | 372 | C    |
| 1   | A     | 373 | A    |
| 1   | A     | 374 | A    |
| 1   | A     | 375 | U    |
| 1   | A     | 377 | G    |
| 1   | A     | 381 | C    |
| 1   | A     | 386 | C    |
| 1   | A     | 387 | U    |
| 1   | A     | 388 | G    |
| 1   | A     | 389 | A    |
| 1   | A     | 390 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 391 | G    |
| 1   | A     | 397 | A    |
| 1   | A     | 398 | U    |
| 1   | A     | 399 | G    |
| 1   | A     | 401 | C    |
| 1   | A     | 404 | G    |
| 1   | A     | 406 | G    |
| 1   | A     | 408 | A    |
| 1   | A     | 411 | A    |
| 1   | A     | 413 | G    |
| 1   | A     | 414 | A    |
| 1   | A     | 416 | G    |
| 1   | A     | 429 | U    |
| 1   | A     | 430 | A    |
| 1   | A     | 435 | A    |
| 1   | A     | 437 | U    |
| 1   | A     | 439 | U    |
| 1   | A     | 448 | A    |
| 1   | A     | 451 | A    |
| 1   | A     | 452 | A    |
| 1   | A     | 455 | G    |
| 1   | A     | 456 | A    |
| 1   | A     | 457 | G    |
| 1   | A     | 461 | A    |
| 1   | A     | 462 | G    |
| 1   | A     | 463 | U    |
| 1   | A     | 464 | U    |
| 1   | A     | 466 | A    |
| 1   | A     | 468 | A    |
| 1   | A     | 469 | C    |
| 1   | A     | 475 | C    |
| 1   | A     | 476 | U    |
| 1   | A     | 479 | U    |
| 1   | A     | 481 | G    |
| 1   | A     | 483 | C    |
| 1   | A     | 484 | G    |
| 1   | A     | 485 | U    |
| 1   | A     | 486 | U    |
| 1   | A     | 492 | C    |
| 1   | A     | 497 | G    |
| 1   | A     | 499 | A    |
| 1   | A     | 501 | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 511 | C    |
| 1   | A     | 517 | G    |
| 1   | A     | 518 | C    |
| 1   | A     | 527 | G    |
| 1   | A     | 532 | A    |
| 1   | A     | 533 | A    |
| 1   | A     | 540 | G    |
| 1   | A     | 541 | G    |
| 1   | A     | 542 | G    |
| 1   | A     | 543 | U    |
| 1   | A     | 547 | A    |
| 1   | A     | 548 | G    |
| 1   | A     | 549 | C    |
| 1   | A     | 557 | G    |
| 1   | A     | 563 | A    |
| 1   | A     | 564 | C    |
| 1   | A     | 572 | A    |
| 1   | A     | 573 | A    |
| 1   | A     | 575 | G    |
| 1   | A     | 576 | C    |
| 1   | A     | 577 | G    |
| 1   | A     | 579 | A    |
| 1   | A     | 588 | G    |
| 1   | A     | 589 | U    |
| 1   | A     | 591 | U    |
| 1   | A     | 592 | G    |
| 1   | A     | 593 | U    |
| 1   | A     | 598 | U    |
| 1   | A     | 607 | A    |
| 1   | A     | 608 | A    |
| 1   | A     | 614 | C    |
| 1   | A     | 615 | G    |
| 1   | A     | 618 | C    |
| 1   | A     | 619 | U    |
| 1   | A     | 621 | A    |
| 1   | A     | 632 | U    |
| 1   | A     | 633 | G    |
| 1   | A     | 636 | U    |
| 1   | A     | 637 | C    |
| 1   | A     | 638 | U    |
| 1   | A     | 639 | G    |
| 1   | A     | 648 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 653 | U    |
| 1   | A     | 654 | G    |
| 1   | A     | 665 | A    |
| 1   | A     | 683 | G    |
| 1   | A     | 687 | A    |
| 1   | A     | 696 | A    |
| 1   | A     | 697 | U    |
| 1   | A     | 698 | G    |
| 1   | A     | 699 | C    |
| 1   | A     | 700 | G    |
| 1   | A     | 701 | U    |
| 1   | A     | 702 | A    |
| 1   | A     | 703 | G    |
| 1   | A     | 711 | G    |
| 1   | A     | 718 | A    |
| 1   | A     | 719 | C    |
| 1   | A     | 721 | G    |
| 1   | A     | 723 | U    |
| 1   | A     | 724 | G    |
| 1   | A     | 729 | A    |
| 1   | A     | 731 | G    |
| 1   | A     | 747 | A    |
| 1   | A     | 753 | A    |
| 1   | A     | 755 | G    |
| 1   | A     | 763 | G    |
| 1   | A     | 765 | G    |
| 1   | A     | 766 | A    |
| 1   | A     | 780 | A    |
| 1   | A     | 785 | G    |
| 1   | A     | 792 | A    |
| 1   | A     | 793 | U    |
| 1   | A     | 794 | A    |
| 1   | A     | 795 | C    |
| 1   | A     | 809 | G    |
| 1   | A     | 810 | C    |
| 1   | A     | 815 | A    |
| 1   | A     | 817 | C    |
| 1   | A     | 819 | A    |
| 1   | A     | 823 | C    |
| 1   | A     | 828 | U    |
| 1   | A     | 832 | G    |
| 1   | A     | 840 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 841  | C    |
| 1   | A     | 842  | U    |
| 1   | A     | 843  | U    |
| 1   | A     | 846  | G    |
| 1   | A     | 849  | G    |
| 1   | A     | 851  | G    |
| 1   | A     | 854  | U    |
| 1   | A     | 868  | C    |
| 1   | A     | 873  | A    |
| 1   | A     | 884  | U    |
| 1   | A     | 885  | G    |
| 1   | A     | 891  | U    |
| 1   | A     | 900  | A    |
| 1   | A     | 914  | A    |
| 1   | A     | 915  | A    |
| 1   | A     | 918  | A    |
| 1   | A     | 927  | G    |
| 1   | A     | 934  | C    |
| 1   | A     | 935  | A    |
| 1   | A     | 936  | C    |
| 1   | A     | 939  | G    |
| 1   | A     | 955  | U    |
| 1   | A     | 960  | U    |
| 1   | A     | 961  | U    |
| 1   | A     | 966  | G    |
| 1   | A     | 968  | A    |
| 1   | A     | 969  | A    |
| 1   | A     | 971  | G    |
| 1   | A     | 974  | A    |
| 1   | A     | 975  | A    |
| 1   | A     | 976  | G    |
| 1   | A     | 977  | A    |
| 1   | A     | 985  | C    |
| 1   | A     | 989  | U    |
| 1   | A     | 992  | U    |
| 1   | A     | 993  | G    |
| 1   | A     | 994  | A    |
| 1   | A     | 996  | A    |
| 1   | A     | 1004 | A    |
| 1   | A     | 1006 | G    |
| 1   | A     | 1010 | U    |
| 1   | A     | 1013 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1020 | G    |
| 1   | A     | 1022 | A    |
| 1   | A     | 1025 | U    |
| 1   | A     | 1026 | G    |
| 1   | A     | 1028 | C    |
| 1   | A     | 1030 | U    |
| 1   | A     | 1031 | C    |
| 1   | A     | 1032 | G    |
| 1   | A     | 1036 | A    |
| 1   | A     | 1051 | C    |
| 1   | A     | 1064 | G    |
| 1   | A     | 1065 | U    |
| 1   | A     | 1066 | C    |
| 1   | A     | 1070 | U    |
| 1   | A     | 1073 | U    |
| 1   | A     | 1086 | U    |
| 1   | A     | 1093 | A    |
| 1   | A     | 1094 | G    |
| 1   | A     | 1095 | U    |
| 1   | A     | 1100 | C    |
| 1   | A     | 1101 | A    |
| 1   | A     | 1108 | G    |
| 1   | A     | 1112 | C    |
| 1   | A     | 1118 | U    |
| 1   | A     | 1121 | U    |
| 1   | A     | 1130 | A    |
| 1   | A     | 1135 | U    |
| 1   | A     | 1136 | C    |
| 1   | A     | 1137 | C    |
| 1   | A     | 1139 | G    |
| 1   | A     | 1140 | C    |
| 1   | A     | 1143 | G    |
| 1   | A     | 1158 | C    |
| 1   | A     | 1159 | U    |
| 1   | A     | 1161 | C    |
| 1   | A     | 1167 | A    |
| 1   | A     | 1168 | U    |
| 1   | A     | 1184 | G    |
| 1   | A     | 1192 | C    |
| 1   | A     | 1196 | A    |
| 1   | A     | 1197 | A    |
| 1   | A     | 1198 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1199 | U    |
| 1   | A     | 1202 | U    |
| 1   | A     | 1209 | C    |
| 1   | A     | 1210 | C    |
| 1   | A     | 1215 | G    |
| 1   | A     | 1218 | C    |
| 1   | A     | 1225 | A    |
| 1   | A     | 1226 | C    |
| 1   | A     | 1227 | A    |
| 1   | A     | 1236 | A    |
| 1   | A     | 1238 | A    |
| 1   | A     | 1240 | U    |
| 1   | A     | 1241 | G    |
| 1   | A     | 1249 | C    |
| 1   | A     | 1251 | A    |
| 1   | A     | 1253 | G    |
| 1   | A     | 1256 | A    |
| 1   | A     | 1258 | G    |
| 1   | A     | 1274 | A    |
| 1   | A     | 1278 | G    |
| 1   | A     | 1279 | G    |
| 1   | A     | 1280 | A    |
| 1   | A     | 1281 | C    |
| 1   | A     | 1282 | C    |
| 1   | A     | 1287 | A    |
| 1   | A     | 1290 | G    |
| 1   | A     | 1295 | U    |
| 1   | A     | 1300 | G    |
| 1   | A     | 1301 | U    |
| 1   | A     | 1302 | C    |
| 1   | A     | 1303 | C    |
| 1   | A     | 1305 | G    |
| 1   | A     | 1312 | G    |
| 1   | A     | 1317 | C    |
| 1   | A     | 1318 | A    |
| 1   | A     | 1319 | A    |
| 1   | A     | 1320 | C    |
| 1   | A     | 1323 | G    |
| 1   | A     | 1333 | A    |
| 1   | A     | 1335 | U    |
| 1   | A     | 1336 | C    |
| 1   | A     | 1338 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1341 | U    |
| 1   | A     | 1342 | C    |
| 1   | A     | 1343 | G    |
| 1   | A     | 1345 | U    |
| 1   | A     | 1346 | A    |
| 1   | A     | 1349 | A    |
| 1   | A     | 1353 | G    |
| 1   | A     | 1357 | A    |
| 1   | A     | 1361 | G    |
| 1   | A     | 1362 | A    |
| 1   | A     | 1363 | A    |
| 1   | A     | 1364 | U    |
| 1   | A     | 1368 | A    |
| 1   | A     | 1379 | G    |
| 1   | A     | 1398 | A    |
| 1   | A     | 1402 | C    |
| 1   | A     | 1415 | G    |
| 1   | A     | 1419 | G    |
| 1   | A     | 1422 | G    |
| 1   | A     | 1425 | U    |
| 1   | A     | 1441 | A    |
| 1   | A     | 1446 | A    |
| 1   | A     | 1451 | U    |
| 1   | A     | 1452 | C    |
| 1   | A     | 1470 | U    |
| 1   | A     | 1490 | U    |
| 1   | A     | 1493 | A    |
| 1   | A     | 1494 | G    |
| 1   | A     | 1496 | C    |
| 1   | A     | 1497 | G    |
| 1   | A     | 1503 | A    |
| 1   | A     | 1506 | U    |
| 1   | A     | 1517 | G    |
| 1   | A     | 1518 | A    |
| 1   | A     | 1520 | C    |
| 1   | A     | 1523 | G    |
| 1   | A     | 1528 | U    |
| 1   | A     | 1530 | G    |
| 1   | A     | 1534 | A    |
| 22  | V     | 2    | C    |
| 22  | V     | 3    | C    |
| 22  | V     | 4    | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 22  | V     | 5   | G    |
| 22  | V     | 6   | G    |
| 22  | V     | 8   | U    |
| 22  | V     | 15  | G    |
| 22  | V     | 16  | U    |
| 22  | V     | 17  | C    |
| 22  | V     | 18  | G    |
| 22  | V     | 19  | G    |
| 22  | V     | 20  | U    |
| 22  | V     | 21  | A    |
| 22  | V     | 22  | G    |
| 22  | V     | 26  | A    |
| 22  | V     | 28  | G    |
| 22  | V     | 37  | A    |
| 22  | V     | 38  | A    |
| 22  | V     | 39  | U    |
| 22  | V     | 40  | C    |
| 22  | V     | 41  | C    |
| 22  | V     | 42  | C    |
| 22  | V     | 43  | C    |
| 22  | V     | 44  | G    |
| 22  | V     | 46  | G    |
| 22  | V     | 47  | U    |
| 22  | V     | 48  | C    |
| 22  | V     | 51  | U    |
| 22  | V     | 53  | G    |
| 22  | V     | 54  | U    |
| 22  | V     | 55  | U    |
| 22  | V     | 57  | G    |
| 22  | V     | 59  | U    |
| 22  | V     | 60  | U    |
| 22  | V     | 62  | C    |
| 22  | V     | 64  | A    |
| 22  | V     | 65  | G    |
| 22  | V     | 66  | U    |
| 22  | V     | 68  | C    |
| 22  | V     | 71  | G    |
| 22  | V     | 72  | C    |
| 22  | V     | 73  | A    |
| 22  | V     | 74  | C    |
| 22  | V     | 75  | C    |
| 22  | V     | 76  | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 23  | W     | 2   | G    |
| 23  | W     | 6   | C    |
| 23  | W     | 8   | U    |
| 23  | W     | 13  | C    |
| 23  | W     | 15  | G    |
| 23  | W     | 16  | C    |
| 23  | W     | 17  | U    |
| 23  | W     | 18  | G    |
| 23  | W     | 19  | G    |
| 23  | W     | 20  | U    |
| 23  | W     | 21  | A    |
| 23  | W     | 22  | G    |
| 23  | W     | 28  | C    |
| 23  | W     | 34  | G    |
| 23  | W     | 35  | C    |
| 23  | W     | 37  | G    |
| 23  | W     | 40  | U    |
| 23  | W     | 42  | G    |
| 23  | W     | 43  | G    |
| 23  | W     | 46  | G    |
| 23  | W     | 48  | C    |
| 23  | W     | 49  | G    |
| 23  | W     | 50  | G    |
| 23  | W     | 52  | G    |
| 23  | W     | 55  | U    |
| 23  | W     | 56  | C    |
| 23  | W     | 57  | A    |
| 23  | W     | 58  | A    |
| 23  | W     | 59  | A    |
| 23  | W     | 60  | U    |
| 23  | W     | 61  | C    |
| 23  | W     | 62  | C    |
| 23  | W     | 66  | C    |
| 23  | W     | 67  | G    |
| 23  | W     | 69  | G    |
| 23  | W     | 71  | C    |
| 23  | W     | 72  | G    |
| 23  | W     | 73  | A    |
| 23  | W     | 74  | C    |
| 23  | W     | 75  | A    |
| 24  | X     | 13  | U    |
| 24  | X     | 14  | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 24  | X     | 16  | C    |
| 24  | X     | 17  | C    |
| 24  | X     | 18  | C    |
| 24  | X     | 19  | U    |
| 24  | X     | 20  | C    |
| 24  | X     | 21  | A    |
| 33  | a     | 4   | C    |
| 33  | a     | 7   | G    |
| 33  | a     | 9   | G    |
| 33  | a     | 10  | G    |
| 33  | a     | 12  | C    |
| 33  | a     | 13  | G    |
| 33  | a     | 15  | A    |
| 33  | a     | 21  | G    |
| 33  | a     | 24  | G    |
| 33  | a     | 26  | C    |
| 33  | a     | 30  | C    |
| 33  | a     | 34  | A    |
| 33  | a     | 35  | C    |
| 33  | a     | 42  | C    |
| 33  | a     | 43  | C    |
| 33  | a     | 44  | G    |
| 33  | a     | 46  | A    |
| 33  | a     | 52  | A    |
| 33  | a     | 53  | A    |
| 33  | a     | 54  | G    |
| 33  | a     | 56  | G    |
| 33  | a     | 57  | A    |
| 33  | a     | 59  | A    |
| 33  | a     | 65  | U    |
| 33  | a     | 67  | G    |
| 33  | a     | 84  | G    |
| 33  | a     | 85  | G    |
| 33  | a     | 86  | G    |
| 33  | a     | 87  | U    |
| 33  | a     | 88  | C    |
| 33  | a     | 89  | U    |
| 33  | a     | 90  | C    |
| 33  | a     | 91  | C    |
| 33  | a     | 93  | C    |
| 33  | a     | 98  | G    |
| 33  | a     | 99  | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 33  | a     | 100 | G    |
| 33  | a     | 103 | U    |
| 33  | a     | 106 | G    |
| 33  | a     | 108 | A    |
| 33  | a     | 109 | A    |
| 33  | a     | 110 | C    |
| 33  | a     | 115 | A    |
| 34  | b     | 3   | U    |
| 34  | b     | 4   | U    |
| 34  | b     | 7   | G    |
| 34  | b     | 10  | A    |
| 34  | b     | 12  | U    |
| 34  | b     | 13  | A    |
| 34  | b     | 14  | A    |
| 34  | b     | 20  | C    |
| 34  | b     | 23  | G    |
| 34  | b     | 24  | G    |
| 34  | b     | 28  | A    |
| 34  | b     | 33  | C    |
| 34  | b     | 34  | U    |
| 34  | b     | 35  | G    |
| 34  | b     | 39  | G    |
| 34  | b     | 45  | G    |
| 34  | b     | 46  | G    |
| 34  | b     | 49  | A    |
| 34  | b     | 50  | U    |
| 34  | b     | 51  | G    |
| 34  | b     | 55  | G    |
| 34  | b     | 62  | U    |
| 34  | b     | 63  | A    |
| 34  | b     | 64  | A    |
| 34  | b     | 69  | C    |
| 34  | b     | 71  | A    |
| 34  | b     | 72  | U    |
| 34  | b     | 73  | A    |
| 34  | b     | 74  | A    |
| 34  | b     | 75  | G    |
| 34  | b     | 76  | C    |
| 34  | b     | 77  | G    |
| 34  | b     | 84  | A    |
| 34  | b     | 86  | G    |
| 34  | b     | 88  | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 34  | b     | 90  | U    |
| 34  | b     | 91  | A    |
| 34  | b     | 92  | U    |
| 34  | b     | 96  | C    |
| 34  | b     | 100 | U    |
| 34  | b     | 101 | A    |
| 34  | b     | 102 | U    |
| 34  | b     | 103 | A    |
| 34  | b     | 109 | C    |
| 34  | b     | 114 | U    |
| 34  | b     | 116 | C    |
| 34  | b     | 118 | A    |
| 34  | b     | 119 | A    |
| 34  | b     | 120 | U    |
| 34  | b     | 125 | A    |
| 34  | b     | 126 | A    |
| 34  | b     | 127 | A    |
| 34  | b     | 136 | G    |
| 34  | b     | 140 | C    |
| 34  | b     | 142 | A    |
| 34  | b     | 160 | A    |
| 34  | b     | 163 | C    |
| 34  | b     | 166 | U    |
| 34  | b     | 169 | G    |
| 34  | b     | 172 | A    |
| 34  | b     | 174 | U    |
| 34  | b     | 181 | A    |
| 34  | b     | 186 | G    |
| 34  | b     | 187 | G    |
| 34  | b     | 188 | G    |
| 34  | b     | 195 | A    |
| 34  | b     | 196 | A    |
| 34  | b     | 197 | A    |
| 34  | b     | 199 | A    |
| 34  | b     | 200 | U    |
| 34  | b     | 201 | C    |
| 34  | b     | 204 | A    |
| 34  | b     | 210 | C    |
| 34  | b     | 215 | G    |
| 34  | b     | 216 | A    |
| 34  | b     | 218 | A    |
| 34  | b     | 221 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 34  | b     | 222 | A    |
| 34  | b     | 223 | A    |
| 34  | b     | 224 | U    |
| 34  | b     | 225 | C    |
| 34  | b     | 228 | C    |
| 34  | b     | 229 | C    |
| 34  | b     | 231 | A    |
| 34  | b     | 233 | A    |
| 34  | b     | 234 | U    |
| 34  | b     | 235 | U    |
| 34  | b     | 239 | C    |
| 34  | b     | 240 | C    |
| 34  | b     | 241 | A    |
| 34  | b     | 242 | G    |
| 34  | b     | 243 | U    |
| 34  | b     | 245 | G    |
| 34  | b     | 248 | G    |
| 34  | b     | 249 | C    |
| 34  | b     | 250 | G    |
| 34  | b     | 251 | A    |
| 34  | b     | 252 | G    |
| 34  | b     | 255 | A    |
| 34  | b     | 256 | A    |
| 34  | b     | 264 | C    |
| 34  | b     | 265 | A    |
| 34  | b     | 266 | G    |
| 34  | b     | 268 | C    |
| 34  | b     | 270 | A    |
| 34  | b     | 271 | G    |
| 34  | b     | 272 | A    |
| 34  | b     | 274 | C    |
| 34  | b     | 275 | C    |
| 34  | b     | 277 | G    |
| 34  | b     | 278 | A    |
| 34  | b     | 279 | A    |
| 34  | b     | 280 | U    |
| 34  | b     | 281 | C    |
| 34  | b     | 282 | A    |
| 34  | b     | 288 | U    |
| 34  | b     | 290 | U    |
| 34  | b     | 294 | A    |
| 34  | b     | 295 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 34  | b     | 298 | G    |
| 34  | b     | 299 | A    |
| 34  | b     | 300 | A    |
| 34  | b     | 303 | G    |
| 34  | b     | 304 | U    |
| 34  | b     | 307 | G    |
| 34  | b     | 309 | A    |
| 34  | b     | 310 | A    |
| 34  | b     | 311 | A    |
| 34  | b     | 317 | G    |
| 34  | b     | 322 | A    |
| 34  | b     | 323 | C    |
| 34  | b     | 324 | A    |
| 34  | b     | 329 | G    |
| 34  | b     | 330 | A    |
| 34  | b     | 331 | C    |
| 34  | b     | 332 | A    |
| 34  | b     | 342 | A    |
| 34  | b     | 343 | C    |
| 34  | b     | 345 | A    |
| 34  | b     | 347 | A    |
| 34  | b     | 349 | U    |
| 34  | b     | 353 | C    |
| 34  | b     | 356 | G    |
| 34  | b     | 358 | U    |
| 34  | b     | 362 | A    |
| 34  | b     | 363 | G    |
| 34  | b     | 365 | U    |
| 34  | b     | 366 | C    |
| 34  | b     | 367 | G    |
| 34  | b     | 368 | A    |
| 34  | b     | 369 | U    |
| 34  | b     | 370 | G    |
| 34  | b     | 371 | A    |
| 34  | b     | 372 | G    |
| 34  | b     | 373 | U    |
| 34  | b     | 375 | G    |
| 34  | b     | 383 | C    |
| 34  | b     | 385 | C    |
| 34  | b     | 386 | G    |
| 34  | b     | 387 | U    |
| 34  | b     | 388 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 34  | b     | 389 | G    |
| 34  | b     | 391 | A    |
| 34  | b     | 396 | G    |
| 34  | b     | 400 | G    |
| 34  | b     | 401 | A    |
| 34  | b     | 403 | U    |
| 34  | b     | 404 | A    |
| 34  | b     | 405 | U    |
| 34  | b     | 406 | G    |
| 34  | b     | 411 | G    |
| 34  | b     | 412 | A    |
| 34  | b     | 413 | C    |
| 34  | b     | 419 | U    |
| 34  | b     | 425 | G    |
| 34  | b     | 434 | U    |
| 34  | b     | 436 | C    |
| 34  | b     | 442 | G    |
| 34  | b     | 443 | A    |
| 34  | b     | 444 | C    |
| 34  | b     | 446 | G    |
| 34  | b     | 447 | A    |
| 34  | b     | 448 | U    |
| 34  | b     | 449 | A    |
| 34  | b     | 451 | U    |
| 34  | b     | 453 | A    |
| 34  | b     | 454 | A    |
| 34  | b     | 456 | C    |
| 34  | b     | 457 | A    |
| 34  | b     | 459 | U    |
| 34  | b     | 461 | C    |
| 34  | b     | 464 | U    |
| 34  | b     | 466 | A    |
| 34  | b     | 478 | A    |
| 34  | b     | 479 | A    |
| 34  | b     | 480 | A    |
| 34  | b     | 481 | G    |
| 34  | b     | 482 | A    |
| 34  | b     | 483 | A    |
| 34  | b     | 489 | G    |
| 34  | b     | 490 | C    |
| 34  | b     | 491 | G    |
| 34  | b     | 493 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 34  | b     | 494 | G    |
| 34  | b     | 501 | A    |
| 34  | b     | 502 | A    |
| 34  | b     | 503 | A    |
| 34  | b     | 504 | A    |
| 34  | b     | 505 | A    |
| 34  | b     | 507 | A    |
| 34  | b     | 508 | A    |
| 34  | b     | 509 | C    |
| 34  | b     | 513 | A    |
| 34  | b     | 517 | C    |
| 34  | b     | 518 | G    |
| 34  | b     | 519 | U    |
| 34  | b     | 521 | U    |
| 34  | b     | 527 | C    |
| 34  | b     | 528 | A    |
| 34  | b     | 529 | A    |
| 34  | b     | 530 | G    |
| 34  | b     | 531 | C    |
| 34  | b     | 532 | A    |
| 34  | b     | 538 | A    |
| 34  | b     | 539 | G    |
| 34  | b     | 544 | C    |
| 34  | b     | 545 | U    |
| 34  | b     | 546 | U    |
| 34  | b     | 547 | A    |
| 34  | b     | 548 | G    |
| 34  | b     | 549 | G    |
| 34  | b     | 550 | C    |
| 34  | b     | 551 | G    |
| 34  | b     | 556 | A    |
| 34  | b     | 560 | C    |
| 34  | b     | 563 | A    |
| 34  | b     | 567 | U    |
| 34  | b     | 568 | U    |
| 34  | b     | 569 | U    |
| 34  | b     | 573 | U    |
| 34  | b     | 574 | A    |
| 34  | b     | 575 | A    |
| 34  | b     | 578 | G    |
| 34  | b     | 584 | C    |
| 34  | b     | 585 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 34  | b     | 586 | A    |
| 34  | b     | 587 | C    |
| 34  | b     | 589 | U    |
| 34  | b     | 591 | U    |
| 34  | b     | 592 | A    |
| 34  | b     | 603 | A    |
| 34  | b     | 604 | G    |
| 34  | b     | 605 | G    |
| 34  | b     | 606 | U    |
| 34  | b     | 612 | G    |
| 34  | b     | 613 | A    |
| 34  | b     | 614 | A    |
| 34  | b     | 619 | G    |
| 34  | b     | 621 | A    |
| 34  | b     | 622 | G    |
| 34  | b     | 625 | G    |
| 34  | b     | 626 | A    |
| 34  | b     | 627 | A    |
| 34  | b     | 633 | A    |
| 34  | b     | 637 | A    |
| 34  | b     | 638 | G    |
| 34  | b     | 640 | C    |
| 34  | b     | 643 | A    |
| 34  | b     | 644 | A    |
| 34  | b     | 646 | U    |
| 34  | b     | 647 | G    |
| 34  | b     | 651 | G    |
| 34  | b     | 652 | U    |
| 34  | b     | 653 | U    |
| 34  | b     | 654 | A    |
| 34  | b     | 655 | A    |
| 34  | b     | 656 | G    |
| 34  | b     | 659 | G    |
| 34  | b     | 664 | G    |
| 34  | b     | 665 | U    |
| 34  | b     | 667 | U    |
| 34  | b     | 668 | A    |
| 34  | b     | 669 | G    |
| 34  | b     | 670 | A    |
| 34  | b     | 675 | A    |
| 34  | b     | 679 | C    |
| 34  | b     | 683 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 34  | b     | 686 | U    |
| 34  | b     | 687 | C    |
| 34  | b     | 695 | G    |
| 34  | b     | 701 | G    |
| 34  | b     | 704 | G    |
| 34  | b     | 705 | A    |
| 34  | b     | 711 | G    |
| 34  | b     | 715 | A    |
| 34  | b     | 716 | A    |
| 34  | b     | 718 | A    |
| 34  | b     | 719 | C    |
| 34  | b     | 723 | C    |
| 34  | b     | 724 | U    |
| 34  | b     | 727 | A    |
| 34  | b     | 729 | G    |
| 34  | b     | 730 | A    |
| 34  | b     | 731 | C    |
| 34  | b     | 733 | G    |
| 34  | b     | 738 | G    |
| 34  | b     | 740 | C    |
| 34  | b     | 745 | G    |
| 34  | b     | 747 | U    |
| 34  | b     | 750 | A    |
| 34  | b     | 752 | A    |
| 34  | b     | 757 | G    |
| 34  | b     | 758 | C    |
| 34  | b     | 764 | A    |
| 34  | b     | 765 | C    |
| 34  | b     | 766 | U    |
| 34  | b     | 770 | G    |
| 34  | b     | 775 | G    |
| 34  | b     | 776 | G    |
| 34  | b     | 777 | G    |
| 34  | b     | 781 | A    |
| 34  | b     | 782 | A    |
| 34  | b     | 783 | A    |
| 34  | b     | 784 | G    |
| 34  | b     | 785 | G    |
| 34  | b     | 788 | A    |
| 34  | b     | 789 | A    |
| 34  | b     | 790 | U    |
| 34  | b     | 792 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 34  | b     | 793 | A    |
| 34  | b     | 794 | A    |
| 34  | b     | 797 | G    |
| 34  | b     | 801 | G    |
| 34  | b     | 805 | G    |
| 34  | b     | 807 | U    |
| 34  | b     | 810 | U    |
| 34  | b     | 812 | C    |
| 34  | b     | 814 | C    |
| 34  | b     | 819 | A    |
| 34  | b     | 822 | G    |
| 34  | b     | 827 | U    |
| 34  | b     | 828 | U    |
| 34  | b     | 829 | A    |
| 34  | b     | 830 | G    |
| 34  | b     | 836 | G    |
| 34  | b     | 842 | U    |
| 34  | b     | 844 | A    |
| 34  | b     | 845 | A    |
| 34  | b     | 846 | U    |
| 34  | b     | 847 | U    |
| 34  | b     | 852 | U    |
| 34  | b     | 856 | G    |
| 34  | b     | 858 | G    |
| 34  | b     | 859 | G    |
| 34  | b     | 866 | A    |
| 34  | b     | 867 | C    |
| 34  | b     | 872 | U    |
| 34  | b     | 873 | C    |
| 34  | b     | 874 | G    |
| 34  | b     | 876 | C    |
| 34  | b     | 877 | A    |
| 34  | b     | 878 | A    |
| 34  | b     | 879 | G    |
| 34  | b     | 880 | G    |
| 34  | b     | 881 | G    |
| 34  | b     | 882 | G    |
| 34  | b     | 886 | A    |
| 34  | b     | 887 | U    |
| 34  | b     | 888 | C    |
| 34  | b     | 889 | C    |
| 34  | b     | 891 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 34  | b     | 893  | C    |
| 34  | b     | 894  | U    |
| 34  | b     | 895  | U    |
| 34  | b     | 896  | A    |
| 34  | b     | 897  | C    |
| 34  | b     | 898  | C    |
| 34  | b     | 899  | A    |
| 34  | b     | 900  | A    |
| 34  | b     | 910  | A    |
| 34  | b     | 911  | A    |
| 34  | b     | 912  | C    |
| 34  | b     | 914  | G    |
| 34  | b     | 915  | C    |
| 34  | b     | 929  | U    |
| 34  | b     | 931  | U    |
| 34  | b     | 932  | U    |
| 34  | b     | 933  | A    |
| 34  | b     | 934  | U    |
| 34  | b     | 941  | A    |
| 34  | b     | 945  | A    |
| 34  | b     | 946  | C    |
| 34  | b     | 947  | A    |
| 34  | b     | 954  | G    |
| 34  | b     | 958  | U    |
| 34  | b     | 959  | A    |
| 34  | b     | 961  | C    |
| 34  | b     | 967  | U    |
| 34  | b     | 969  | G    |
| 34  | b     | 973  | A    |
| 34  | b     | 974  | G    |
| 34  | b     | 975  | A    |
| 34  | b     | 979  | A    |
| 34  | b     | 980  | A    |
| 34  | b     | 983  | A    |
| 34  | b     | 985  | C    |
| 34  | b     | 986  | C    |
| 34  | b     | 988  | A    |
| 34  | b     | 990  | A    |
| 34  | b     | 996  | A    |
| 34  | b     | 999  | U    |
| 34  | b     | 1003 | G    |
| 34  | b     | 1004 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 34  | b     | 1006 | C    |
| 34  | b     | 1007 | C    |
| 34  | b     | 1008 | A    |
| 34  | b     | 1010 | A    |
| 34  | b     | 1011 | G    |
| 34  | b     | 1012 | U    |
| 34  | b     | 1013 | C    |
| 34  | b     | 1017 | G    |
| 34  | b     | 1018 | U    |
| 34  | b     | 1021 | A    |
| 34  | b     | 1022 | G    |
| 34  | b     | 1023 | U    |
| 34  | b     | 1025 | G    |
| 34  | b     | 1026 | G    |
| 34  | b     | 1027 | A    |
| 34  | b     | 1028 | A    |
| 34  | b     | 1032 | A    |
| 34  | b     | 1033 | U    |
| 34  | b     | 1034 | G    |
| 34  | b     | 1037 | G    |
| 34  | b     | 1038 | G    |
| 34  | b     | 1039 | A    |
| 34  | b     | 1045 | C    |
| 34  | b     | 1047 | G    |
| 34  | b     | 1051 | G    |
| 34  | b     | 1052 | C    |
| 34  | b     | 1054 | A    |
| 34  | b     | 1055 | G    |
| 34  | b     | 1056 | G    |
| 34  | b     | 1057 | A    |
| 34  | b     | 1058 | U    |
| 34  | b     | 1059 | G    |
| 34  | b     | 1060 | U    |
| 34  | b     | 1061 | U    |
| 34  | b     | 1062 | G    |
| 34  | b     | 1063 | G    |
| 34  | b     | 1064 | C    |
| 34  | b     | 1068 | G    |
| 34  | b     | 1069 | A    |
| 34  | b     | 1070 | A    |
| 34  | b     | 1071 | G    |
| 34  | b     | 1072 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 34  | b     | 1073 | A    |
| 34  | b     | 1075 | C    |
| 34  | b     | 1077 | A    |
| 34  | b     | 1078 | U    |
| 34  | b     | 1079 | C    |
| 34  | b     | 1080 | A    |
| 34  | b     | 1081 | U    |
| 34  | b     | 1082 | U    |
| 34  | b     | 1084 | A    |
| 34  | b     | 1085 | A    |
| 34  | b     | 1086 | A    |
| 34  | b     | 1087 | G    |
| 34  | b     | 1088 | A    |
| 34  | b     | 1089 | A    |
| 34  | b     | 1090 | A    |
| 34  | b     | 1091 | G    |
| 34  | b     | 1092 | C    |
| 34  | b     | 1094 | U    |
| 34  | b     | 1095 | A    |
| 34  | b     | 1096 | A    |
| 34  | b     | 1097 | U    |
| 34  | b     | 1098 | A    |
| 34  | b     | 1099 | G    |
| 34  | b     | 1100 | C    |
| 34  | b     | 1102 | C    |
| 34  | b     | 1103 | A    |
| 34  | b     | 1104 | C    |
| 34  | b     | 1105 | U    |
| 34  | b     | 1106 | G    |
| 34  | b     | 1107 | G    |
| 34  | b     | 1109 | C    |
| 34  | b     | 1110 | G    |
| 34  | b     | 1111 | A    |
| 34  | b     | 1112 | G    |
| 34  | b     | 1115 | G    |
| 34  | b     | 1116 | G    |
| 34  | b     | 1117 | C    |
| 34  | b     | 1121 | C    |
| 34  | b     | 1122 | G    |
| 34  | b     | 1130 | U    |
| 34  | b     | 1132 | U    |
| 34  | b     | 1133 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 34  | b     | 1134 | A    |
| 34  | b     | 1135 | C    |
| 34  | b     | 1136 | G    |
| 34  | b     | 1141 | U    |
| 34  | b     | 1142 | A    |
| 34  | b     | 1143 | A    |
| 34  | b     | 1144 | A    |
| 34  | b     | 1151 | A    |
| 34  | b     | 1155 | A    |
| 34  | b     | 1156 | A    |
| 34  | b     | 1163 | G    |
| 34  | b     | 1169 | A    |
| 34  | b     | 1171 | G    |
| 34  | b     | 1172 | C    |
| 34  | b     | 1173 | U    |
| 34  | b     | 1174 | U    |
| 34  | b     | 1175 | A    |
| 34  | b     | 1176 | U    |
| 34  | b     | 1177 | G    |
| 34  | b     | 1178 | C    |
| 34  | b     | 1179 | G    |
| 34  | b     | 1180 | U    |
| 34  | b     | 1184 | U    |
| 34  | b     | 1185 | G    |
| 34  | b     | 1187 | G    |
| 34  | b     | 1188 | U    |
| 34  | b     | 1195 | G    |
| 34  | b     | 1197 | G    |
| 34  | b     | 1200 | C    |
| 34  | b     | 1202 | G    |
| 34  | b     | 1204 | A    |
| 34  | b     | 1205 | A    |
| 34  | b     | 1206 | G    |
| 34  | b     | 1209 | U    |
| 34  | b     | 1210 | G    |
| 34  | b     | 1211 | C    |
| 34  | b     | 1212 | G    |
| 34  | b     | 1218 | G    |
| 34  | b     | 1222 | U    |
| 34  | b     | 1223 | G    |
| 34  | b     | 1224 | U    |
| 34  | b     | 1225 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 34  | b     | 1227 | G    |
| 34  | b     | 1232 | G    |
| 34  | b     | 1236 | G    |
| 34  | b     | 1237 | A    |
| 34  | b     | 1238 | G    |
| 34  | b     | 1239 | G    |
| 34  | b     | 1240 | U    |
| 34  | b     | 1241 | A    |
| 34  | b     | 1242 | U    |
| 34  | b     | 1244 | A    |
| 34  | b     | 1247 | A    |
| 34  | b     | 1248 | G    |
| 34  | b     | 1249 | U    |
| 34  | b     | 1252 | G    |
| 34  | b     | 1253 | A    |
| 34  | b     | 1255 | U    |
| 34  | b     | 1256 | G    |
| 34  | b     | 1260 | A    |
| 34  | b     | 1265 | A    |
| 34  | b     | 1266 | G    |
| 34  | b     | 1268 | A    |
| 34  | b     | 1271 | G    |
| 34  | b     | 1272 | A    |
| 34  | b     | 1273 | U    |
| 34  | b     | 1274 | A    |
| 34  | b     | 1276 | A    |
| 34  | b     | 1280 | G    |
| 34  | b     | 1287 | A    |
| 34  | b     | 1294 | U    |
| 34  | b     | 1296 | G    |
| 34  | b     | 1299 | G    |
| 34  | b     | 1300 | G    |
| 34  | b     | 1301 | A    |
| 34  | b     | 1302 | A    |
| 34  | b     | 1306 | C    |
| 34  | b     | 1312 | U    |
| 34  | b     | 1314 | C    |
| 34  | b     | 1318 | U    |
| 34  | b     | 1320 | C    |
| 34  | b     | 1321 | A    |
| 34  | b     | 1322 | A    |
| 34  | b     | 1330 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 34  | b     | 1332 | G    |
| 34  | b     | 1338 | G    |
| 34  | b     | 1340 | U    |
| 34  | b     | 1341 | G    |
| 34  | b     | 1345 | C    |
| 34  | b     | 1347 | A    |
| 34  | b     | 1348 | C    |
| 34  | b     | 1349 | C    |
| 34  | b     | 1352 | U    |
| 34  | b     | 1354 | A    |
| 34  | b     | 1355 | G    |
| 34  | b     | 1365 | A    |
| 34  | b     | 1368 | G    |
| 34  | b     | 1370 | C    |
| 34  | b     | 1374 | G    |
| 34  | b     | 1378 | A    |
| 34  | b     | 1379 | U    |
| 34  | b     | 1381 | G    |
| 34  | b     | 1382 | G    |
| 34  | b     | 1383 | A    |
| 34  | b     | 1386 | C    |
| 34  | b     | 1390 | U    |
| 34  | b     | 1392 | A    |
| 34  | b     | 1394 | U    |
| 34  | b     | 1395 | A    |
| 34  | b     | 1396 | U    |
| 34  | b     | 1400 | U    |
| 34  | b     | 1414 | C    |
| 34  | b     | 1415 | U    |
| 34  | b     | 1416 | G    |
| 34  | b     | 1418 | G    |
| 34  | b     | 1419 | A    |
| 34  | b     | 1420 | A    |
| 34  | b     | 1421 | G    |
| 34  | b     | 1424 | G    |
| 34  | b     | 1425 | G    |
| 34  | b     | 1427 | A    |
| 34  | b     | 1428 | C    |
| 34  | b     | 1444 | G    |
| 34  | b     | 1449 | G    |
| 34  | b     | 1451 | C    |
| 34  | b     | 1452 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 34  | b     | 1453 | A    |
| 34  | b     | 1454 | C    |
| 34  | b     | 1455 | G    |
| 34  | b     | 1458 | U    |
| 34  | b     | 1459 | G    |
| 34  | b     | 1460 | U    |
| 34  | b     | 1461 | C    |
| 34  | b     | 1467 | U    |
| 34  | b     | 1469 | A    |
| 34  | b     | 1470 | A    |
| 34  | b     | 1476 | U    |
| 34  | b     | 1477 | A    |
| 34  | b     | 1478 | G    |
| 34  | b     | 1482 | G    |
| 34  | b     | 1485 | U    |
| 34  | b     | 1488 | C    |
| 34  | b     | 1490 | A    |
| 34  | b     | 1491 | G    |
| 34  | b     | 1493 | C    |
| 34  | b     | 1494 | A    |
| 34  | b     | 1496 | A    |
| 34  | b     | 1497 | U    |
| 34  | b     | 1498 | C    |
| 34  | b     | 1501 | G    |
| 34  | b     | 1503 | A    |
| 34  | b     | 1504 | A    |
| 34  | b     | 1506 | U    |
| 34  | b     | 1507 | C    |
| 34  | b     | 1508 | A    |
| 34  | b     | 1509 | A    |
| 34  | b     | 1510 | G    |
| 34  | b     | 1511 | G    |
| 34  | b     | 1512 | C    |
| 34  | b     | 1521 | G    |
| 34  | b     | 1522 | A    |
| 34  | b     | 1523 | U    |
| 34  | b     | 1524 | G    |
| 34  | b     | 1529 | G    |
| 34  | b     | 1530 | G    |
| 34  | b     | 1535 | A    |
| 34  | b     | 1536 | C    |
| 34  | b     | 1537 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 34  | b     | 1539 | U    |
| 34  | b     | 1542 | U    |
| 34  | b     | 1550 | C    |
| 34  | b     | 1552 | A    |
| 34  | b     | 1556 | C    |
| 34  | b     | 1562 | U    |
| 34  | b     | 1565 | C    |
| 34  | b     | 1566 | A    |
| 34  | b     | 1568 | G    |
| 34  | b     | 1569 | A    |
| 34  | b     | 1570 | A    |
| 34  | b     | 1576 | U    |
| 34  | b     | 1578 | U    |
| 34  | b     | 1583 | A    |
| 34  | b     | 1585 | C    |
| 34  | b     | 1587 | G    |
| 34  | b     | 1600 | C    |
| 34  | b     | 1602 | U    |
| 34  | b     | 1603 | A    |
| 34  | b     | 1607 | C    |
| 34  | b     | 1608 | A    |
| 34  | b     | 1609 | A    |
| 34  | b     | 1610 | A    |
| 34  | b     | 1613 | G    |
| 34  | b     | 1614 | A    |
| 34  | b     | 1616 | A    |
| 34  | b     | 1617 | C    |
| 34  | b     | 1618 | A    |
| 34  | b     | 1627 | G    |
| 34  | b     | 1631 | G    |
| 34  | b     | 1633 | G    |
| 34  | b     | 1634 | A    |
| 34  | b     | 1637 | A    |
| 34  | b     | 1644 | C    |
| 34  | b     | 1646 | C    |
| 34  | b     | 1647 | U    |
| 34  | b     | 1648 | U    |
| 34  | b     | 1649 | G    |
| 34  | b     | 1654 | A    |
| 34  | b     | 1656 | C    |
| 34  | b     | 1657 | U    |
| 34  | b     | 1658 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 34  | b     | 1660 | G    |
| 34  | b     | 1663 | G    |
| 34  | b     | 1667 | G    |
| 34  | b     | 1668 | A    |
| 34  | b     | 1670 | C    |
| 34  | b     | 1672 | A    |
| 34  | b     | 1673 | G    |
| 34  | b     | 1674 | G    |
| 34  | b     | 1677 | A    |
| 34  | b     | 1689 | A    |
| 34  | b     | 1691 | C    |
| 34  | b     | 1693 | U    |
| 34  | b     | 1694 | C    |
| 34  | b     | 1698 | A    |
| 34  | b     | 1699 | G    |
| 34  | b     | 1700 | A    |
| 34  | b     | 1702 | G    |
| 34  | b     | 1703 | G    |
| 34  | b     | 1705 | A    |
| 34  | b     | 1706 | C    |
| 34  | b     | 1710 | G    |
| 34  | b     | 1713 | A    |
| 34  | b     | 1715 | G    |
| 34  | b     | 1716 | U    |
| 34  | b     | 1728 | C    |
| 34  | b     | 1730 | C    |
| 34  | b     | 1731 | G    |
| 34  | b     | 1732 | C    |
| 34  | b     | 1733 | G    |
| 34  | b     | 1735 | A    |
| 34  | b     | 1746 | A    |
| 34  | b     | 1750 | G    |
| 34  | b     | 1754 | A    |
| 34  | b     | 1756 | G    |
| 34  | b     | 1757 | A    |
| 34  | b     | 1758 | U    |
| 34  | b     | 1763 | G    |
| 34  | b     | 1764 | C    |
| 34  | b     | 1766 | G    |
| 34  | b     | 1773 | A    |
| 34  | b     | 1774 | C    |
| 34  | b     | 1775 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 34  | b     | 1776 | G    |
| 34  | b     | 1778 | U    |
| 34  | b     | 1780 | A    |
| 34  | b     | 1782 | U    |
| 34  | b     | 1783 | A    |
| 34  | b     | 1784 | A    |
| 34  | b     | 1786 | A    |
| 34  | b     | 1787 | A    |
| 34  | b     | 1800 | C    |
| 34  | b     | 1801 | A    |
| 34  | b     | 1802 | A    |
| 34  | b     | 1805 | A    |
| 34  | b     | 1806 | C    |
| 34  | b     | 1807 | G    |
| 34  | b     | 1808 | A    |
| 34  | b     | 1809 | A    |
| 34  | b     | 1811 | G    |
| 34  | b     | 1819 | A    |
| 34  | b     | 1820 | U    |
| 34  | b     | 1827 | U    |
| 34  | b     | 1828 | G    |
| 34  | b     | 1829 | A    |
| 34  | b     | 1833 | C    |
| 34  | b     | 1839 | G    |
| 34  | b     | 1842 | G    |
| 34  | b     | 1845 | G    |
| 34  | b     | 1847 | A    |
| 34  | b     | 1848 | A    |
| 34  | b     | 1849 | G    |
| 34  | b     | 1853 | A    |
| 34  | b     | 1857 | G    |
| 34  | b     | 1862 | G    |
| 34  | b     | 1866 | A    |
| 34  | b     | 1867 | G    |
| 34  | b     | 1868 | C    |
| 34  | b     | 1870 | C    |
| 34  | b     | 1871 | A    |
| 34  | b     | 1875 | G    |
| 34  | b     | 1877 | A    |
| 34  | b     | 1885 | A    |
| 34  | b     | 1890 | A    |
| 34  | b     | 1896 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 34  | b     | 1901 | A    |
| 34  | b     | 1902 | C    |
| 34  | b     | 1905 | C    |
| 34  | b     | 1907 | G    |
| 34  | b     | 1908 | C    |
| 34  | b     | 1911 | U    |
| 34  | b     | 1912 | A    |
| 34  | b     | 1913 | A    |
| 34  | b     | 1914 | C    |
| 34  | b     | 1915 | U    |
| 34  | b     | 1924 | C    |
| 34  | b     | 1928 | A    |
| 34  | b     | 1929 | G    |
| 34  | b     | 1930 | G    |
| 34  | b     | 1931 | U    |
| 34  | b     | 1932 | A    |
| 34  | b     | 1936 | A    |
| 34  | b     | 1937 | A    |
| 34  | b     | 1938 | A    |
| 34  | b     | 1940 | U    |
| 34  | b     | 1941 | C    |
| 34  | b     | 1942 | C    |
| 34  | b     | 1943 | U    |
| 34  | b     | 1952 | A    |
| 34  | b     | 1953 | A    |
| 34  | b     | 1955 | U    |
| 34  | b     | 1958 | C    |
| 34  | b     | 1960 | A    |
| 34  | b     | 1961 | C    |
| 34  | b     | 1963 | U    |
| 34  | b     | 1964 | G    |
| 34  | b     | 1965 | C    |
| 34  | b     | 1967 | C    |
| 34  | b     | 1970 | A    |
| 34  | b     | 1971 | U    |
| 34  | b     | 1972 | G    |
| 34  | b     | 1977 | A    |
| 34  | b     | 1980 | G    |
| 34  | b     | 1981 | A    |
| 34  | b     | 1982 | U    |
| 34  | b     | 1989 | G    |
| 34  | b     | 1991 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 34  | b     | 1993 | U    |
| 34  | b     | 1997 | C    |
| 34  | b     | 2006 | C    |
| 34  | b     | 2007 | U    |
| 34  | b     | 2011 | U    |
| 34  | b     | 2014 | A    |
| 34  | b     | 2020 | A    |
| 34  | b     | 2022 | U    |
| 34  | b     | 2023 | C    |
| 34  | b     | 2025 | C    |
| 34  | b     | 2027 | G    |
| 34  | b     | 2030 | A    |
| 34  | b     | 2031 | A    |
| 34  | b     | 2032 | G    |
| 34  | b     | 2033 | A    |
| 34  | b     | 2034 | U    |
| 34  | b     | 2036 | C    |
| 34  | b     | 2042 | A    |
| 34  | b     | 2043 | C    |
| 34  | b     | 2044 | C    |
| 34  | b     | 2046 | G    |
| 34  | b     | 2049 | G    |
| 34  | b     | 2055 | C    |
| 34  | b     | 2056 | G    |
| 34  | b     | 2060 | A    |
| 34  | b     | 2061 | G    |
| 34  | b     | 2062 | A    |
| 34  | b     | 2063 | C    |
| 34  | b     | 2068 | U    |
| 34  | b     | 2069 | G    |
| 34  | b     | 2070 | A    |
| 34  | b     | 2076 | U    |
| 34  | b     | 2077 | A    |
| 34  | b     | 2080 | A    |
| 34  | b     | 2087 | G    |
| 34  | b     | 2092 | U    |
| 34  | b     | 2095 | A    |
| 34  | b     | 2098 | U    |
| 34  | b     | 2103 | C    |
| 34  | b     | 2104 | C    |
| 34  | b     | 2105 | U    |
| 34  | b     | 2106 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 34  | b     | 2107 | G    |
| 34  | b     | 2109 | U    |
| 34  | b     | 2110 | G    |
| 34  | b     | 2111 | U    |
| 34  | b     | 2112 | G    |
| 34  | b     | 2113 | U    |
| 34  | b     | 2114 | A    |
| 34  | b     | 2115 | G    |
| 34  | b     | 2117 | A    |
| 34  | b     | 2118 | U    |
| 34  | b     | 2119 | A    |
| 34  | b     | 2120 | G    |
| 34  | b     | 2121 | G    |
| 34  | b     | 2123 | G    |
| 34  | b     | 2124 | G    |
| 34  | b     | 2125 | G    |
| 34  | b     | 2126 | A    |
| 34  | b     | 2127 | G    |
| 34  | b     | 2128 | G    |
| 34  | b     | 2130 | U    |
| 34  | b     | 2131 | U    |
| 34  | b     | 2132 | U    |
| 34  | b     | 2133 | G    |
| 34  | b     | 2139 | U    |
| 34  | b     | 2142 | A    |
| 34  | b     | 2143 | C    |
| 34  | b     | 2144 | G    |
| 34  | b     | 2145 | C    |
| 34  | b     | 2147 | A    |
| 34  | b     | 2148 | G    |
| 34  | b     | 2149 | U    |
| 34  | b     | 2152 | G    |
| 34  | b     | 2153 | C    |
| 34  | b     | 2156 | G    |
| 34  | b     | 2158 | A    |
| 34  | b     | 2159 | G    |
| 34  | b     | 2160 | C    |
| 34  | b     | 2161 | C    |
| 34  | b     | 2162 | G    |
| 34  | b     | 2163 | A    |
| 34  | b     | 2164 | C    |
| 34  | b     | 2165 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 34  | b     | 2166 | U    |
| 34  | b     | 2167 | U    |
| 34  | b     | 2168 | G    |
| 34  | b     | 2169 | A    |
| 34  | b     | 2170 | A    |
| 34  | b     | 2171 | A    |
| 34  | b     | 2172 | U    |
| 34  | b     | 2173 | A    |
| 34  | b     | 2174 | C    |
| 34  | b     | 2175 | C    |
| 34  | b     | 2176 | A    |
| 34  | b     | 2177 | C    |
| 34  | b     | 2178 | C    |
| 34  | b     | 2179 | C    |
| 34  | b     | 2183 | A    |
| 34  | b     | 2185 | U    |
| 34  | b     | 2190 | G    |
| 34  | b     | 2191 | A    |
| 34  | b     | 2193 | G    |
| 34  | b     | 2198 | A    |
| 34  | b     | 2199 | A    |
| 34  | b     | 2203 | U    |
| 34  | b     | 2204 | G    |
| 34  | b     | 2210 | U    |
| 34  | b     | 2211 | A    |
| 34  | b     | 2212 | A    |
| 34  | b     | 2213 | U    |
| 34  | b     | 2214 | C    |
| 34  | b     | 2215 | C    |
| 34  | b     | 2218 | G    |
| 34  | b     | 2225 | A    |
| 34  | b     | 2238 | G    |
| 34  | b     | 2239 | G    |
| 34  | b     | 2243 | U    |
| 34  | b     | 2250 | G    |
| 34  | b     | 2251 | G    |
| 34  | b     | 2252 | G    |
| 34  | b     | 2255 | G    |
| 34  | b     | 2256 | G    |
| 34  | b     | 2257 | U    |
| 34  | b     | 2261 | C    |
| 34  | b     | 2265 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 34  | b     | 2267 | A    |
| 34  | b     | 2268 | A    |
| 34  | b     | 2273 | A    |
| 34  | b     | 2275 | C    |
| 34  | b     | 2276 | G    |
| 34  | b     | 2279 | G    |
| 34  | b     | 2280 | G    |
| 34  | b     | 2282 | G    |
| 34  | b     | 2283 | C    |
| 34  | b     | 2284 | A    |
| 34  | b     | 2286 | G    |
| 34  | b     | 2287 | A    |
| 34  | b     | 2288 | A    |
| 34  | b     | 2289 | G    |
| 34  | b     | 2294 | G    |
| 34  | b     | 2297 | A    |
| 34  | b     | 2298 | A    |
| 34  | b     | 2305 | U    |
| 34  | b     | 2307 | G    |
| 34  | b     | 2308 | G    |
| 34  | b     | 2311 | A    |
| 34  | b     | 2312 | U    |
| 34  | b     | 2316 | G    |
| 34  | b     | 2319 | G    |
| 34  | b     | 2320 | U    |
| 34  | b     | 2322 | A    |
| 34  | b     | 2325 | G    |
| 34  | b     | 2327 | A    |
| 34  | b     | 2331 | G    |
| 34  | b     | 2333 | A    |
| 34  | b     | 2334 | U    |
| 34  | b     | 2335 | A    |
| 34  | b     | 2336 | A    |
| 34  | b     | 2345 | G    |
| 34  | b     | 2347 | C    |
| 34  | b     | 2350 | C    |
| 34  | b     | 2353 | G    |
| 34  | b     | 2354 | C    |
| 34  | b     | 2357 | G    |
| 34  | b     | 2358 | A    |
| 34  | b     | 2361 | G    |
| 34  | b     | 2366 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 34  | b     | 2367 | G    |
| 34  | b     | 2371 | G    |
| 34  | b     | 2372 | U    |
| 34  | b     | 2376 | A    |
| 34  | b     | 2379 | G    |
| 34  | b     | 2382 | G    |
| 34  | b     | 2383 | G    |
| 34  | b     | 2385 | C    |
| 34  | b     | 2388 | A    |
| 34  | b     | 2396 | G    |
| 34  | b     | 2402 | U    |
| 34  | b     | 2403 | C    |
| 34  | b     | 2404 | U    |
| 34  | b     | 2406 | A    |
| 34  | b     | 2407 | A    |
| 34  | b     | 2410 | G    |
| 34  | b     | 2411 | A    |
| 34  | b     | 2413 | G    |
| 34  | b     | 2421 | G    |
| 34  | b     | 2422 | C    |
| 34  | b     | 2423 | U    |
| 34  | b     | 2425 | A    |
| 34  | b     | 2426 | A    |
| 34  | b     | 2427 | C    |
| 34  | b     | 2428 | G    |
| 34  | b     | 2429 | G    |
| 34  | b     | 2430 | A    |
| 34  | b     | 2431 | U    |
| 34  | b     | 2434 | A    |
| 34  | b     | 2435 | A    |
| 34  | b     | 2439 | A    |
| 34  | b     | 2440 | C    |
| 34  | b     | 2441 | U    |
| 34  | b     | 2445 | G    |
| 34  | b     | 2447 | G    |
| 34  | b     | 2448 | A    |
| 34  | b     | 2449 | U    |
| 34  | b     | 2450 | A    |
| 34  | b     | 2455 | G    |
| 34  | b     | 2456 | C    |
| 34  | b     | 2458 | G    |
| 34  | b     | 2459 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 34  | b     | 2465 | C    |
| 34  | b     | 2470 | G    |
| 34  | b     | 2472 | G    |
| 34  | b     | 2474 | U    |
| 34  | b     | 2476 | A    |
| 34  | b     | 2478 | A    |
| 34  | b     | 2481 | G    |
| 34  | b     | 2482 | A    |
| 34  | b     | 2484 | G    |
| 34  | b     | 2490 | G    |
| 34  | b     | 2491 | U    |
| 34  | b     | 2497 | A    |
| 34  | b     | 2500 | U    |
| 34  | b     | 2502 | G    |
| 34  | b     | 2503 | A    |
| 34  | b     | 2505 | G    |
| 34  | b     | 2506 | U    |
| 34  | b     | 2507 | C    |
| 34  | b     | 2513 | A    |
| 34  | b     | 2517 | C    |
| 34  | b     | 2518 | A    |
| 34  | b     | 2519 | U    |
| 34  | b     | 2525 | G    |
| 34  | b     | 2527 | C    |
| 34  | b     | 2529 | G    |
| 34  | b     | 2530 | A    |
| 34  | b     | 2534 | A    |
| 34  | b     | 2535 | G    |
| 34  | b     | 2536 | G    |
| 34  | b     | 2544 | G    |
| 34  | b     | 2547 | A    |
| 34  | b     | 2554 | U    |
| 34  | b     | 2556 | C    |
| 34  | b     | 2557 | G    |
| 34  | b     | 2562 | U    |
| 34  | b     | 2564 | A    |
| 34  | b     | 2565 | A    |
| 34  | b     | 2566 | A    |
| 34  | b     | 2567 | G    |
| 34  | b     | 2571 | U    |
| 34  | b     | 2573 | C    |
| 34  | b     | 2576 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 34  | b     | 2577 | A    |
| 34  | b     | 2578 | G    |
| 34  | b     | 2582 | G    |
| 34  | b     | 2584 | U    |
| 34  | b     | 2585 | U    |
| 34  | b     | 2586 | U    |
| 34  | b     | 2590 | A    |
| 34  | b     | 2595 | G    |
| 34  | b     | 2596 | U    |
| 34  | b     | 2600 | A    |
| 34  | b     | 2601 | C    |
| 34  | b     | 2602 | A    |
| 34  | b     | 2603 | G    |
| 34  | b     | 2604 | U    |
| 34  | b     | 2607 | G    |
| 34  | b     | 2609 | U    |
| 34  | b     | 2610 | C    |
| 34  | b     | 2611 | C    |
| 34  | b     | 2613 | U    |
| 34  | b     | 2614 | A    |
| 34  | b     | 2615 | U    |
| 34  | b     | 2618 | G    |
| 34  | b     | 2623 | G    |
| 34  | b     | 2628 | C    |
| 34  | b     | 2629 | U    |
| 34  | b     | 2634 | A    |
| 34  | b     | 2635 | A    |
| 34  | b     | 2638 | G    |
| 34  | b     | 2639 | A    |
| 34  | b     | 2640 | G    |
| 34  | b     | 2641 | G    |
| 34  | b     | 2645 | G    |
| 34  | b     | 2646 | C    |
| 34  | b     | 2655 | G    |
| 34  | b     | 2659 | G    |
| 34  | b     | 2660 | A    |
| 34  | b     | 2661 | G    |
| 34  | b     | 2666 | C    |
| 34  | b     | 2670 | A    |
| 34  | b     | 2673 | G    |
| 34  | b     | 2688 | G    |
| 34  | b     | 2689 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 34  | b     | 2690 | U    |
| 34  | b     | 2692 | G    |
| 34  | b     | 2700 | A    |
| 34  | b     | 2702 | G    |
| 34  | b     | 2707 | U    |
| 34  | b     | 2712 | C    |
| 34  | b     | 2713 | U    |
| 34  | b     | 2716 | C    |
| 34  | b     | 2718 | G    |
| 34  | b     | 2726 | A    |
| 34  | b     | 2727 | A    |
| 34  | b     | 2732 | G    |
| 34  | b     | 2733 | A    |
| 34  | b     | 2735 | G    |
| 34  | b     | 2736 | A    |
| 34  | b     | 2744 | G    |
| 34  | b     | 2745 | C    |
| 34  | b     | 2746 | U    |
| 34  | b     | 2749 | A    |
| 34  | b     | 2750 | A    |
| 34  | b     | 2751 | G    |
| 34  | b     | 2752 | C    |
| 34  | b     | 2753 | A    |
| 34  | b     | 2755 | C    |
| 34  | b     | 2757 | A    |
| 34  | b     | 2758 | A    |
| 34  | b     | 2761 | A    |
| 34  | b     | 2762 | C    |
| 34  | b     | 2765 | A    |
| 34  | b     | 2767 | C    |
| 34  | b     | 2772 | C    |
| 34  | b     | 2778 | A    |
| 34  | b     | 2779 | U    |
| 34  | b     | 2780 | G    |
| 34  | b     | 2781 | A    |
| 34  | b     | 2782 | G    |
| 34  | b     | 2784 | U    |
| 34  | b     | 2792 | A    |
| 34  | b     | 2793 | C    |
| 34  | b     | 2795 | C    |
| 34  | b     | 2796 | U    |
| 34  | b     | 2797 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 34  | b     | 2798 | U    |
| 34  | b     | 2799 | A    |
| 34  | b     | 2800 | A    |
| 34  | b     | 2805 | C    |
| 34  | b     | 2808 | G    |
| 34  | b     | 2818 | U    |
| 34  | b     | 2819 | G    |
| 34  | b     | 2820 | A    |
| 34  | b     | 2821 | A    |
| 34  | b     | 2823 | A    |
| 34  | b     | 2824 | C    |
| 34  | b     | 2826 | A    |
| 34  | b     | 2833 | U    |
| 34  | b     | 2835 | A    |
| 34  | b     | 2838 | G    |
| 34  | b     | 2849 | U    |
| 34  | b     | 2850 | A    |
| 34  | b     | 2858 | C    |
| 34  | b     | 2861 | U    |
| 34  | b     | 2866 | U    |
| 34  | b     | 2868 | A    |
| 34  | b     | 2872 | A    |
| 34  | b     | 2873 | A    |
| 34  | b     | 2874 | C    |
| 34  | b     | 2883 | A    |
| 34  | b     | 2884 | U    |
| 34  | b     | 2885 | G    |
| 34  | b     | 2886 | A    |
| 34  | b     | 2888 | C    |
| 34  | b     | 2891 | U    |
| 34  | b     | 2893 | A    |
| 34  | b     | 2894 | G    |
| 34  | b     | 2895 | G    |
| 34  | b     | 2901 | C    |
| 34  | b     | 2903 | U    |

All (52) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 5   | U    |
| 1   | A     | 51  | A    |
| 1   | A     | 66  | A    |

*Continued on next page...*

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 94   | G    |
| 1   | A     | 109  | A    |
| 1   | A     | 125  | U    |
| 1   | A     | 148  | G    |
| 1   | A     | 218  | U    |
| 1   | A     | 243  | A    |
| 1   | A     | 254  | G    |
| 1   | A     | 301  | G    |
| 1   | A     | 429  | U    |
| 1   | A     | 447  | G    |
| 1   | A     | 478  | A    |
| 1   | A     | 484  | G    |
| 1   | A     | 572  | A    |
| 1   | A     | 695  | A    |
| 1   | A     | 701  | U    |
| 1   | A     | 722  | G    |
| 1   | A     | 960  | U    |
| 1   | A     | 1065 | U    |
| 1   | A     | 1117 | A    |
| 1   | A     | 1129 | C    |
| 1   | A     | 1157 | A    |
| 1   | A     | 1201 | A    |
| 1   | A     | 1226 | C    |
| 1   | A     | 1300 | G    |
| 1   | A     | 1332 | A    |
| 1   | A     | 1348 | U    |
| 1   | A     | 1492 | A    |
| 22  | V     | 9    | A    |
| 22  | V     | 15   | G    |
| 22  | V     | 18   | G    |
| 22  | V     | 38   | A    |
| 22  | V     | 39   | U    |
| 22  | V     | 40   | C    |
| 22  | V     | 48   | C    |
| 22  | V     | 74   | C    |
| 22  | V     | 75   | C    |
| 23  | W     | 1    | C    |
| 23  | W     | 7    | G    |
| 23  | W     | 18   | G    |
| 23  | W     | 20   | U    |
| 23  | W     | 42   | G    |
| 23  | W     | 49   | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 23  | W     | 57  | A    |
| 23  | W     | 60  | U    |
| 23  | W     | 73  | A    |
| 23  | W     | 74  | C    |
| 24  | X     | 12  | C    |
| 24  | X     | 18  | C    |
| 24  | X     | 19  | U    |

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

1 ligand is 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$ |
| 57  | CLM  | b     | 9000 | -    | 19,20,20     | 0.88 | 1 (5%)      | 23,27,27    | 0.80 | 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   |
|-----|------|-------|------|------|---------|-------------|---------|
| 57  | CLM  | b     | 9000 | -    | -       | 10/20/22/22 | 0/1/1/1 |



All (1) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 57  | b     | 9000 | CLM  | C9-N9 | -2.07 | 1.40        | 1.45     |

There are no bond angle outliers.

There are no chirality outliers.

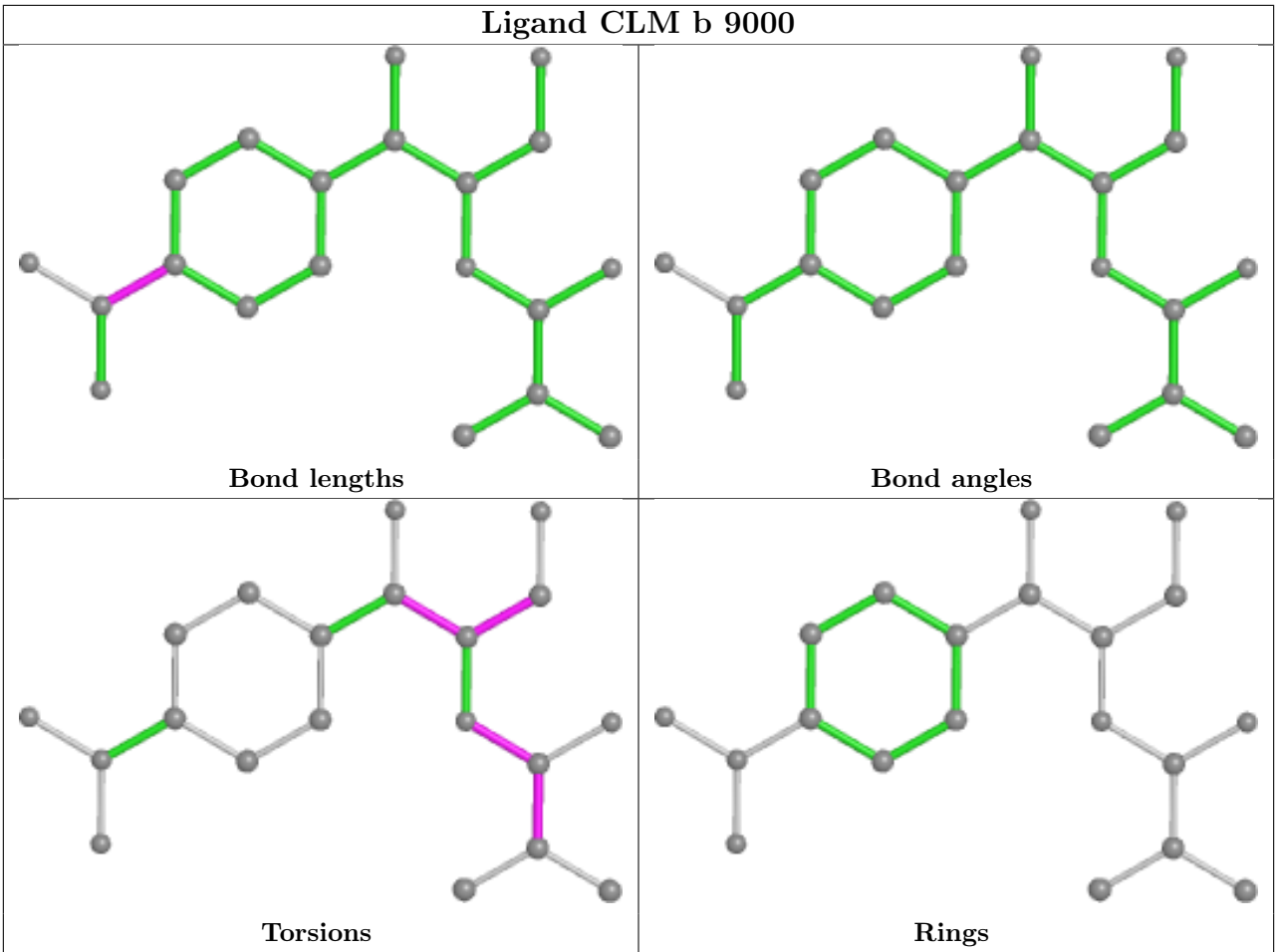
All (10) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms        |
|-----|-------|------|------|--------------|
| 57  | b     | 9000 | CLM  | N2-C3-C5-O5  |
| 57  | b     | 9000 | CLM  | N2-C3-C5-C6  |
| 57  | b     | 9000 | CLM  | C4-C3-C5-O5  |
| 57  | b     | 9000 | CLM  | O2-C2-N2-C3  |
| 57  | b     | 9000 | CLM  | C1-C2-N2-C3  |
| 57  | b     | 9000 | CLM  | N2-C3-C4-O4  |
| 57  | b     | 9000 | CLM  | C5-C3-C4-O4  |
| 57  | b     | 9000 | CLM  | C4-C3-C5-C6  |
| 57  | b     | 9000 | CLM  | CL1-C1-C2-O2 |
| 57  | b     | 9000 | CLM  | CL1-C1-C2-N2 |

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 34  | b     | 4                |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | b     | 2610:C    | O3'    | 2611:C    | P      | 1.83         |
| 1     | b     | 2504:U    | O3'    | 2505:G    | P      | 1.81         |
| 1     | b     | 2248:C    | O3'    | 2249:U    | P      | 1.78         |
| 1     | b     | 1323:C    | O3'    | 1324:G    | P      | 1.77         |

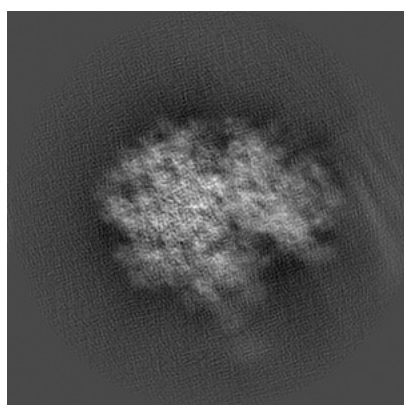
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6486. These allow visual inspection of the internal detail of the map and identification of artifacts.

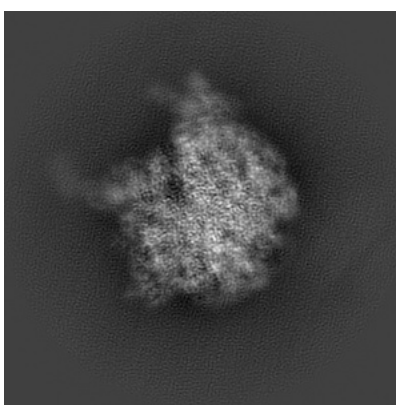
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

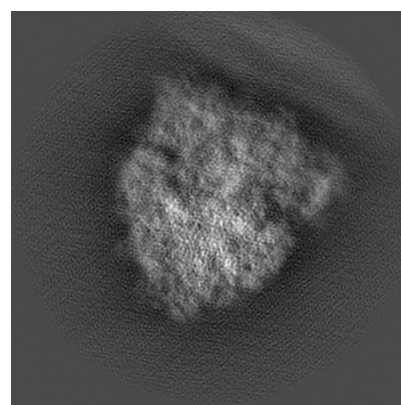
#### 6.1.1 Primary map



X



Y

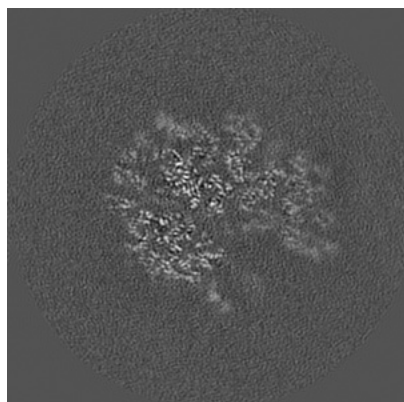


Z

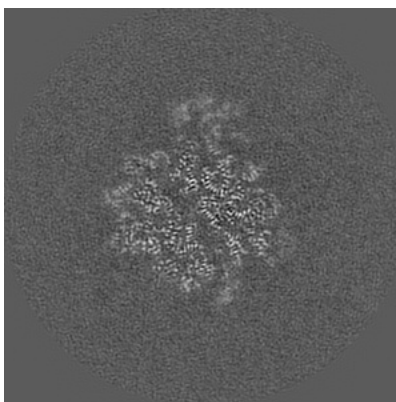
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

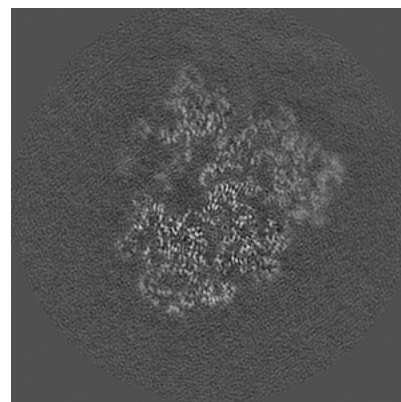
#### 6.2.1 Primary map



X Index: 160



Y Index: 160

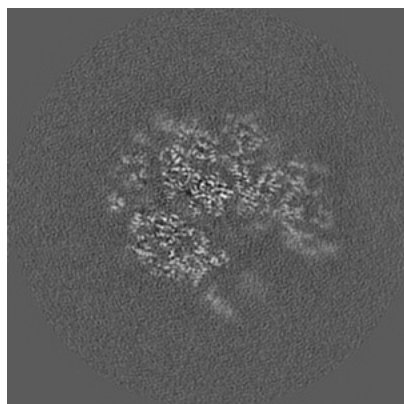


Z Index: 160

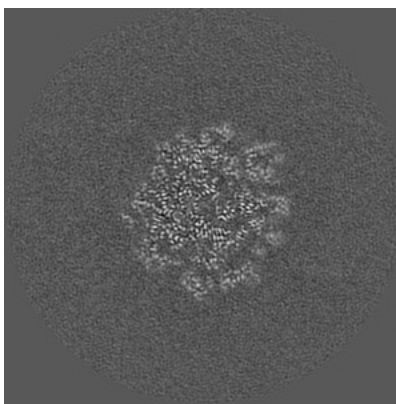
The images above show central slices of the map in three orthogonal directions.

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

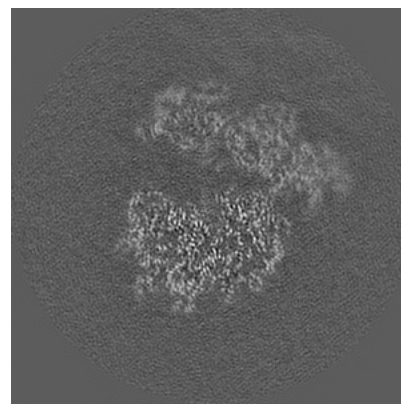
### 6.3.1 Primary map



X Index: 162



Y Index: 136



Z Index: 151

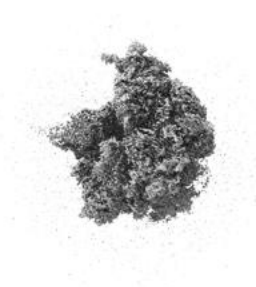
The images above show the largest variance slices of the map in three orthogonal directions.

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

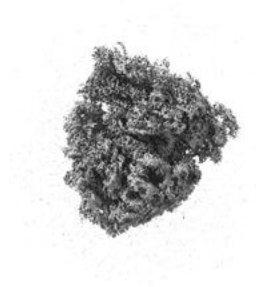
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

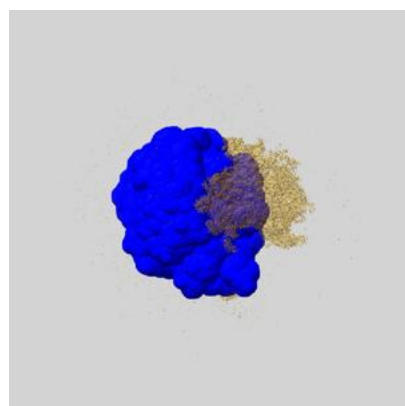
## 6.5 Mask visualisation [i](#)

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

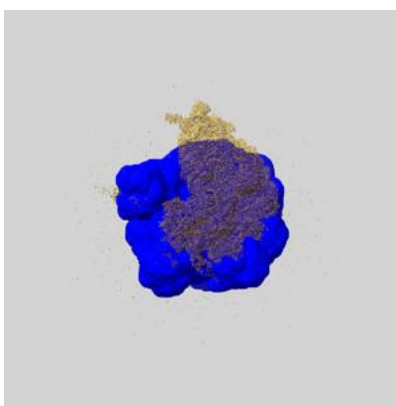
A mask typically either:

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

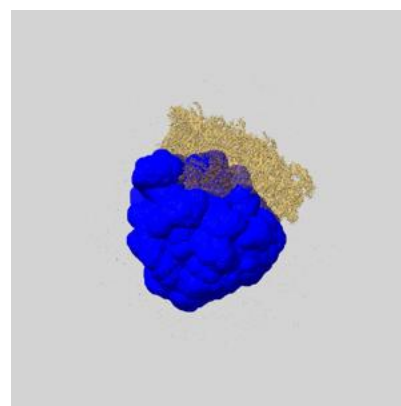
### 6.5.1 emd\_6486\_msk.map [i](#)



X



Y

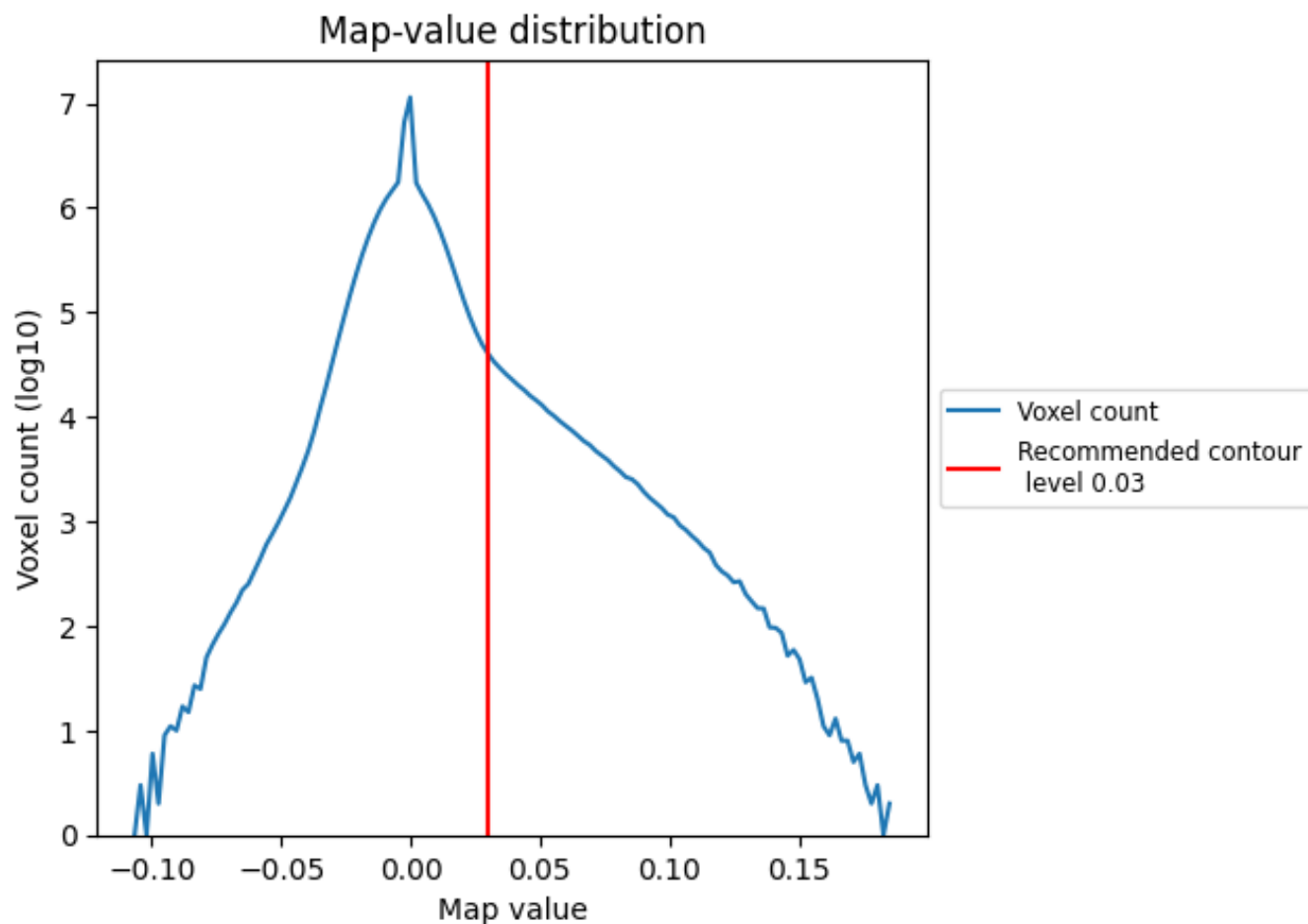


Z

## 7 Map analysis [i](#)

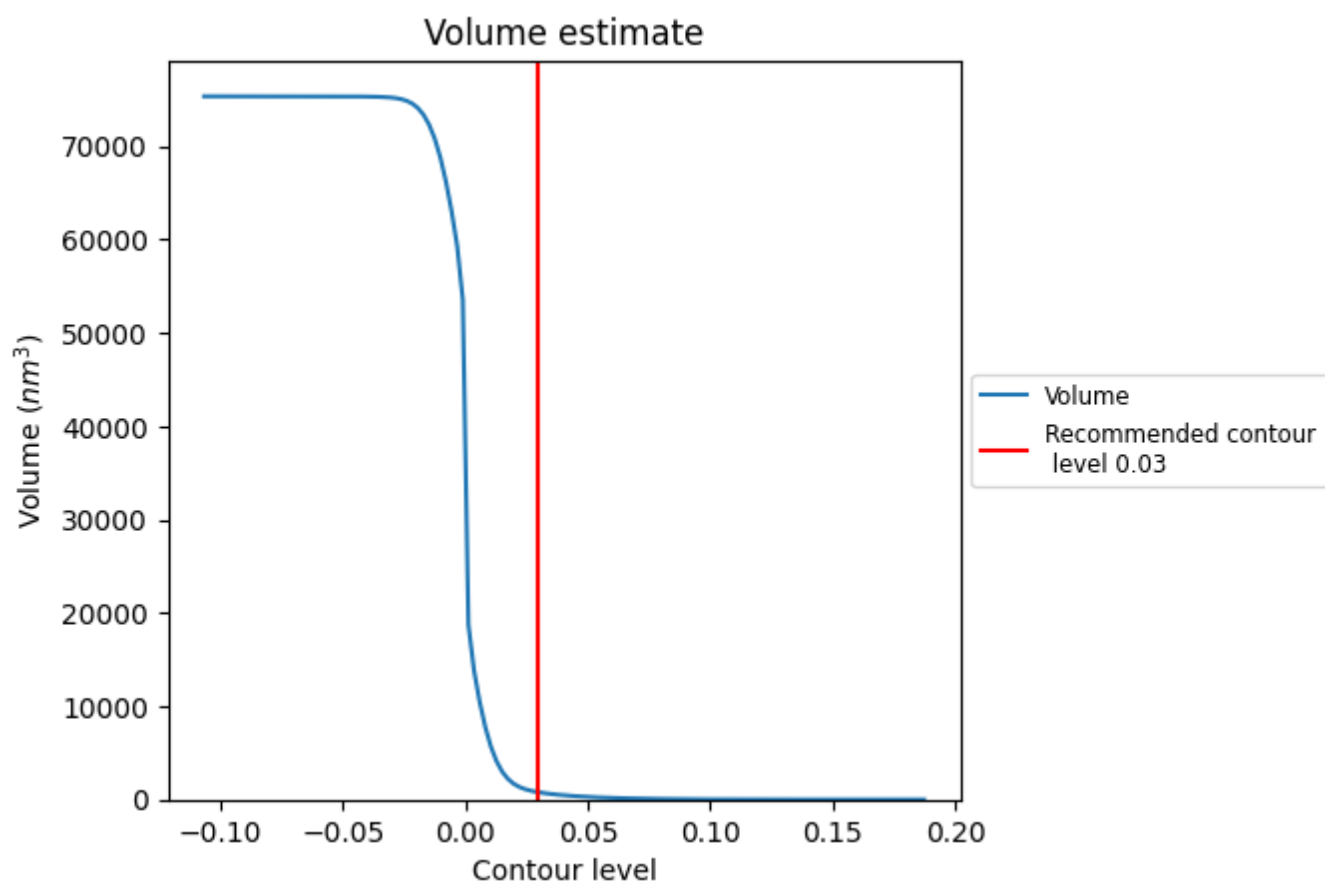
This section contains the results of statistical analysis of the map.

### 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.

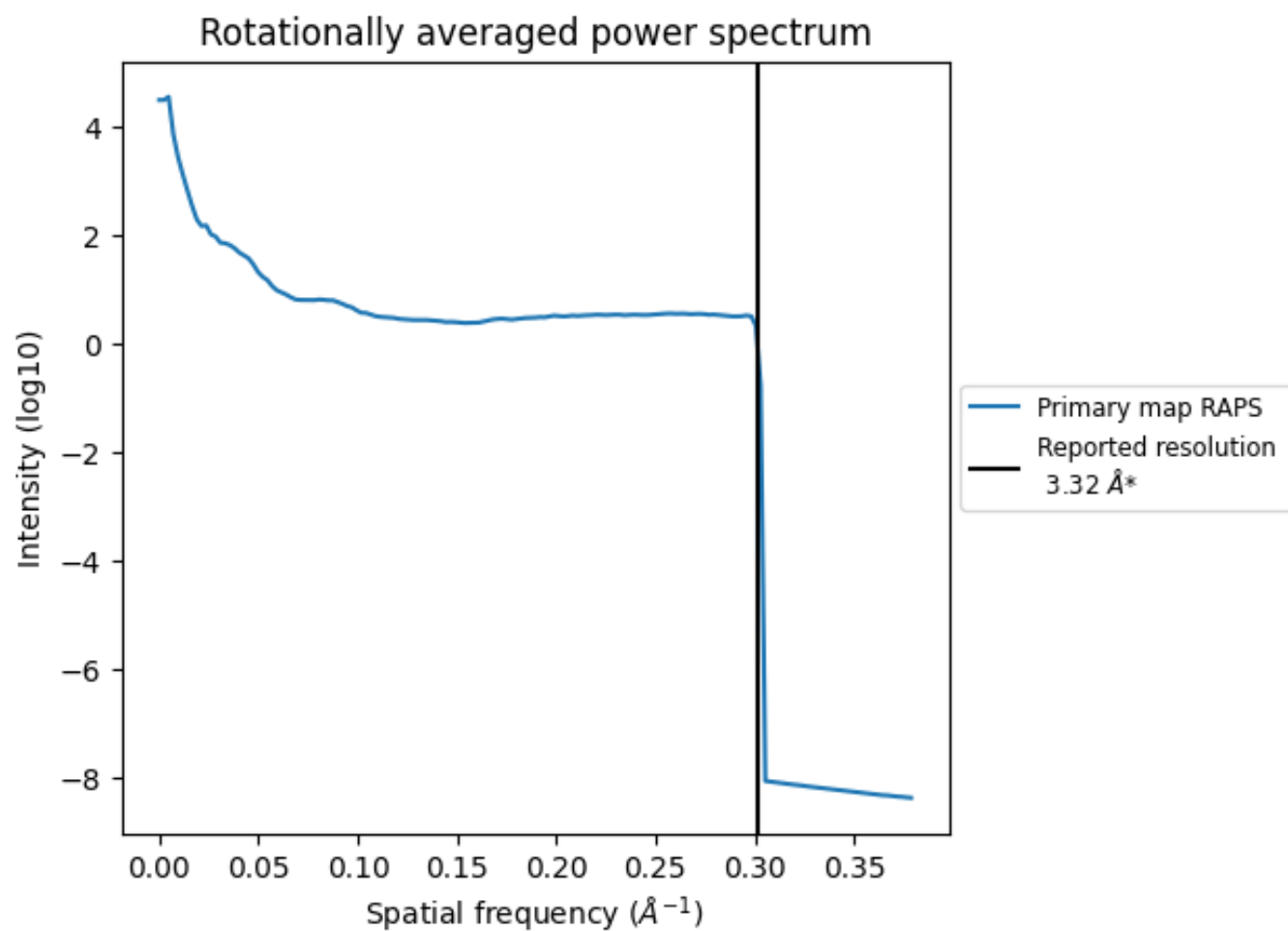
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 781 nm<sup>3</sup>; this corresponds to an approximate mass of 706 kDa.

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

### 7.3 Rotationally averaged power spectrum ⓘ



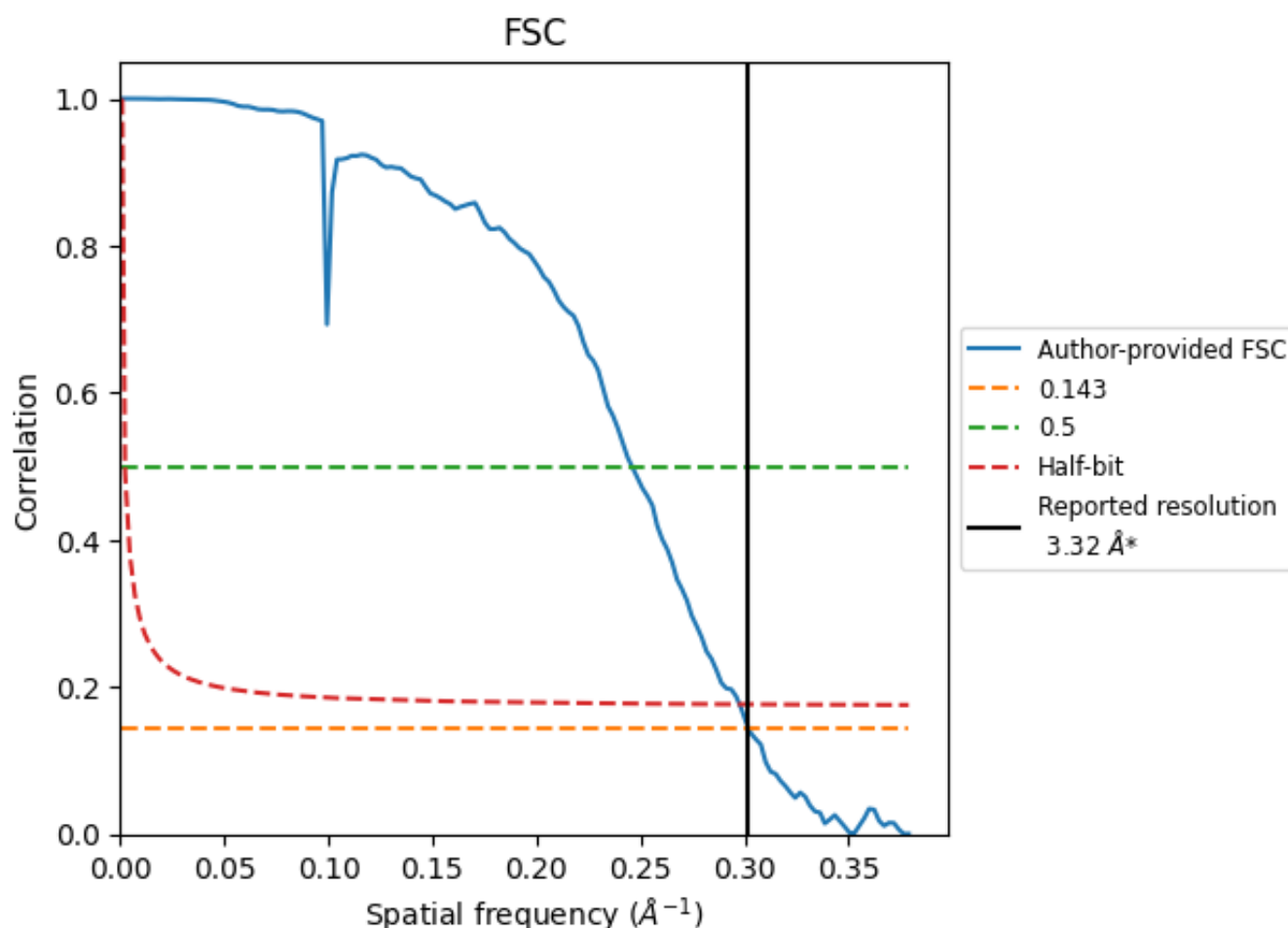
\*Reported resolution corresponds to spatial frequency of 0.301 Å<sup>-1</sup>



## 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 0.301 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

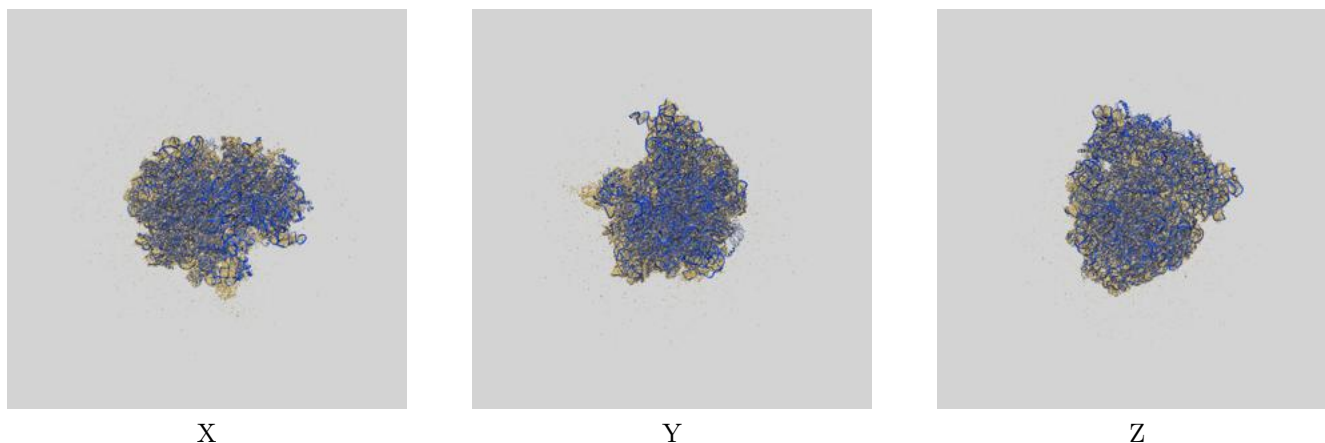
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | -                                  | -    | -        |
| Author-provided FSC curve | 3.31                               | 4.07 | 3.36     |
| Unmasked-calculated*      | -                                  | -    | -        |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

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

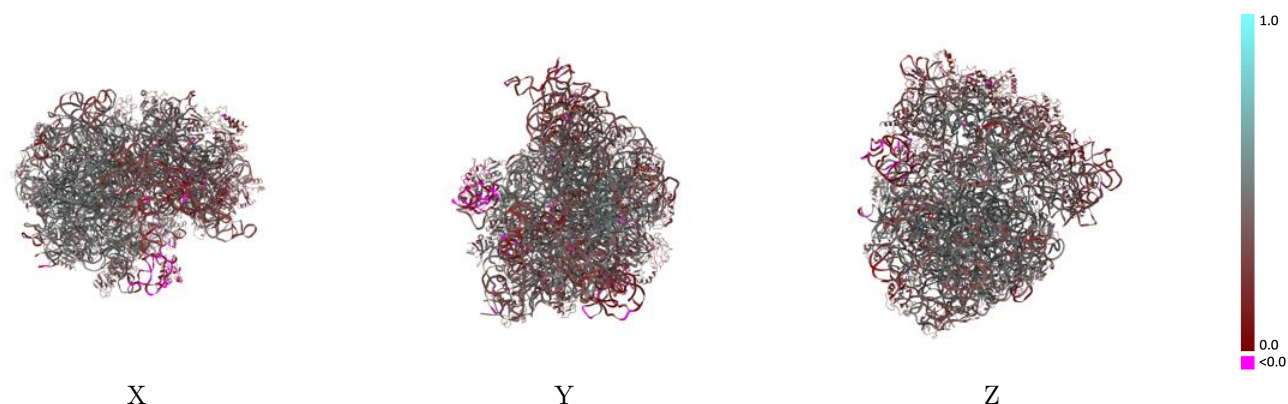
This section contains information regarding the fit between EMDB map EMD-6486 and PDB model 3JBV. Per-residue inclusion information can be found in [section 3](#) on [page 14](#).

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



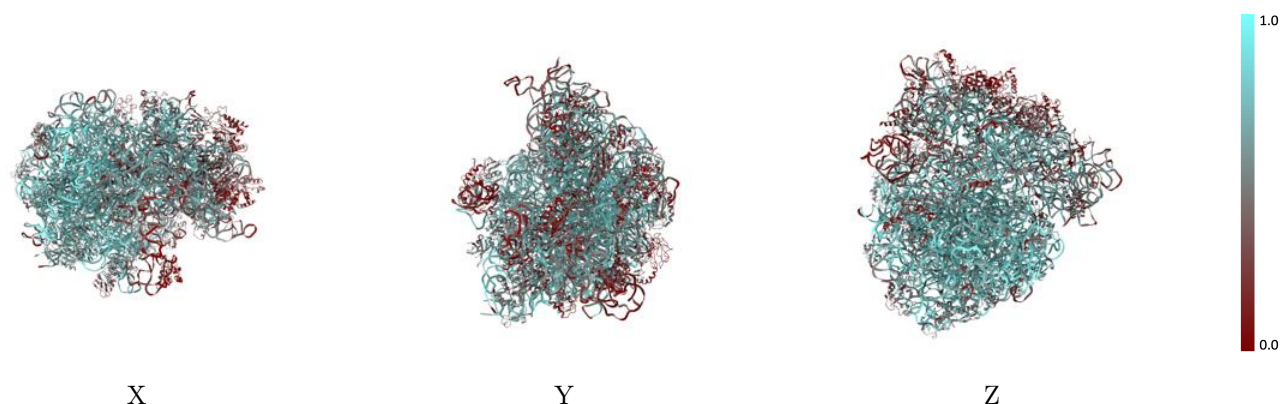
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



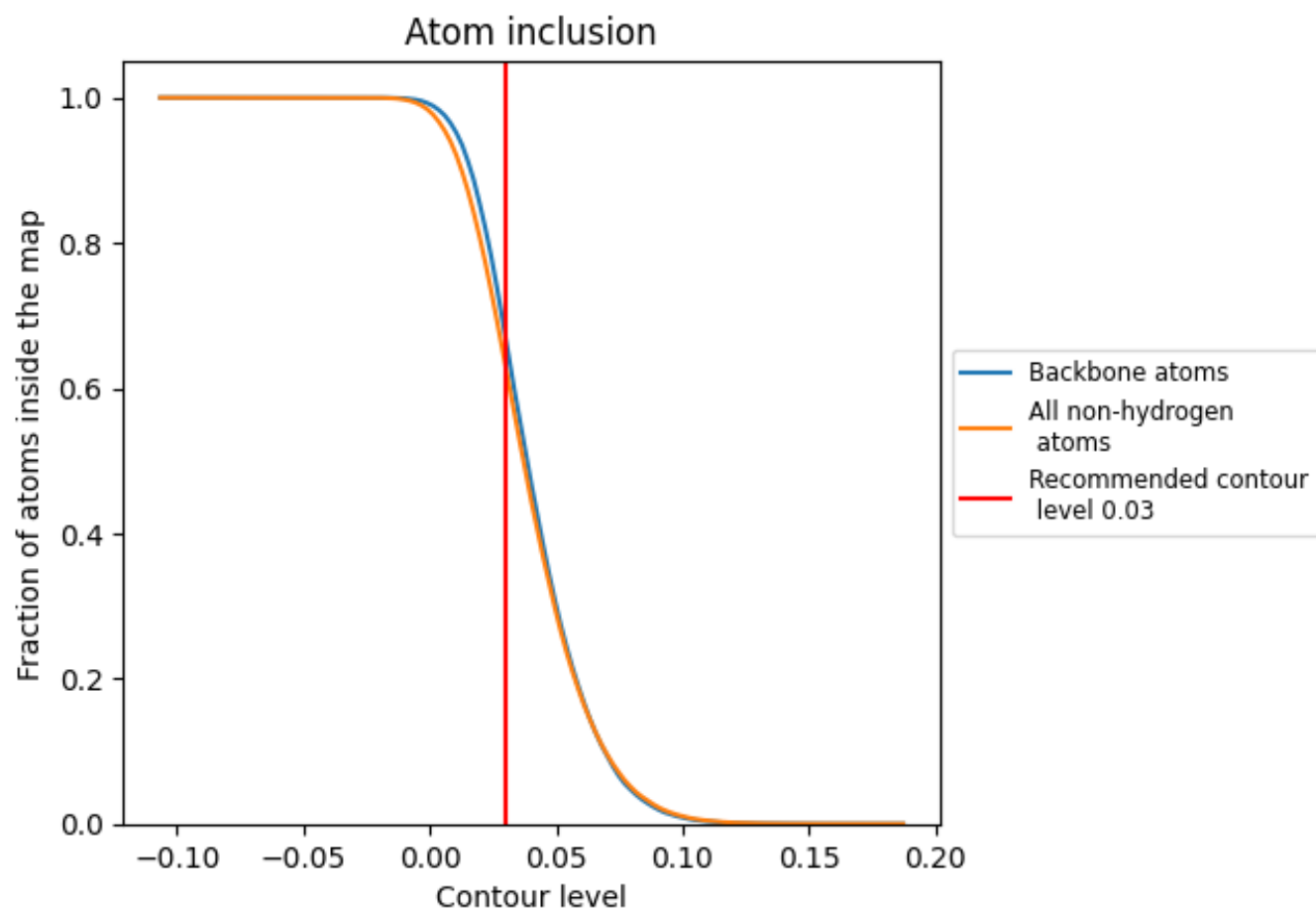
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 67% of all backbone atoms, 63% 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 (0.03) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion   | Q-score  |
|-------|--|--|
| All   |  0.6305   |  0.3940   |
| 0     |  0.5874   |  0.4320   |
| 1     |  0.4560   |  0.3300   |
| 2     |  0.6018   |  0.4520   |
| 3     |  0.6402   |  0.4360   |
| 4     |  0.5536   |  0.3990   |
| 6     |  0.7211   |  0.4850   |
| 7     |  0.6986   |  0.5070   |
| 8     |  0.6541   |  0.4600   |
| A     |  0.6511   |  0.3950   |
| B     |  0.1570   |  0.2650   |
| C     |  0.2478   |  0.3040   |
| D     |  0.1836   |  0.2520   |
| E     |  0.3204   |  0.3460   |
| F     |  0.3681  |  0.3420  |
| G     |  0.2419 |  0.2950 |
| H     |  0.3740 |  0.3520 |
| I     |  0.2717 |  0.2630 |
| J     |  0.2102 |  0.2600 |
| K     |  0.4713 |  0.3920 |
| L     |  0.4365 |  0.3790 |
| M     |  0.3164 |  0.3130 |
| N     |  0.3257 |  0.3420 |
| O     |  0.5000 |  0.3860 |
| P     |  0.2057 |  0.1160 |
| Q     |  0.3418 |  0.3360 |
| R     |  0.4450 |  0.3770 |
| S     |  0.3688 |  0.3650 |
| T     |  0.3354 |  0.2890 |
| U     |  0.3153 |  0.3170 |
| V     |  0.2704 |  0.2560 |
| W     |  0.6123 |  0.3470 |
| X     |  0.5368 |  0.3990 |
| a     |  0.7502 |  0.3890 |
| b     |  0.7591 |  0.4220 |



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| Chain | Atom inclusion   | Q-score  |
|-------|--|--|
| c     |  0.6771   |  0.4680   |
| d     |  0.6027   |  0.4520   |
| e     |  0.5474   |  0.3900   |
| f     |  0.3860   |  0.2860   |
| g     |  0.4133   |  0.3360   |
| h     |  0.1496   |  0.2440   |
| i     |  0.0620   |  0.0360   |
| j     |  0.6227   |  0.4430   |
| k     |  0.5608   |  0.4450   |
| l     |  0.6279   |  0.4350   |
| m     |  0.6137   |  0.4560   |
| n     |  0.6432   |  0.4500   |
| o     |  0.5701   |  0.3650   |
| p     |  0.5169   |  0.4020   |
| q     |  0.6729   |  0.4670   |
| r     |  0.5822   |  0.4160   |
| s     |  0.5909   |  0.4500   |
| t     |  0.5277   |  0.3770   |
| u     |  0.5059   |  0.3570   |
| w     |  0.5528  |  0.4050  |
| y     |  0.6685 |  0.4770 |
| z     |  0.0625 |  0.3120 |