



# wwPDB EM Validation Summary Report ⓘ

May 19, 2024 – 11:31 AM EDT

PDB ID : 7MSM  
EMDB ID : EMD-23969  
Title : Mtb 70SIC in complex with MtbEttA at Trans\_R0 state  
Authors : Cui, Z.; Zhang, J.  
Deposited on : 2021-05-11  
Resolution : 2.79 Å(reported)

This is a wwPDB EM Validation Summary 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.dev92  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36.2

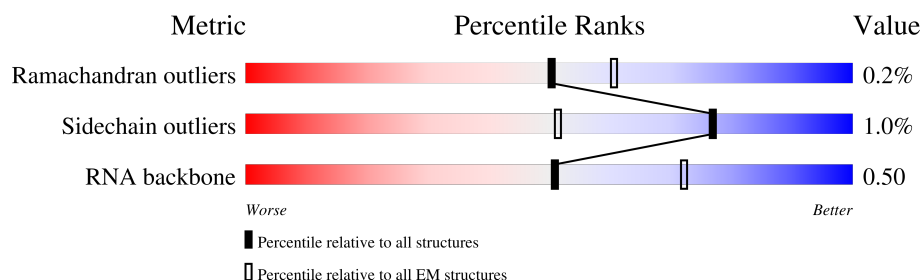
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.79 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   | 0     | 57     |                  |
| 2   | 1     | 55     |                  |
| 3   | 2     | 47     |                  |
| 4   | 3     | 64     |                  |
| 5   | 4     | 37     |                  |
| 6   | 6     | 80     |                  |
| 7   | 7     | 24     |                  |
| 8   | 8     | 235    |                  |



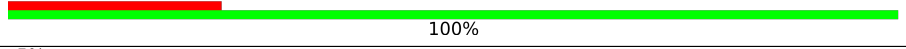

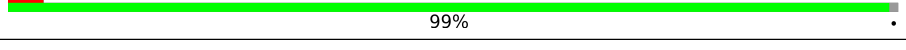
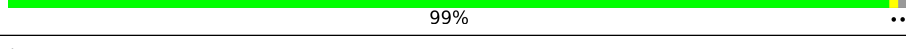
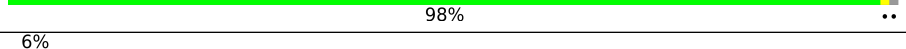
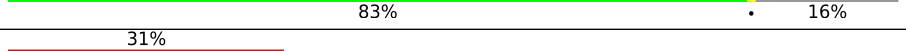
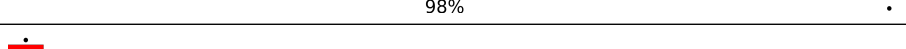
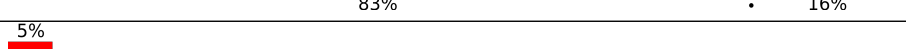
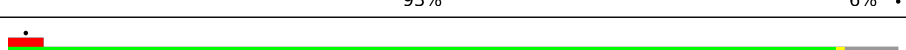
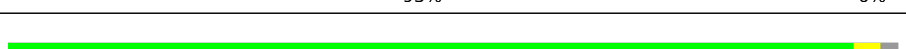
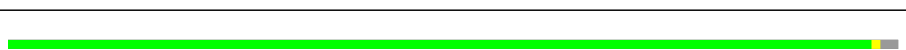

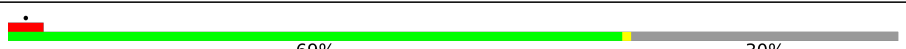


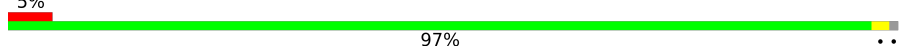
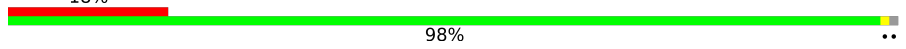



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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 9   | A     | 3138   |                  |
| 10  | B     | 115    |                  |
| 11  | C     | 280    |                  |
| 12  | D     | 217    |                  |
| 13  | E     | 223    |                  |
| 14  | F     | 187    |                  |
| 15  | G     | 179    |                  |
| 16  | H     | 152    |                  |
| 17  | J     | 195    |                  |
| 18  | K     | 122    |                  |
| 19  | L     | 146    |                  |
| 20  | M     | 138    |                  |
| 21  | N     | 180    |                  |
| 22  | O     | 122    |                  |
| 23  | P     | 113    |                  |
| 24  | Q     | 129    |                  |
| 25  | R     | 104    |                  |
| 26  | S     | 197    |                  |
| 27  | T     | 100    |                  |
| 28  | U     | 105    |                  |
| 29  | V     | 215    |                  |
| 30  | W     | 86     |                  |
| 31  | X     | 64     |                  |
| 32  | Y     | 77     |                  |
| 33  | Z     | 65     |                  |

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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 34  | a     | 1537   |    |
| 35  | c     | 274    |    |
| 36  | d     | 201    |    |
| 37  | e     | 220    |    |
| 38  | f     | 96     |    |
| 39  | g     | 156    |    |
| 40  | h     | 132    |    |
| 41  | i     | 151    |    |
| 42  | j     | 101    |    |
| 43  | k     | 139    |    |
| 44  | l     | 124    |    |
| 45  | m     | 124    |  |
| 46  | n     | 61     |  |
| 47  | o     | 89     |  |
| 48  | p     | 162    |  |
| 49  | q     | 135    |  |
| 50  | r     | 84     |  |
| 51  | s     | 93     |  |
| 52  | t     | 86     |  |
| 53  | x     | 558    |  |
| 54  | y     | 77     |  |
| 55  | z     | 26     |  |

## 2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 152436 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 50S ribosomal protein L32.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 1   | 0     | 54       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 429   | 266 | 94 | 69 |         |       |

- Molecule 2 is a protein called 50S ribosomal protein L33 2.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 2   | 1     | 48       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 400   | 245 | 84 | 67 | 4 |         |       |

- Molecule 3 is a protein called 50S ribosomal protein L34.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 3   | 2     | 44       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 374   | 222 | 97 | 54 | 1 |         |       |

- Molecule 4 is a protein called 50S ribosomal protein L35.

| Mol | Chain | Residues | Atoms |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---------|-------|
| 4   | 3     | 62       | Total | C   | N   | O  | 0       | 0     |
|     |       |          | 494   | 298 | 112 | 84 |         |       |

- Molecule 5 is a protein called 50S ribosomal protein L36.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 5   | 4     | 37       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 299   | 182 | 66 | 47 | 4 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| 4     | 1       | VAL      | MET    | conflict | UNP P9WH89 |

- Molecule 6 is a protein called 50S ribosomal protein L31.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 6   | 6     | 57       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 446   | 277 | 82 | 82 | 5 |         |       |

- Molecule 7 is a protein called 50S ribosomal protein L37.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 7   | 7     | 22       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 186   | 111 | 47 | 28 |         |       |

- Molecule 8 is a protein called 50S ribosomal protein L1.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 8   | 8     | 230      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1704  | 1068 | 310 | 323 | 3 |         |       |

- Molecule 9 is a RNA chain called 23S rRNA.

| Mol | Chain | Residues | Atoms |       |       |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|-------|
| 9   | A     | 3118     | Total | C     | N     | O     | P    | 0       | 0     |
|     |       |          | 66958 | 29847 | 12340 | 21653 | 3118 |         |       |

- Molecule 10 is a RNA chain called 5S rRNA.

| Mol | Chain | Residues | Atoms |      |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|-------|
| 10  | B     | 115      | Total | C    | N   | O   | P   | 0       | 0     |
|     |       |          | 2458  | 1097 | 456 | 790 | 115 |         |       |

- Molecule 11 is a protein called 50S ribosomal protein L2.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 11  | C     | 272      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2088  | 1277 | 437 | 369 | 5 |         |       |

- Molecule 12 is a protein called 50S ribosomal protein L3.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 12  | D     | 213      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1590  | 985 | 307 | 292 | 6 |         |       |

- Molecule 13 is a protein called 50S ribosomal protein L4.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 13  | E     | 207      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1552  | 958 | 303 | 289 | 2 |         |       |

- Molecule 14 is a protein called 50S ribosomal protein L5.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 14  | F     | 178      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1408  | 885 | 267 | 251 | 5 |         |       |

- Molecule 15 is a protein called 50S ribosomal protein L6.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 15  | G     | 174      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1330  | 836 | 249 | 244 | 1 |         |       |

- Molecule 16 is a protein called 50S ribosomal protein L9.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 16  | H     | 47       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 350   | 220 | 64 | 65 | 1 |         |       |

- Molecule 17 is a protein called 50S ribosomal protein L13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 17  | J     | 146      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1143  | 724 | 217 | 199 | 3 |         |       |

- Molecule 18 is a protein called 50S ribosomal protein L14.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 18  | K     | 122      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 941   | 590 | 180 | 169 | 2 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference      |
|-------|---------|----------|--------|----------|----------------|
| K     | 1       | VAL      | MET    | conflict | UNP A0A045HTP7 |

- Molecule 19 is a protein called 50S ribosomal protein L15.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 19  | L     | 144      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1075  | 666 | 217 | 190 | 2 |         |       |

- Molecule 20 is a protein called 50S ribosomal protein L16.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 20  | M     | 134      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1072  | 679 | 215 | 177 | 1 |         |       |

- Molecule 21 is a protein called 50S ribosomal protein L17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 21  | N     | 116      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 908   | 574 | 175 | 158 | 1 |         |       |

- Molecule 22 is a protein called 50S ribosomal protein L18.

| Mol | Chain | Residues | Atoms |     |     |     |  | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|-------|
| 22  | O     | 119      | Total | C   | N   | O   |  | 0       | 0     |
|     |       |          | 905   | 552 | 191 | 162 |  |         |       |

- Molecule 23 is a protein called 50S ribosomal protein L19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 23  | P     | 112      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 907   | 573 | 174 | 159 | 1 |         |       |

- Molecule 24 is a protein called 50S ribosomal protein L20.

| Mol | Chain | Residues | Atoms |     |     |     |  | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|-------|
| 24  | Q     | 124      | Total | C   | N   | O   |  | 0       | 0     |
|     |       |          | 993   | 616 | 207 | 170 |  |         |       |

- Molecule 25 is a protein called 50S ribosomal protein L21.

| Mol | Chain | Residues | Atoms |     |     |     |  | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|-------|
| 25  | R     | 100      | Total | C   | N   | O   |  | 0       | 0     |
|     |       |          | 757   | 482 | 138 | 137 |  |         |       |

There is a discrepancy between the modelled and reference sequences:



| Chain | Residue | Modelled | Actual | Comment   | Reference  |
|-------|---------|----------|--------|-----------|------------|
| R     | 1       | MET      | -      | insertion | UNP P9WHC3 |

- Molecule 26 is a protein called 50S ribosomal protein L22.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 26  | S     | 113      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 860   | 533 | 178 | 149 |         |       |

- Molecule 27 is a protein called 50S ribosomal protein L23.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 27  | T     | 95       | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 741   | 469 | 138 | 134 |         |       |

- Molecule 28 is a protein called 50S ribosomal protein L24.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 28  | U     | 90       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 699   | 430 | 138 | 129 | 2 |         |       |

- Molecule 29 is a protein called 50S ribosomal protein L25.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 29  | V     | 177      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 1319  | 822 | 243 | 254 |         |       |

- Molecule 30 is a protein called 50S ribosomal protein L27.

| Mol | Chain | Residues | Atoms |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---------|-------|
| 30  | W     | 74       | Total | C   | N   | O  | 0       | 0     |
|     |       |          | 549   | 337 | 114 | 98 |         |       |

- Molecule 31 is a protein called 50S ribosomal protein L28.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 31  | X     | 62       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 468   | 284 | 100 | 80 | 4 |         |       |

- Molecule 32 is a protein called 50S ribosomal protein L29.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 32  | Y     | 68       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 560   | 343 | 109 | 107 | 1 |         |       |

- Molecule 33 is a protein called 50S ribosomal protein L30.

| Mol | Chain | Residues | Atoms |     |     |    |  | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|--|---------|-------|
| 33  | Z     | 59       | Total | C   | N   | O  |  | 0       | 0     |
|     |       |          | 476   | 293 | 101 | 82 |  |         |       |

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

| Mol | Chain | Residues | Atoms |       |      |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|-------|
| 34  | a     | 1519     | Total | C     | N    | O     | P    | 0       | 0     |
|     |       |          | 32620 | 14535 | 5961 | 10605 | 1519 |         |       |

- Molecule 35 is a protein called 30S ribosomal protein S3.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 35  | c     | 207      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1654  | 1030 | 322 | 298 | 4 |         |       |

- Molecule 36 is a protein called 30S ribosomal protein S4.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 36  | d     | 200      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1650  | 1036 | 316 | 296 | 2 |         |       |

- Molecule 37 is a protein called 30S ribosomal protein S5.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 37  | e     | 169      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1222  | 770 | 231 | 218 | 3 |         |       |

- Molecule 38 is a protein called 30S ribosomal protein S6.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 38  | f     | 95       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 757   | 480 | 133 | 141 | 3 |         |       |

- Molecule 39 is a protein called 30S ribosomal protein S7.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 39  | g     | 155      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1230  | 768 | 241 | 219 | 2 |         |       |

- Molecule 40 is a protein called 30S ribosomal protein S8.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 40  | h     | 131      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1006  | 631 | 188 | 186 | 1 |         |       |

- Molecule 41 is a protein called 30S ribosomal protein S9.

| Mol | Chain | Residues | Atoms |     |     |     |  | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|-------|
| 41  | i     | 127      | Total | C   | N   | O   |  | 0       | 0     |
|     |       |          | 992   | 628 | 195 | 169 |  |         |       |

- Molecule 42 is a protein called 30S ribosomal protein S10.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 42  | j     | 99       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 789   | 496 | 146 | 144 | 3 |         |       |

- Molecule 43 is a protein called 30S ribosomal protein S11.

| Mol | Chain | Residues | Atoms |     |     |     |  | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|-------|
| 43  | k     | 117      | Total | C   | N   | O   |  | 0       | 0     |
|     |       |          | 873   | 540 | 175 | 158 |  |         |       |

- Molecule 44 is a protein called 30S ribosomal protein S12.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 44  | l     | 122      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 959   | 594 | 197 | 166 | 2 |         |       |

- Molecule 45 is a protein called 30S ribosomal protein S13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 45  | m     | 116      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 945   | 578 | 196 | 168 | 3 |         |       |

- Molecule 46 is a protein called 30S ribosomal protein S14 type Z.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 46  | n     | 60       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 468   | 294 | 96 | 73 | 5 |         |       |

- Molecule 47 is a protein called 30S ribosomal protein S15.

| Mol | Chain | Residues | Atoms |     |     |     |  | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|-------|
| 47  | o     | 87       | Total | C   | N   | O   |  | 0       | 0     |
|     |       |          | 718   | 449 | 144 | 125 |  |         |       |

- Molecule 48 is a protein called 30S ribosomal protein S16.

| Mol | Chain | Residues | Atoms |     |     |     |  | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|-------|
| 48  | p     | 113      | Total | C   | N   | O   |  | 0       | 0     |
|     |       |          | 884   | 564 | 166 | 154 |  |         |       |

- Molecule 49 is a protein called 30S ribosomal protein S17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 49  | q     | 95       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 770   | 482 | 152 | 133 | 3 |         |       |

- Molecule 50 is a protein called 30S ribosomal protein S18 1.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 50  | r     | 64       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 506   | 315 | 98 | 90 | 3 |         |       |

- Molecule 51 is a protein called 30S ribosomal protein S19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 51  | s     | 83       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 672   | 432 | 125 | 114 | 1 |         |       |

- Molecule 52 is a protein called 30S ribosomal protein S20.

| Mol | Chain | Residues | Atoms |     |     |     |  | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|-------|
| 52  | t     | 85       | Total | C   | N   | O   |  | 0       | 0     |
|     |       |          | 652   | 394 | 141 | 117 |  |         |       |

- Molecule 53 is a protein called Energy-dependent translational throttle protein EttA.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 53  | x     | 553      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4312  | 2712 | 754 | 834 | 12 |         |       |

- Molecule 54 is a RNA chain called initiator tRNA (Met).

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 54  | y     | 77       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 1644  | 732 | 297 | 538 | 77 |         |       |

- Molecule 55 is a RNA chain called mRNA.

| Mol | Chain | Residues | Atoms |    |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---|---------|-------|
| 55  | z     | 7        | Total | C  | N  | O  | P | 0       | 0     |
|     |       |          | 149   | 67 | 27 | 48 | 7 |         |       |

- Molecule 56 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 56  | 1     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 56  | 4     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 56  | 6     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 56  | X     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 56  | n     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 56  | r     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 57 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

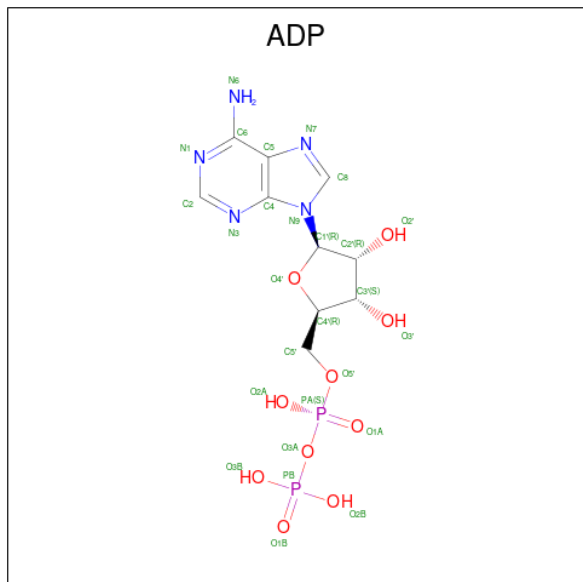
| Mol | Chain | Residues | Atoms |     | AltConf |
|-----|-------|----------|-------|-----|---------|
| 57  | A     | 302      | Total | Mg  | 0       |
|     |       |          | 302   | 302 |         |
| 57  | B     | 5        | Total | Mg  | 0       |
|     |       |          | 5     | 5   |         |
| 57  | C     | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |
| 57  | L     | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |

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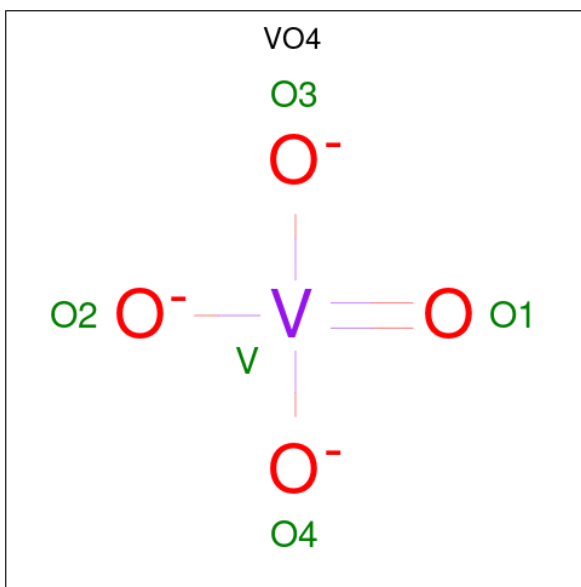
| Mol | Chain | Residues | Atoms |     | AltConf |
|-----|-------|----------|-------|-----|---------|
| 57  | W     | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |
| 57  | a     | 130      | Total | Mg  | 0       |
|     |       |          | 130   | 130 |         |
| 57  | r     | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |
| 57  | x     | 2        | Total | Mg  | 0       |
|     |       |          | 2     | 2   |         |
| 57  | y     | 2        | Total | Mg  | 0       |
|     |       |          | 2     | 2   |         |

- Molecule 58 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



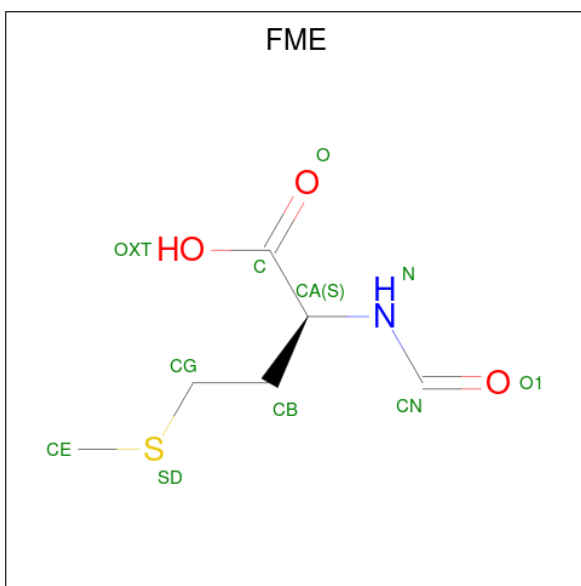
| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 58  | x     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |
| 58  | x     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |

- Molecule 59 is VANADATE ION (three-letter code: VO4) (formula:  $O_4V$ ).



| Mol | Chain | Residues | Atoms |   |   | AltConf |
|-----|-------|----------|-------|---|---|---------|
| 59  | x     | 1        | Total | O | V | 0       |
|     |       |          | 5     | 4 | 1 |         |
| 59  | x     | 1        | Total | O | V | 0       |
|     |       |          | 5     | 4 | 1 |         |

- Molecule 60 is N-FORMYLMETHIONINE (three-letter code: FME) (formula:  $C_6H_{11}NO_3S$ ).



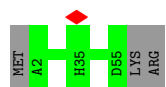
| Mol | Chain | Residues | Atoms |   |   |   |   | AltConf |
|-----|-------|----------|-------|---|---|---|---|---------|
| 60  | y     | 1        | Total | C | N | O | S | 0       |
|     |       |          | 10    | 6 | 1 | 2 | 1 |         |

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


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

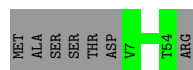
- Molecule 1: 50S ribosomal protein L32

Chain 0:  95% 5%



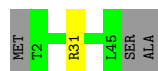
- Molecule 2: 50S ribosomal protein L33 2

Chain 1:  87% 13%



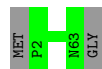
- Molecule 3: 50S ribosomal protein L34

Chain 2:  91% 6%



- Molecule 4: 50S ribosomal protein L35

Chain 3:  97%



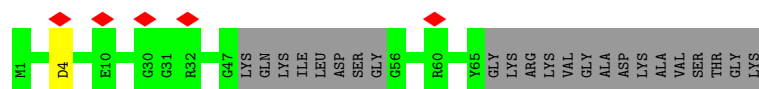
- Molecule 5: 50S ribosomal protein L36

Chain 4:  97%

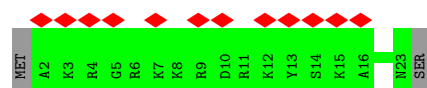
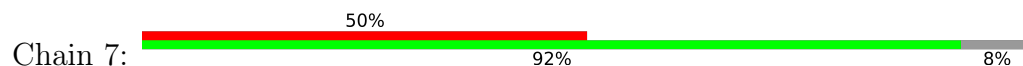


- Molecule 6: 50S ribosomal protein L31

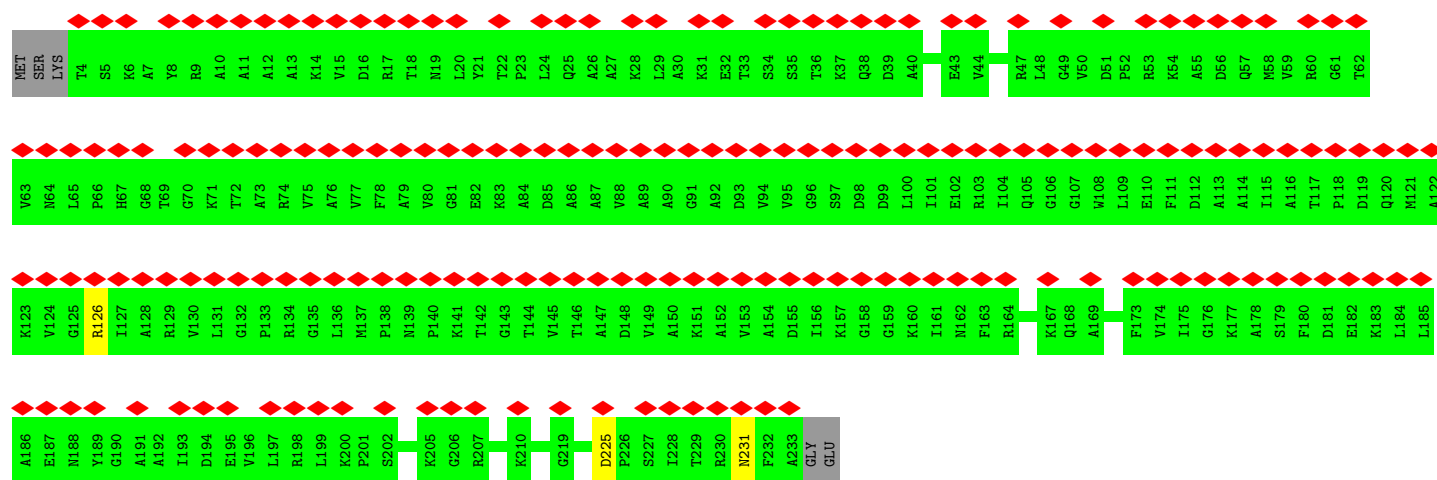
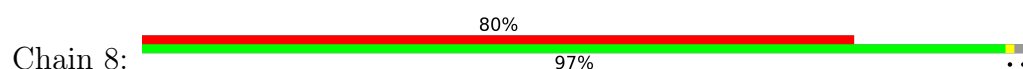




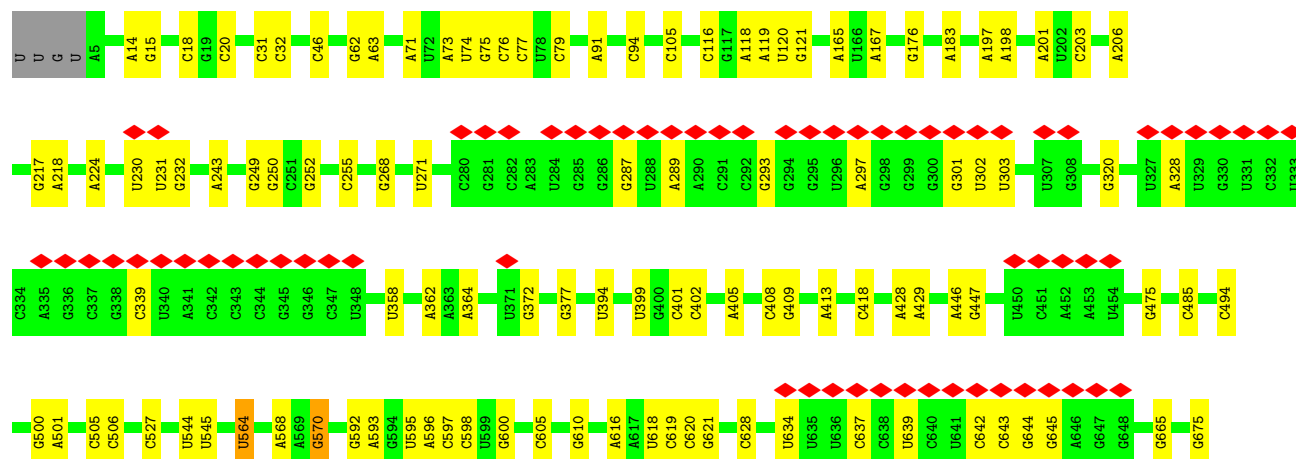
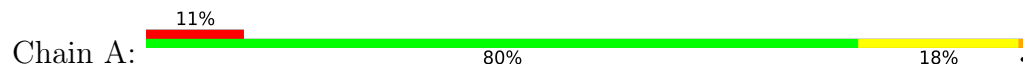
• Molecule 7: 50S ribosomal protein L37



• Molecule 8: 50S ribosomal protein L1



• Molecule 9: 23S rRNA









- Chain G:

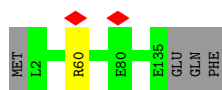
- Chain H:
- 
- 18%
- 30%
- 69%
- M1 R2 L3 L4 L5 T6 A7 D8 V9 D10 H11 I12 G13 S14 I15 G16 D17 T18 A19 V19 E20 R33 V38 A39 S40 R41 G42 A43 Q44 K45 Q46 A47 ASP GLU TLE ARG ARG ARG ARG THR LYS SER VAL ARG ASP LEU GLU HIS ALA ASN GLU ILE LYS ALA TLE GLU
- LEU PRO GLY THR VAL ASP SER ALA HIS ILE LYS ARG PHE LEU VAL THR LYS GLY ASP ALA ASN LEU ASP ARG THR HIS VAL SER VAL

- Chain J:  75% 25%
- |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |    |     |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|----|-----|
| MET | LEU | VAL | GLY | LYS | LEU | GLY | TRP | ARG | ALA | VAL | ARG | ASP | LEU | GLY | SER | MET | SER | VAL | ALA | GLU | THR | ASN | PRO | PRO | PRO | THR | PRO | ASP | ARG | ARG | PRO | GLY | HIS | PRO | GLY | ILE | HIS | PRO | ARG | GLU | LYS | VAL | VAL | SER | ALA | VAL | P2 | GLY |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|----|-----|

- Chain K:  98%

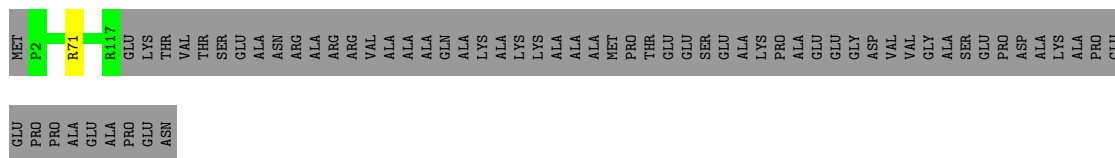
- Chain L:

- Chain M:  96%



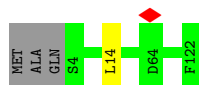
- Molecule 21: 50S ribosomal protein L17

Chain N: 64% 36%



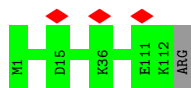
- Molecule 22: 50S ribosomal protein L18

Chain O: 97%



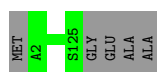
- Molecule 23: 50S ribosomal protein L19

Chain P: 99%



- Molecule 24: 50S ribosomal protein L20

Chain Q: 96%



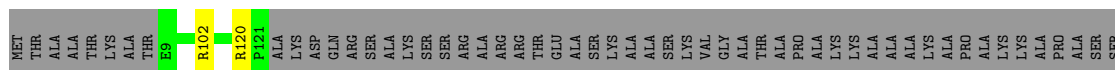
- Molecule 25: 50S ribosomal protein L21

Chain R: 94%



- Molecule 26: 50S ribosomal protein L22

Chain S: 56% 43%




GLY VAL LYS LYS THR PRO ALA LYS LYS ALA ALA PRO PRO LYS LYS LYS ALA ALA ALA LYS LYS GLY GLY SER ASP

- Molecule 27: 50S ribosomal protein L23

Chain T:  94% 5%


MET ALA T3 R70 F96 G97 ALA PRO ALA

- Molecule 28: 50S ribosomal protein L24

Chain U:  84% 14%

M1 D29 A46 ILE SER THR THR GLN ARG GLY ALA ARG SER GLY ILE VAL T61 S76 D88 E89 E90 N101 G102 K103 D104 ILE


- Molecule 29: 50S ribosomal protein L25

Chain V:  81% 18%

MET ALA LYS SER ALA S6 R10 G39 R57 H58 D68 G71 K72 E73 R99 R100 G101 E102 K103 E113 G114 Q115 Q116 G117 P118 D119 T120 L121 M127 S128 E132 A133 E134 A135 L136 S137 I138 Q141 L142 T143 V144 S145 I146 E147 G148 A149 E150 P151 G152 T153

G158 Q159 I160 A161 L162 P163 A164 G165 I169 S170 D171 F172 D173 K181 A182 PRO THR ALA ALA GLU GLU LEU GLY GLU VAL ALA GLY GLY ALA GLU GLU ALA ALA VAL GLU GLU GLY GLY ALA GLU ALA ALA GLY SER GLU

- Molecule 30: 50S ribosomal protein L27

Chain W:  85% 14%


MET ALA HIS LYS LYS GLY ALA ALA SER S9 R14 G82 SER THR ALA

- Molecule 31: 50S ribosomal protein L28

Chain X:  95%

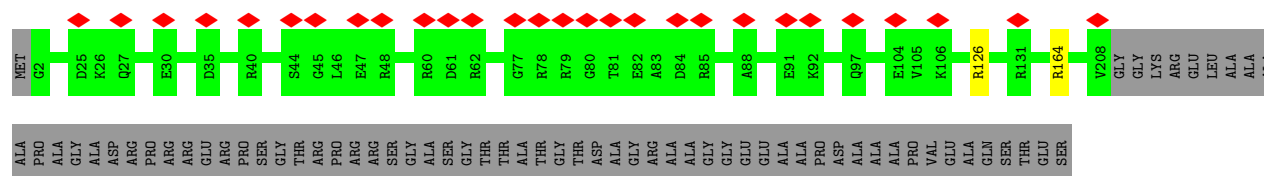
MET A2 R27 R63 GLY

- Molecule 32: 50S ribosomal protein L29

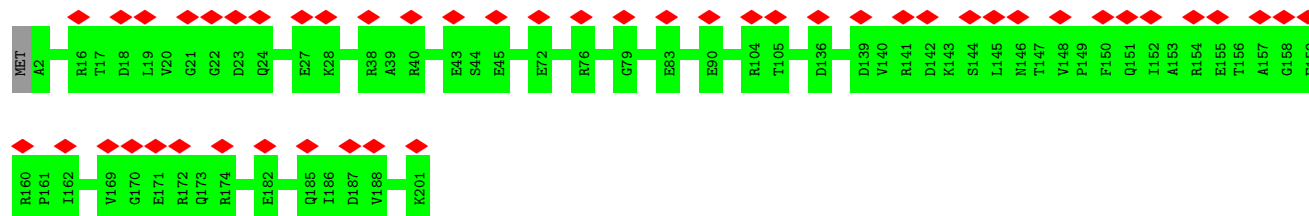
Chain Y:  88% 12%

MET ALA VAL GLY V5 D15 A69 F72 ASP GLY LYS GLU SER

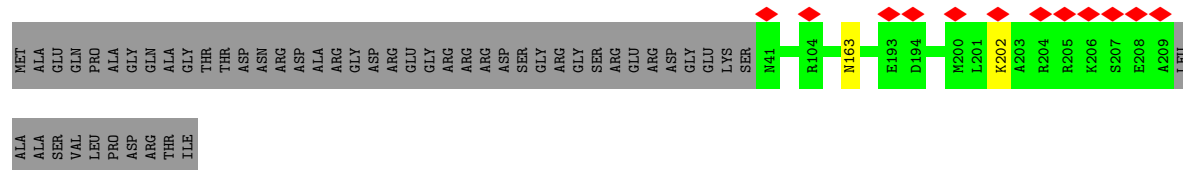
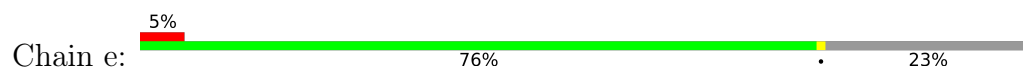




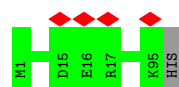
- Molecule 36: 30S ribosomal protein S4



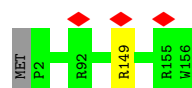
- Molecule 37: 30S ribosomal protein S5



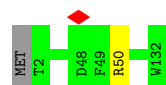
- Molecule 38: 30S ribosomal protein S6



- Molecule 39: 30S ribosomal protein S7

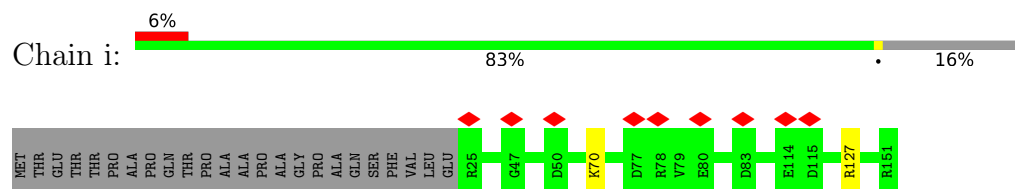


- Molecule 40: 30S ribosomal protein S8

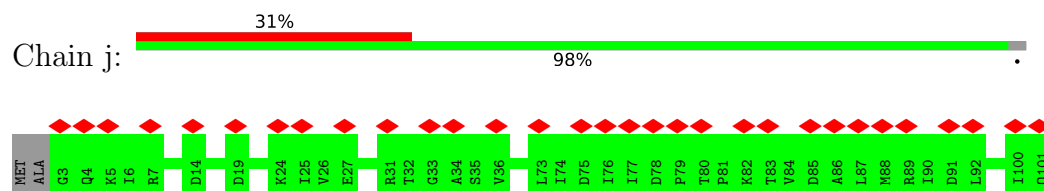




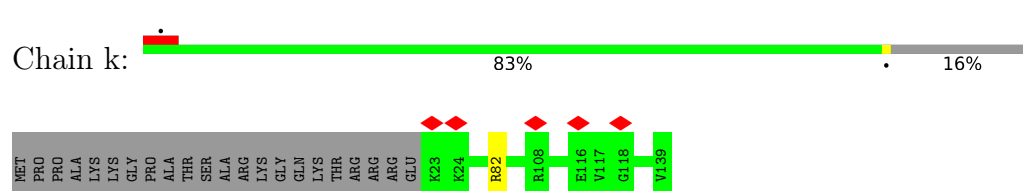
- Molecule 41: 30S ribosomal protein S9



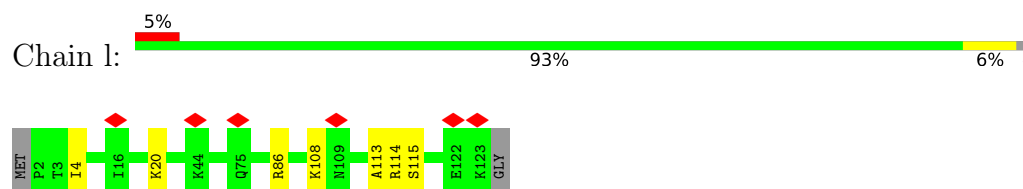
- Molecule 42: 30S ribosomal protein S10



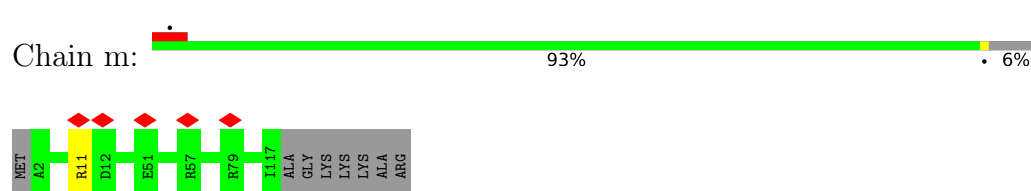
- Molecule 43: 30S ribosomal protein S11



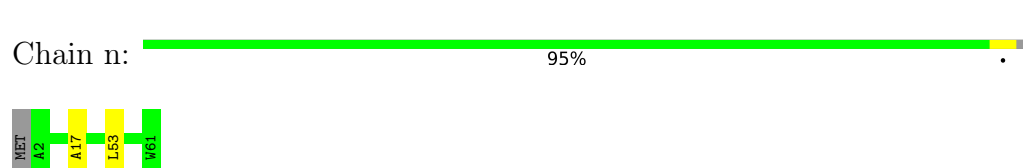
- Molecule 44: 30S ribosomal protein S12



- Molecule 45: 30S ribosomal protein S13



- Molecule 46: 30S ribosomal protein S14 type Z

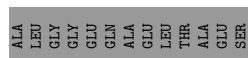
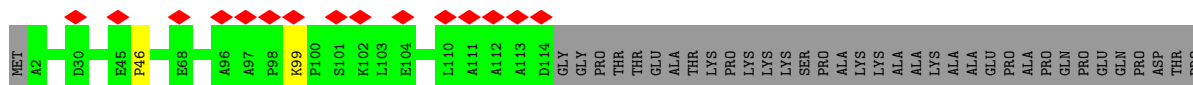


- Molecule 47: 30S ribosomal protein S15

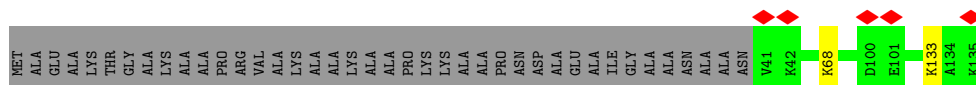




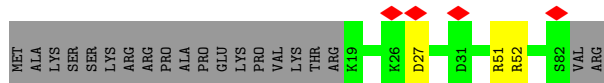
- Molecule 48: 30S ribosomal protein S16



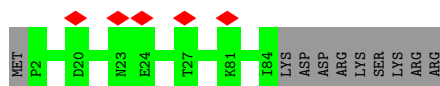
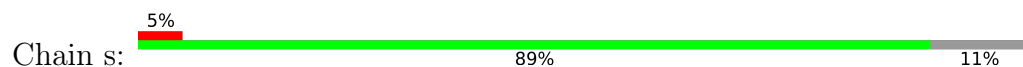
- Molecule 49: 30S ribosomal protein S17



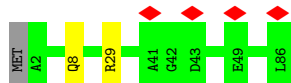
- Molecule 50: 30S ribosomal protein S18 1



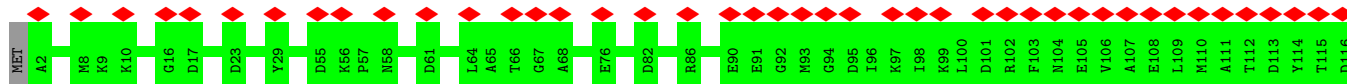
- Molecule 51: 30S ribosomal protein S19

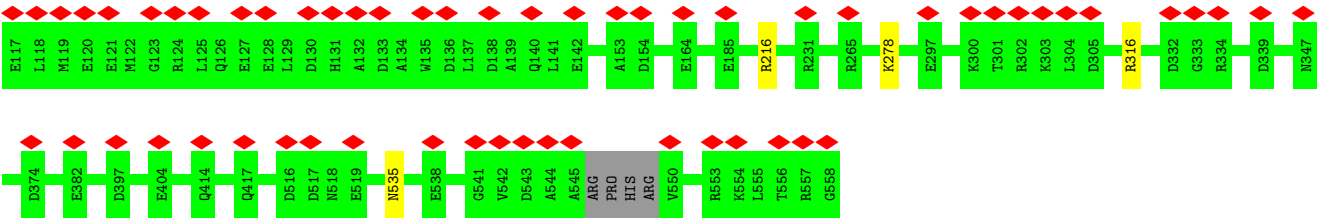


- Molecule 52: 30S ribosomal protein S20

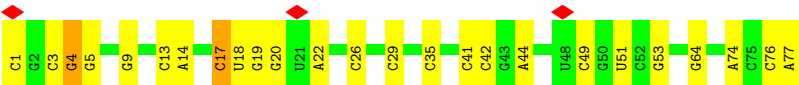


- Molecule 53: Energy-dependent translational throttle protein EttA

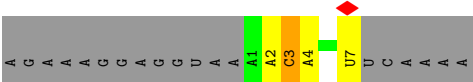




• Molecule 54: initiator tRNA (Met)



• Molecule 55: mRNA



## 4 Experimental information

| Property                             | Value                           | Source    |
|--------------------------------------|---------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                 | Depositor |
| Imposed symmetry                     | POINT, Not provided             |           |
| Number of particles used             | 86692                           | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF               | Depositor |
| CTF correction method                | NONE                            | Depositor |
| Microscope                           | FEI TITAN KRIOS                 | Depositor |
| Voltage (kV)                         | 300                             | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 48                              | Depositor |
| Minimum defocus (nm)                 | Not provided                    |           |
| Maximum defocus (nm)                 | Not provided                    |           |
| Magnification                        | Not provided                    |           |
| Image detector                       | GATAN K2 SUMMIT (4k x 4k)       | Depositor |
| Maximum map value                    | 0.364                           | Depositor |
| Minimum map value                    | -0.005                          | Depositor |
| Average map value                    | 0.001                           | Depositor |
| Map value standard deviation         | 0.012                           | Depositor |
| Recommended contour level            | 0.03                            | Depositor |
| Map size ( $\text{\AA}$ )            | 340.15997, 340.15997, 340.15997 | wwPDB     |
| Map dimensions                       | 320, 320, 320                   | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0                | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 1.063, 1.063, 1.063             | Depositor |

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: UR3, 4OC, OMG, MG, VO4, ADP, G7M, FME, 5MC, 2MG, MA6, ZN, 5MU

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

| Mol | Chain | Bond lengths |                | Bond angles |                   |
|-----|-------|--------------|----------------|-------------|-------------------|
|     |       | RMSZ         | $\# Z  > 5$    | RMSZ        | $\# Z  > 5$       |
| 1   | 0     | 0.47         | 0/435          | 0.58        | 0/581             |
| 2   | 1     | 0.49         | 0/407          | 0.55        | 0/543             |
| 3   | 2     | 0.56         | 0/377          | 0.61        | 0/494             |
| 4   | 3     | 0.44         | 0/499          | 0.57        | 0/664             |
| 5   | 4     | 0.44         | 0/303          | 0.59        | 0/402             |
| 6   | 6     | 0.34         | 0/455          | 0.60        | 1/611 (0.2%)      |
| 7   | 7     | 0.26         | 0/188          | 0.49        | 0/243             |
| 8   | 8     | 0.27         | 0/1728         | 0.51        | 0/2339            |
| 9   | A     | 1.05         | 4/74925 (0.0%) | 1.08        | 287/116904 (0.2%) |
| 10  | B     | 0.75         | 0/2748         | 0.98        | 6/4280 (0.1%)     |
| 11  | C     | 0.56         | 1/2129 (0.0%)  | 0.63        | 0/2861            |
| 12  | D     | 0.51         | 0/1613         | 0.61        | 0/2174            |
| 13  | E     | 0.47         | 0/1575         | 0.62        | 0/2129            |
| 14  | F     | 0.39         | 0/1429         | 0.59        | 0/1921            |
| 15  | G     | 0.31         | 0/1351         | 0.58        | 0/1824            |
| 16  | H     | 0.28         | 0/353          | 0.61        | 0/474             |
| 17  | J     | 0.52         | 0/1170         | 0.60        | 0/1584            |
| 18  | K     | 0.54         | 0/951          | 0.64        | 0/1278            |
| 19  | L     | 0.50         | 0/1088         | 0.64        | 0/1453            |
| 20  | M     | 0.41         | 0/1098         | 0.57        | 0/1481            |
| 21  | N     | 0.50         | 0/925          | 0.59        | 0/1242            |
| 22  | O     | 0.42         | 0/914          | 0.61        | 1/1228 (0.1%)     |
| 23  | P     | 0.51         | 0/922          | 0.60        | 0/1236            |
| 24  | Q     | 0.58         | 0/1006         | 0.60        | 0/1349            |
| 25  | R     | 0.53         | 0/766          | 0.60        | 0/1030            |
| 26  | S     | 0.51         | 0/874          | 0.58        | 0/1186            |
| 27  | T     | 0.46         | 0/751          | 0.62        | 0/1012            |
| 28  | U     | 0.41         | 0/705          | 0.68        | 0/941             |
| 29  | V     | 0.32         | 0/1336         | 0.61        | 0/1820            |
| 30  | W     | 0.51         | 0/554          | 0.63        | 0/737             |
| 31  | X     | 0.51         | 0/476          | 0.63        | 0/638             |
| 32  | Y     | 0.39         | 0/564          | 0.55        | 0/756             |

| Mol | Chain | Bond lengths |                 | Bond angles |                   |
|-----|-------|--------------|-----------------|-------------|-------------------|
|     |       | RMSZ         | # Z  >5         | RMSZ        | # Z  >5           |
| 33  | Z     | 0.44         | 0/480           | 0.59        | 0/645             |
| 34  | a     | 0.88         | 0/36331         | 0.99        | 67/56686 (0.1%)   |
| 35  | c     | 0.36         | 0/1678          | 0.54        | 0/2254            |
| 36  | d     | 0.32         | 0/1683          | 0.53        | 0/2269            |
| 37  | e     | 0.41         | 0/1238          | 0.56        | 0/1673            |
| 38  | f     | 0.39         | 0/767           | 0.56        | 0/1036            |
| 39  | g     | 0.37         | 0/1250          | 0.56        | 0/1686            |
| 40  | h     | 0.44         | 0/1021          | 0.59        | 0/1379            |
| 41  | i     | 0.36         | 0/1010          | 0.60        | 0/1356            |
| 42  | j     | 0.38         | 0/803           | 0.63        | 0/1086            |
| 43  | k     | 0.39         | 0/891           | 0.55        | 0/1204            |
| 44  | l     | 0.45         | 0/970           | 0.65        | 0/1295            |
| 45  | m     | 0.35         | 0/953           | 0.61        | 0/1274            |
| 46  | n     | 0.44         | 0/477           | 0.62        | 1/634 (0.2%)      |
| 47  | o     | 0.40         | 0/727           | 0.58        | 0/973             |
| 48  | p     | 0.36         | 0/901           | 0.62        | 0/1217            |
| 49  | q     | 0.38         | 0/782           | 0.64        | 0/1045            |
| 50  | r     | 0.40         | 0/511           | 0.64        | 1/685 (0.1%)      |
| 51  | s     | 0.35         | 0/690           | 0.54        | 0/928             |
| 52  | t     | 0.31         | 0/654           | 0.48        | 0/867             |
| 53  | x     | 0.34         | 0/4390          | 0.54        | 0/5942            |
| 54  | y     | 0.78         | 1/1836 (0.1%)   | 1.12        | 16/2859 (0.6%)    |
| 55  | z     | 0.93         | 0/166           | 1.26        | 2/256 (0.8%)      |
| All | All   | 0.86         | 6/164824 (0.0%) | 0.95        | 382/246664 (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 |
|-----|-------|---------------------|---------------------|
| 8   | 8     | 0                   | 1                   |
| 14  | F     | 0                   | 1                   |
| 25  | R     | 0                   | 1                   |
| 28  | U     | 0                   | 1                   |
| 29  | V     | 0                   | 2                   |
| 44  | l     | 0                   | 2                   |
| 53  | x     | 0                   | 1                   |
| All | All   | 0                   | 9                   |

The worst 5 of 6 bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|--------|-------------|----------|
| 54  | y     | 1    | C    | OP3-P | -10.61 | 1.48        | 1.61     |
| 11  | C     | 226  | MET  | C-N   | -7.50  | 1.16        | 1.34     |
| 9   | A     | 616  | A    | N9-C4 | -7.12  | 1.33        | 1.37     |
| 9   | A     | 2668 | A    | N9-C4 | -6.71  | 1.33        | 1.37     |
| 9   | A     | 2025 | A    | N9-C4 | -5.25  | 1.34        | 1.37     |

The worst 5 of 382 bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|--------|-------------|----------|
| 54  | y     | 17   | C    | N1-C2-O2  | 13.07  | 126.74      | 118.90   |
| 54  | y     | 17   | C    | C2-N1-C1' | 12.05  | 132.06      | 118.80   |
| 9   | A     | 3060 | C    | N3-C2-O2  | -10.76 | 114.37      | 121.90   |
| 9   | A     | 3060 | C    | N1-C2-O2  | 10.55  | 125.23      | 118.90   |
| 9   | A     | 739  | C    | C2-N1-C1' | 10.22  | 130.04      | 118.80   |

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 8   | 8     | 225 | ASP  | Mainchain |
| 14  | F     | 143 | ALA  | Peptide   |
| 25  | R     | 50  | THR  | Peptide   |
| 28  | U     | 101 | ASN  | Peptide   |
| 29  | V     | 135 | ALA  | 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 |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 1   | 0     | 52/57 (91%)   | 52 (100%) | 0        | 0        | 100         | 100 |
| 2   | 1     | 46/55 (84%)   | 45 (98%)  | 1 (2%)   | 0        | 100         | 100 |
| 3   | 2     | 42/47 (89%)   | 41 (98%)  | 1 (2%)   | 0        | 100         | 100 |
| 4   | 3     | 60/64 (94%)   | 57 (95%)  | 3 (5%)   | 0        | 100         | 100 |
| 5   | 4     | 35/37 (95%)   | 33 (94%)  | 2 (6%)   | 0        | 100         | 100 |
| 6   | 6     | 53/80 (66%)   | 48 (91%)  | 5 (9%)   | 0        | 100         | 100 |
| 7   | 7     | 20/24 (83%)   | 19 (95%)  | 1 (5%)   | 0        | 100         | 100 |
| 8   | 8     | 228/235 (97%) | 206 (90%) | 22 (10%) | 0        | 100         | 100 |
| 11  | C     | 270/280 (96%) | 257 (95%) | 13 (5%)  | 0        | 100         | 100 |
| 12  | D     | 211/217 (97%) | 201 (95%) | 10 (5%)  | 0        | 100         | 100 |
| 13  | E     | 205/223 (92%) | 199 (97%) | 6 (3%)   | 0        | 100         | 100 |
| 14  | F     | 176/187 (94%) | 157 (89%) | 17 (10%) | 2 (1%)   | 14          | 41  |
| 15  | G     | 172/179 (96%) | 161 (94%) | 11 (6%)  | 0        | 100         | 100 |
| 16  | H     | 45/152 (30%)  | 40 (89%)  | 5 (11%)  | 0        | 100         | 100 |
| 17  | J     | 144/195 (74%) | 141 (98%) | 3 (2%)   | 0        | 100         | 100 |
| 18  | K     | 120/122 (98%) | 116 (97%) | 4 (3%)   | 0        | 100         | 100 |
| 19  | L     | 142/146 (97%) | 133 (94%) | 9 (6%)   | 0        | 100         | 100 |
| 20  | M     | 132/138 (96%) | 124 (94%) | 8 (6%)   | 0        | 100         | 100 |
| 21  | N     | 114/180 (63%) | 113 (99%) | 1 (1%)   | 0        | 100         | 100 |
| 22  | O     | 117/122 (96%) | 112 (96%) | 5 (4%)   | 0        | 100         | 100 |
| 23  | P     | 110/113 (97%) | 99 (90%)  | 11 (10%) | 0        | 100         | 100 |
| 24  | Q     | 122/129 (95%) | 121 (99%) | 1 (1%)   | 0        | 100         | 100 |
| 25  | R     | 98/104 (94%)  | 91 (93%)  | 6 (6%)   | 1 (1%)   | 15          | 44  |
| 26  | S     | 111/197 (56%) | 108 (97%) | 3 (3%)   | 0        | 100         | 100 |
| 27  | T     | 93/100 (93%)  | 89 (96%)  | 4 (4%)   | 0        | 100         | 100 |
| 28  | U     | 86/105 (82%)  | 75 (87%)  | 11 (13%) | 0        | 100         | 100 |
| 29  | V     | 175/215 (81%) | 154 (88%) | 19 (11%) | 2 (1%)   | 14          | 41  |
| 30  | W     | 72/86 (84%)   | 63 (88%)  | 9 (12%)  | 0        | 100         | 100 |
| 31  | X     | 60/64 (94%)   | 58 (97%)  | 2 (3%)   | 0        | 100         | 100 |
| 32  | Y     | 66/77 (86%)   | 63 (96%)  | 3 (4%)   | 0        | 100         | 100 |
| 33  | Z     | 57/65 (88%)   | 55 (96%)  | 2 (4%)   | 0        | 100         | 100 |
| 35  | c     | 205/274 (75%) | 189 (92%) | 16 (8%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 36  | d     | 198/201 (98%)   | 177 (89%)  | 21 (11%) | 0        | 100         | 100 |
| 37  | e     | 167/220 (76%)   | 153 (92%)  | 14 (8%)  | 0        | 100         | 100 |
| 38  | f     | 93/96 (97%)     | 90 (97%)   | 3 (3%)   | 0        | 100         | 100 |
| 39  | g     | 153/156 (98%)   | 150 (98%)  | 3 (2%)   | 0        | 100         | 100 |
| 40  | h     | 129/132 (98%)   | 121 (94%)  | 8 (6%)   | 0        | 100         | 100 |
| 41  | i     | 125/151 (83%)   | 110 (88%)  | 15 (12%) | 0        | 100         | 100 |
| 42  | j     | 97/101 (96%)    | 88 (91%)   | 9 (9%)   | 0        | 100         | 100 |
| 43  | k     | 115/139 (83%)   | 107 (93%)  | 8 (7%)   | 0        | 100         | 100 |
| 44  | l     | 120/124 (97%)   | 95 (79%)   | 23 (19%) | 2 (2%)   | 9           | 29  |
| 45  | m     | 114/124 (92%)   | 104 (91%)  | 10 (9%)  | 0        | 100         | 100 |
| 46  | n     | 58/61 (95%)     | 55 (95%)   | 2 (3%)   | 1 (2%)   | 9           | 29  |
| 47  | o     | 85/89 (96%)     | 80 (94%)   | 4 (5%)   | 1 (1%)   | 13          | 39  |
| 48  | p     | 111/162 (68%)   | 99 (89%)   | 11 (10%) | 1 (1%)   | 17          | 46  |
| 49  | q     | 93/135 (69%)    | 78 (84%)   | 15 (16%) | 0        | 100         | 100 |
| 50  | r     | 62/84 (74%)     | 58 (94%)   | 4 (6%)   | 0        | 100         | 100 |
| 51  | s     | 81/93 (87%)     | 73 (90%)   | 8 (10%)  | 0        | 100         | 100 |
| 52  | t     | 83/86 (96%)     | 82 (99%)   | 1 (1%)   | 0        | 100         | 100 |
| 53  | x     | 549/558 (98%)   | 511 (93%)  | 38 (7%)  | 0        | 100         | 100 |
| All | All   | 6072/6981 (87%) | 5651 (93%) | 411 (7%) | 10 (0%)  | 50          | 78  |

5 of 10 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 14  | F     | 143 | ALA  |
| 14  | F     | 144 | VAL  |
| 25  | R     | 51  | THR  |
| 44  | l     | 114 | ARG  |
| 46  | n     | 17  | ALA  |

### 5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 1   | 0     | 44/47 (94%)    | 44 (100%)  | 0        | 100         | 100 |
| 2   | 1     | 45/51 (88%)    | 45 (100%)  | 0        | 100         | 100 |
| 3   | 2     | 38/40 (95%)    | 37 (97%)   | 1 (3%)   | 46          | 79  |
| 4   | 3     | 53/54 (98%)    | 53 (100%)  | 0        | 100         | 100 |
| 5   | 4     | 35/35 (100%)   | 34 (97%)   | 1 (3%)   | 42          | 76  |
| 6   | 6     | 49/66 (74%)    | 49 (100%)  | 0        | 100         | 100 |
| 7   | 7     | 18/20 (90%)    | 18 (100%)  | 0        | 100         | 100 |
| 8   | 8     | 175/179 (98%)  | 173 (99%)  | 2 (1%)   | 73          | 92  |
| 11  | C     | 212/219 (97%)  | 211 (100%) | 1 (0%)   | 88          | 96  |
| 12  | D     | 163/166 (98%)  | 163 (100%) | 0        | 100         | 100 |
| 13  | E     | 159/172 (92%)  | 156 (98%)  | 3 (2%)   | 57          | 85  |
| 14  | F     | 147/155 (95%)  | 145 (99%)  | 2 (1%)   | 67          | 90  |
| 15  | G     | 143/147 (97%)  | 142 (99%)  | 1 (1%)   | 84          | 95  |
| 16  | H     | 36/121 (30%)   | 35 (97%)   | 1 (3%)   | 43          | 77  |
| 17  | J     | 120/161 (74%)  | 120 (100%) | 0        | 100         | 100 |
| 18  | K     | 101/101 (100%) | 99 (98%)   | 2 (2%)   | 55          | 84  |
| 19  | L     | 108/110 (98%)  | 107 (99%)  | 1 (1%)   | 78          | 94  |
| 20  | M     | 110/114 (96%)  | 109 (99%)  | 1 (1%)   | 78          | 94  |
| 21  | N     | 94/139 (68%)   | 93 (99%)   | 1 (1%)   | 73          | 92  |
| 22  | O     | 91/93 (98%)    | 91 (100%)  | 0        | 100         | 100 |
| 23  | P     | 98/99 (99%)    | 98 (100%)  | 0        | 100         | 100 |
| 24  | Q     | 97/99 (98%)    | 97 (100%)  | 0        | 100         | 100 |
| 25  | R     | 81/83 (98%)    | 81 (100%)  | 0        | 100         | 100 |
| 26  | S     | 87/140 (62%)   | 85 (98%)   | 2 (2%)   | 50          | 82  |
| 27  | T     | 81/83 (98%)    | 80 (99%)   | 1 (1%)   | 71          | 92  |
| 28  | U     | 77/88 (88%)    | 76 (99%)   | 1 (1%)   | 69          | 91  |
| 29  | V     | 142/164 (87%)  | 141 (99%)  | 1 (1%)   | 84          | 95  |
| 30  | W     | 54/62 (87%)    | 53 (98%)   | 1 (2%)   | 57          | 85  |
| 31  | X     | 51/52 (98%)    | 50 (98%)   | 1 (2%)   | 55          | 84  |
| 32  | Y     | 60/66 (91%)    | 60 (100%)  | 0        | 100         | 100 |
| 33  | Z     | 51/55 (93%)    | 49 (96%)   | 2 (4%)   | 32          | 66  |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 35  | c     | 170/210 (81%)   | 168 (99%)  | 2 (1%)   | 71          | 92  |
| 36  | d     | 176/177 (99%)   | 176 (100%) | 0        | 100         | 100 |
| 37  | e     | 121/159 (76%)   | 119 (98%)  | 2 (2%)   | 60          | 87  |
| 38  | f     | 84/85 (99%)     | 84 (100%)  | 0        | 100         | 100 |
| 39  | g     | 130/131 (99%)   | 129 (99%)  | 1 (1%)   | 81          | 94  |
| 40  | h     | 107/108 (99%)   | 106 (99%)  | 1 (1%)   | 78          | 94  |
| 41  | i     | 102/120 (85%)   | 100 (98%)  | 2 (2%)   | 55          | 84  |
| 42  | j     | 89/90 (99%)     | 89 (100%)  | 0        | 100         | 100 |
| 43  | k     | 90/107 (84%)    | 89 (99%)   | 1 (1%)   | 73          | 92  |
| 44  | l     | 104/105 (99%)   | 101 (97%)  | 3 (3%)   | 42          | 76  |
| 45  | m     | 99/104 (95%)    | 98 (99%)   | 1 (1%)   | 76          | 93  |
| 46  | n     | 46/47 (98%)     | 46 (100%)  | 0        | 100         | 100 |
| 47  | o     | 77/79 (98%)     | 77 (100%)  | 0        | 100         | 100 |
| 48  | p     | 90/125 (72%)    | 89 (99%)   | 1 (1%)   | 73          | 92  |
| 49  | q     | 85/105 (81%)    | 83 (98%)   | 2 (2%)   | 49          | 81  |
| 50  | r     | 54/72 (75%)     | 52 (96%)   | 2 (4%)   | 34          | 68  |
| 51  | s     | 75/85 (88%)     | 75 (100%)  | 0        | 100         | 100 |
| 52  | t     | 64/65 (98%)     | 62 (97%)   | 2 (3%)   | 40          | 74  |
| 53  | x     | 455/460 (99%)   | 452 (99%)  | 3 (1%)   | 84          | 95  |
| All | All   | 5038/5615 (90%) | 4989 (99%) | 49 (1%)  | 77          | 93  |

5 of 49 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 37  | e     | 163 | ASN  |
| 44  | l     | 20  | LYS  |
| 37  | e     | 202 | LYS  |
| 41  | i     | 70  | LYS  |
| 44  | l     | 108 | LYS  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 24  | Q     | 122 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 29  | V     | 124 | GLN  |
| 53  | x     | 40  | ASN  |
| 29  | V     | 44  | HIS  |
| 36  | d     | 115 | HIS  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 10  | B     | 113/115 (98%)   | 10 (8%)           | 0               |
| 34  | a     | 1515/1537 (98%) | 231 (15%)         | 0               |
| 54  | y     | 76/77 (98%)     | 18 (23%)          | 0               |
| 55  | z     | 6/26 (23%)      | 4 (66%)           | 0               |
| 9   | A     | 3116/3138 (99%) | 460 (14%)         | 5 (0%)          |
| All | All   | 4826/4893 (98%) | 723 (14%)         | 5 (0%)          |

5 of 723 RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9   | A     | 14  | A    |
| 9   | A     | 15  | G    |
| 9   | A     | 62  | G    |
| 9   | A     | 63  | A    |
| 9   | A     | 71  | A    |

All (5) RNA pucker outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 9   | A     | 913  | G    |
| 9   | A     | 2177 | 5MU  |
| 9   | A     | 2355 | U    |
| 9   | A     | 2384 | A    |
| 9   | A     | 3127 | A    |

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 9   | 5MU  | A     | 2177 | 9    | 19,22,23     | 4.55 | 7 (36%)  | 28,32,35    | 3.75 | 9 (32%)  |
| 34  | 5MC  | a     | 960  | 34   | 18,22,23     | 3.38 | 7 (38%)  | 26,32,35    | 1.20 | 2 (7%)   |
| 34  | 4OC  | a     | 1395 | 34   | 20,23,24     | 2.80 | 8 (40%)  | 26,32,35    | 0.97 | 3 (11%)  |
| 34  | MA6  | a     | 1511 | 34   | 18,26,27     | 1.03 | 2 (11%)  | 19,38,41    | 3.29 | 2 (10%)  |
| 9   | OMG  | A     | 2791 | 9    | 18,26,27     | 2.37 | 8 (44%)  | 19,38,41    | 1.52 | 4 (21%)  |
| 34  | UR3  | a     | 1491 | 34   | 19,22,23     | 2.56 | 7 (36%)  | 26,32,35    | 1.19 | 3 (11%)  |
| 34  | 2MG  | a     | 959  | 34   | 18,26,27     | 2.37 | 7 (38%)  | 16,38,41    | 1.40 | 4 (25%)  |
| 34  | MA6  | a     | 1512 | 34   | 18,26,27     | 1.10 | 1 (5%)   | 19,38,41    | 3.39 | 2 (10%)  |
| 34  | G7M  | a     | 518  | 34   | 20,26,27     | 3.88 | 10 (50%) | 17,39,42    | 1.12 | 1 (5%)   |

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   |
|-----|------|-------|------|------|---------|-----------|---------|
| 9   | 5MU  | A     | 2177 | 9    | -       | 1/7/25/26 | 0/2/2/2 |
| 34  | 5MC  | a     | 960  | 34   | -       | 1/7/25/26 | 0/2/2/2 |
| 34  | 4OC  | a     | 1395 | 34   | -       | 2/9/29/30 | 0/2/2/2 |
| 34  | MA6  | a     | 1511 | 34   | -       | 1/7/29/30 | 0/3/3/3 |
| 9   | OMG  | A     | 2791 | 9    | -       | 2/5/27/28 | 0/3/3/3 |
| 34  | UR3  | a     | 1491 | 34   | -       | 2/7/25/26 | 0/2/2/2 |
| 34  | 2MG  | a     | 959  | 34   | -       | 0/5/27/28 | 0/3/3/3 |
| 34  | MA6  | a     | 1512 | 34   | -       | 2/7/29/30 | 0/3/3/3 |
| 34  | G7M  | a     | 518  | 34   | -       | 1/3/25/26 | 0/3/3/3 |

The worst 5 of 57 bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 9   | A     | 2177 | 5MU  | C6-N1 | 10.06 | 1.55        | 1.38     |
| 34  | a     | 518  | G7M  | C8-N7 | 9.69  | 1.50        | 1.33     |
| 9   | A     | 2177 | 5MU  | C2-N1 | 9.51  | 1.53        | 1.38     |
| 34  | a     | 518  | G7M  | C8-N9 | 9.43  | 1.50        | 1.33     |
| 9   | A     | 2177 | 5MU  | C4-C5 | 8.87  | 1.59        | 1.44     |

The worst 5 of 30 bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms    | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 34  | a     | 1512 | MA6  | N1-C6-N6 | -13.36 | 103.00      | 117.06   |
| 34  | a     | 1511 | MA6  | N1-C6-N6 | -12.89 | 103.49      | 117.06   |
| 9   | A     | 2177 | 5MU  | C5-C4-N3 | 12.42  | 125.91      | 115.31   |
| 9   | A     | 2177 | 5MU  | C5-C6-N1 | -10.16 | 112.88      | 123.34   |
| 34  | a     | 1512 | MA6  | N3-C2-N1 | -5.82  | 119.58      | 128.68   |

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 34  | a     | 1512 | MA6  | O4'-C4'-C5'-O5' |
| 34  | a     | 1512 | MA6  | C3'-C4'-C5'-O5' |
| 34  | a     | 1395 | 4OC  | O4'-C4'-C5'-O5' |
| 9   | A     | 2791 | OMG  | O4'-C4'-C5'-O5' |
| 9   | A     | 2791 | OMG  | C3'-C4'-C5'-O5' |

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 456 ligands modelled in this entry, 451 are monoatomic - leaving 5 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link  | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|-------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |       | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 58  | ADP  | x     | 603 | 57    | 24,29,29     | 0.92 | 1 (4%)      | 29,45,45    | 1.58 | 4 (13%)     |
| 59  | VO4  | x     | 604 | 53,57 | 1,4,4        | 4.73 | 1 (100%)    | -           |      |             |
| 60  | FME  | y     | 101 | 54    | 8,9,10       | 1.00 | 0           | 7,9,11      | 1.23 | 1 (14%)     |
| 59  | VO4  | x     | 602 | 57    | 1,4,4        | 4.77 | 1 (100%)    | -           |      |             |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 58  | ADP  | x     | 601 | 57   | 24,29,29     | 0.95 | 1 (4%)   | 29,45,45    | 1.66 | 5 (17%)  |

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   |
|-----|------|-------|-----|------|---------|------------|---------|
| 58  | ADP  | x     | 601 | 57   | -       | 2/12/32/32 | 0/3/3/3 |
| 58  | ADP  | x     | 603 | 57   | -       | 2/12/32/32 | 0/3/3/3 |
| 60  | FME  | y     | 101 | 54   | -       | 1/7/9/11   | -       |

All (4) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 59  | x     | 602 | VO4  | O1-V  | 4.77 | 1.90        | 1.63     |
| 59  | x     | 604 | VO4  | O1-V  | 4.73 | 1.90        | 1.63     |
| 58  | x     | 603 | ADP  | C5-C4 | 2.31 | 1.47        | 1.40     |
| 58  | x     | 601 | ADP  | C5-C4 | 2.28 | 1.47        | 1.40     |

The worst 5 of 10 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 58  | x     | 601 | ADP  | PA-O3A-PB   | -4.77 | 116.47      | 132.83   |
| 58  | x     | 603 | ADP  | PA-O3A-PB   | -4.74 | 116.55      | 132.83   |
| 58  | x     | 601 | ADP  | C3'-C2'-C1' | 3.55  | 106.33      | 100.98   |
| 58  | x     | 603 | ADP  | N3-C2-N1    | -3.17 | 123.73      | 128.68   |
| 58  | x     | 601 | ADP  | N3-C2-N1    | -2.99 | 124.00      | 128.68   |

There are no chirality outliers.

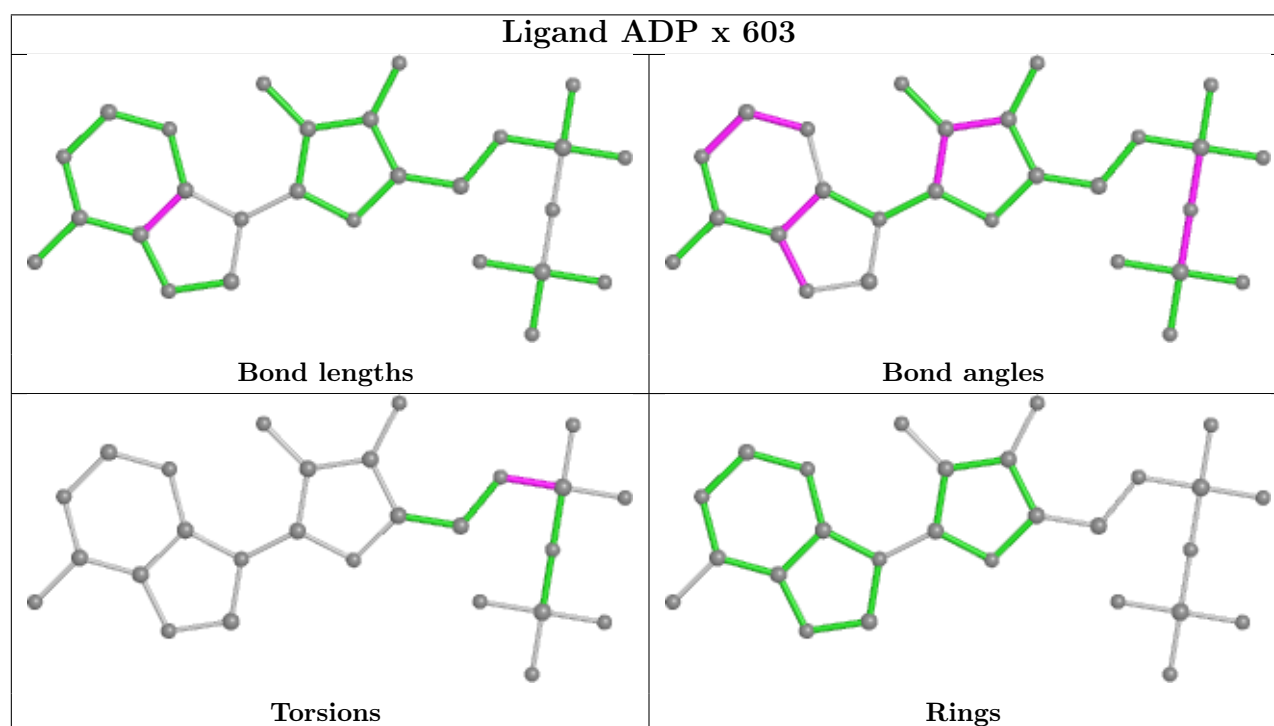
All (5) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 58  | x     | 601 | ADP  | O4'-C4'-C5'-O5' |
| 58  | x     | 603 | ADP  | C5'-O5'-PA-O3A  |
| 58  | x     | 601 | ADP  | C3'-C4'-C5'-O5' |
| 60  | y     | 101 | FME  | CB-CG-SD-CE     |
| 58  | x     | 603 | ADP  | C5'-O5'-PA-O2A  |

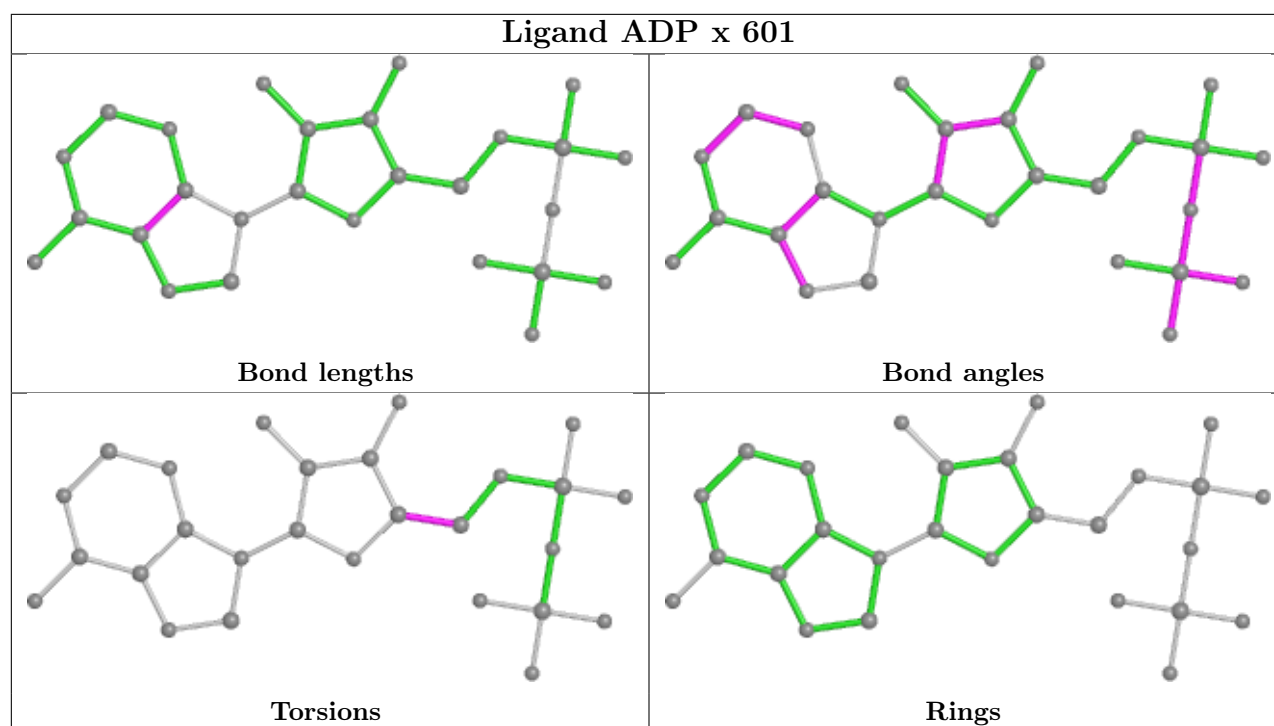
There are no ring outliers.

No monomer is involved in short contacts.

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







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 10  | B     | 1                |
| 11  | C     | 1                |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | B     | 76:U      | O3'    | 77:A      | P      | 3.18         |
| 1     | C     | 226:MET   | C      | 227:ASN   | N      | 1.16         |

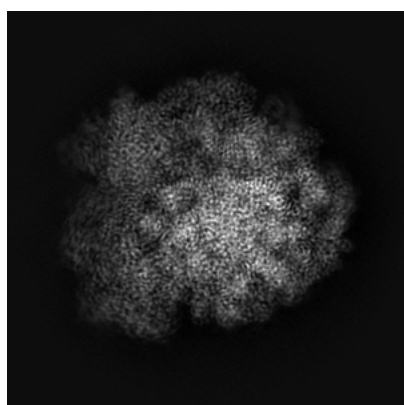
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23969. These allow visual inspection of the internal detail of the map and identification of artifacts.

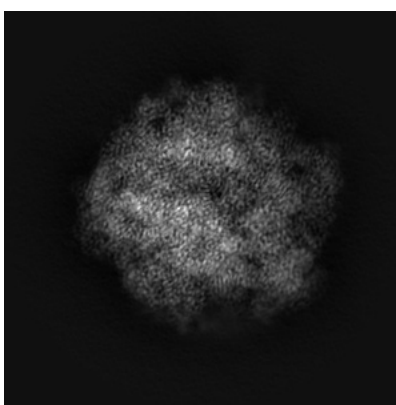
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

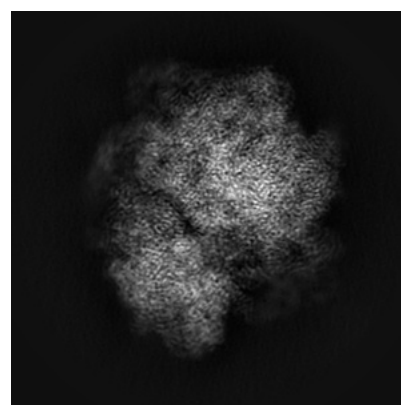
#### 6.1.1 Primary map



X



Y

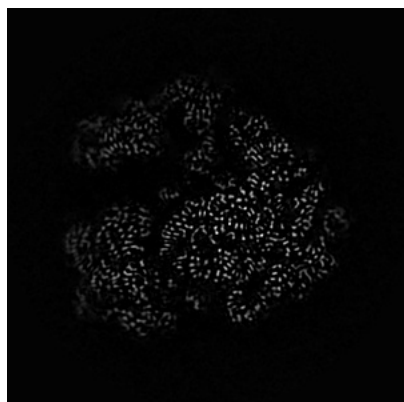


Z

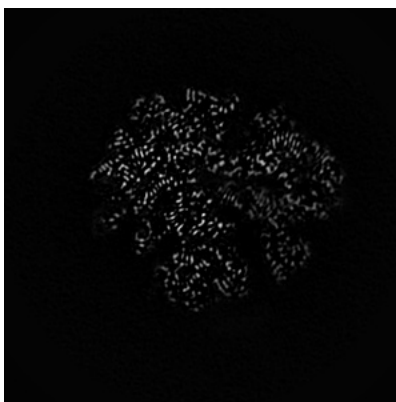
The images above show the map projected in three orthogonal directions.

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

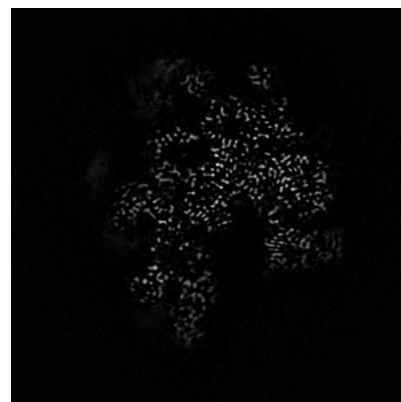
#### 6.2.1 Primary map



X Index: 160



Y Index: 160

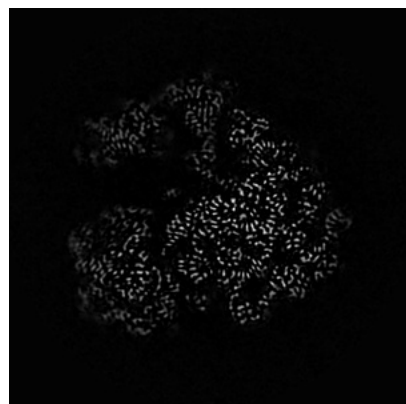


Z Index: 160

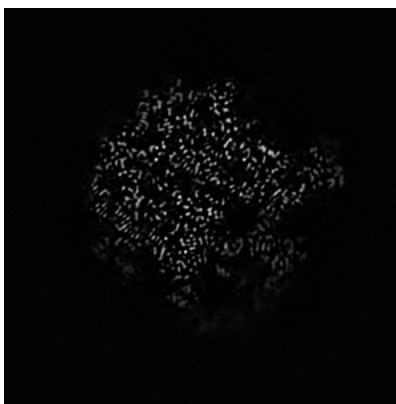
The images above show central slices of the map in three orthogonal directions.

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

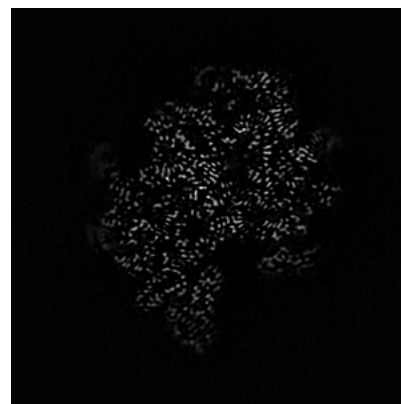
### 6.3.1 Primary map



X Index: 162



Y Index: 183

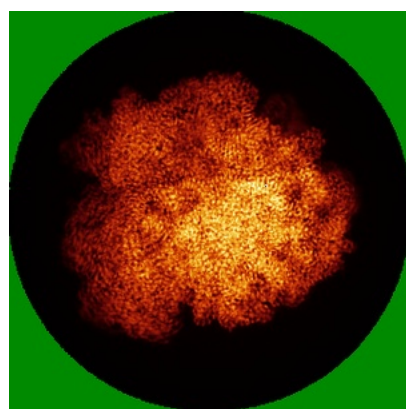


Z Index: 145

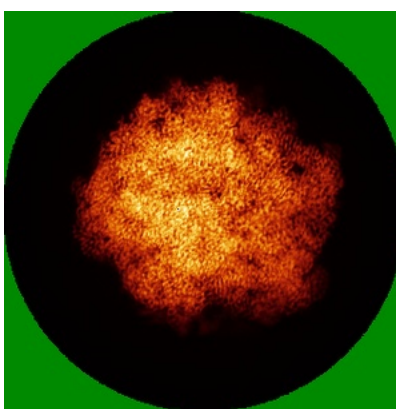
The images above show the largest variance slices of the map in three orthogonal directions.

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

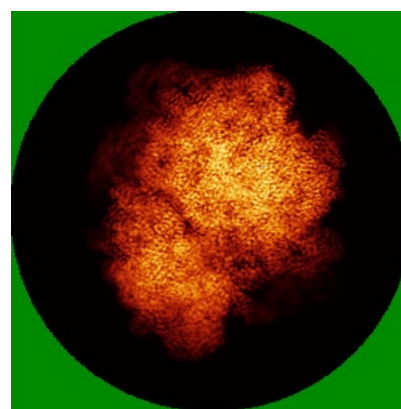
### 6.4.1 Primary map



X



Y

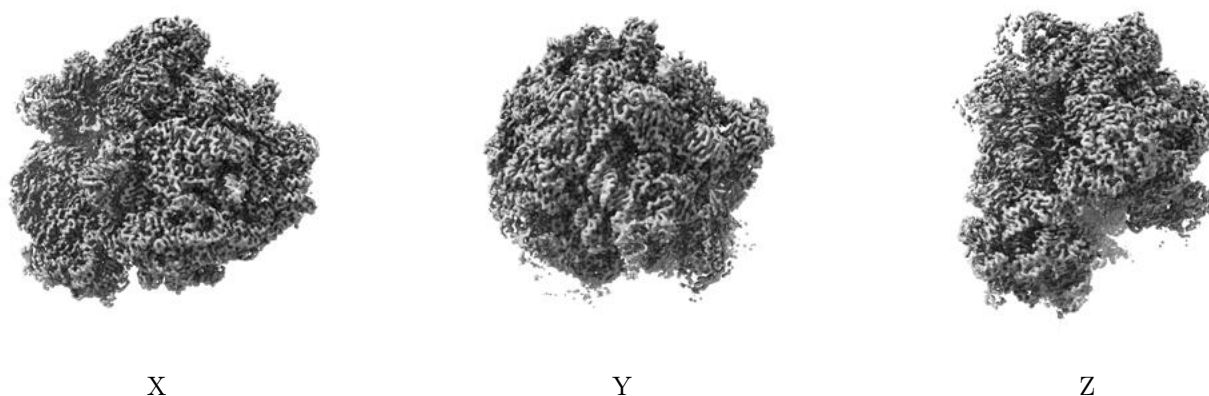


Z

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

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

### 6.5.1 Primary map



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

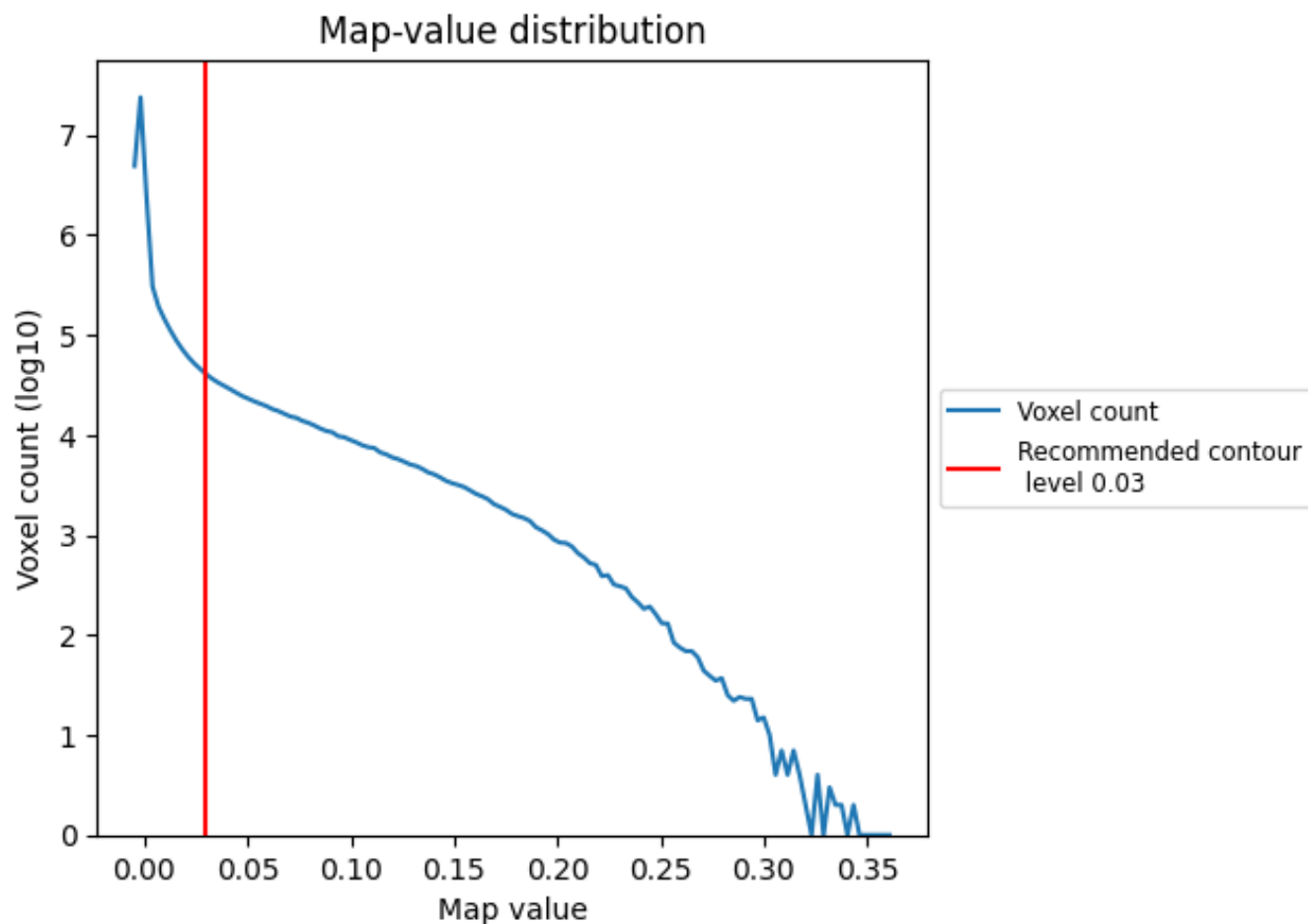
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

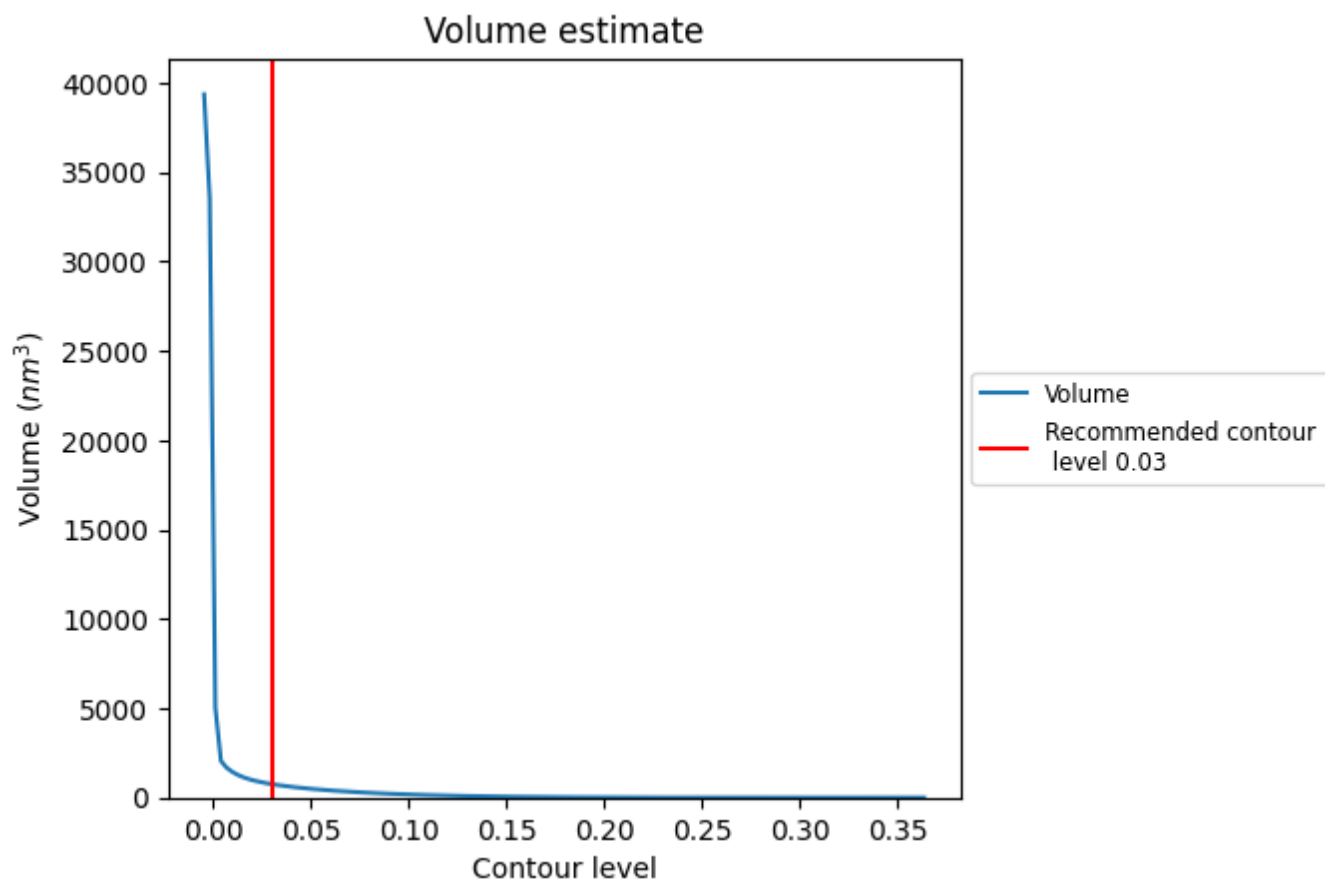
This section contains the results of statistical analysis of the map.

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



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

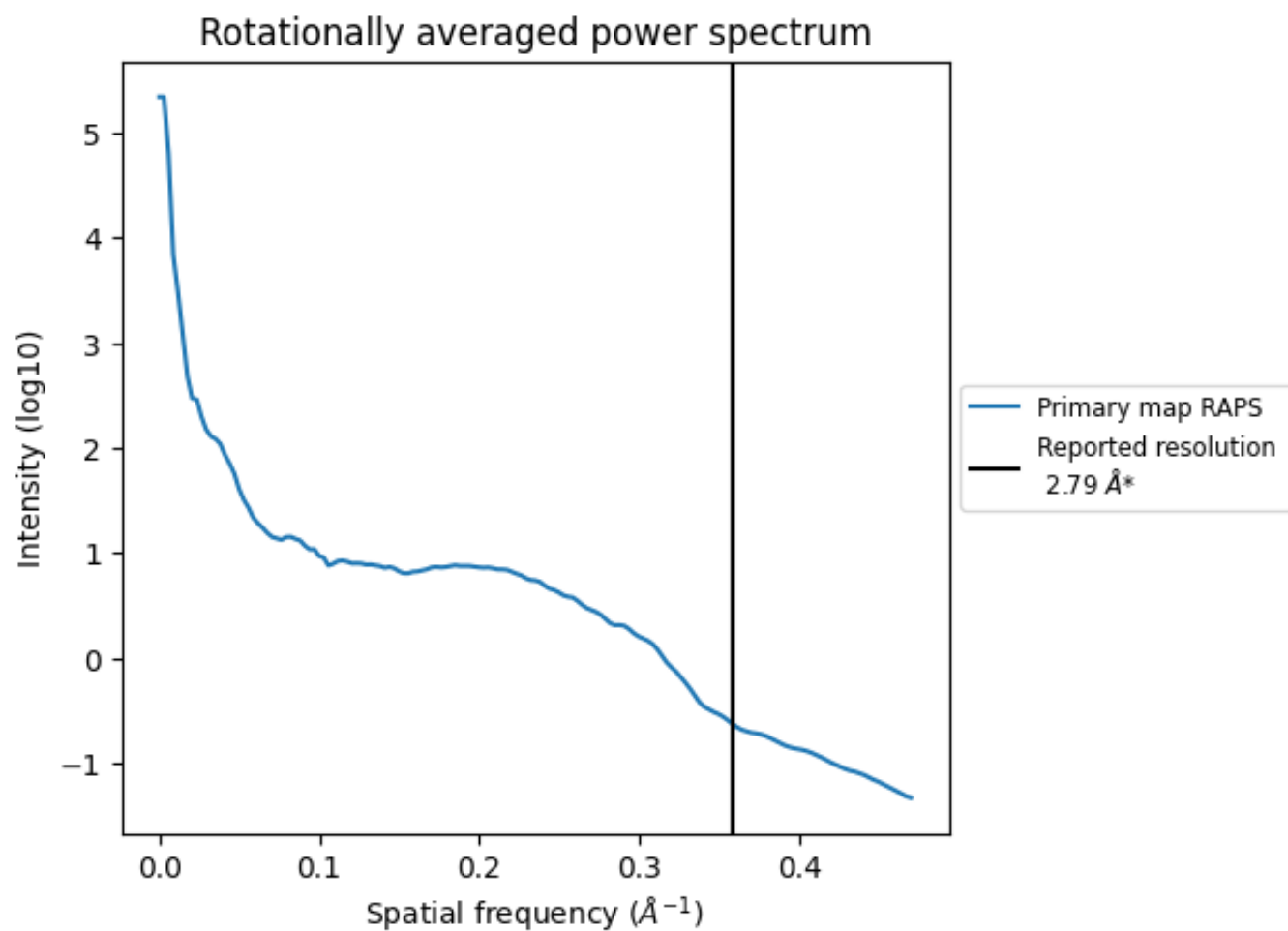
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 751  $\text{nm}^3$ ; this corresponds to an approximate mass of 678 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 ⓘ

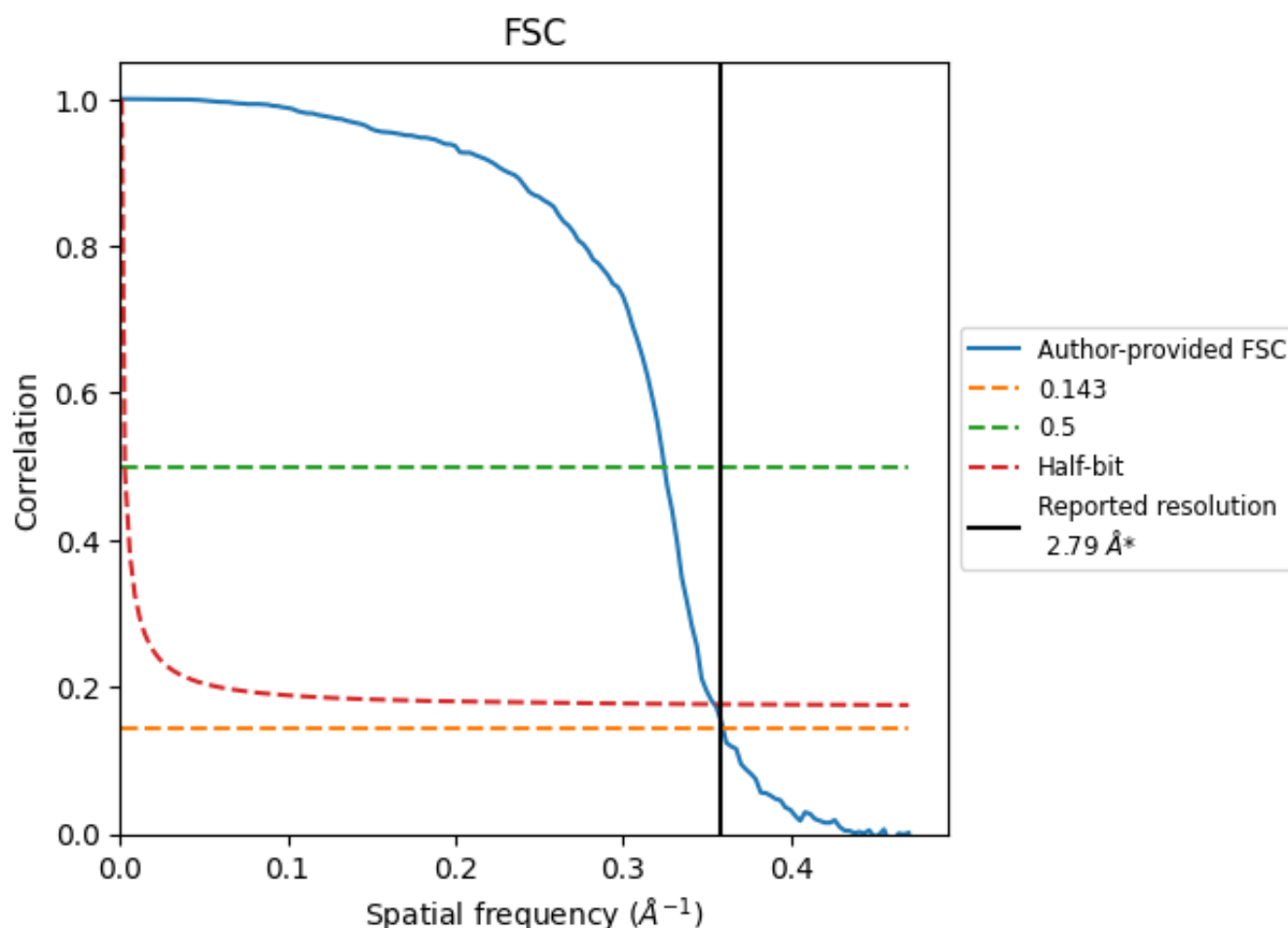


\*Reported resolution corresponds to spatial frequency of 0.358  $\text{\AA}^{-1}$

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.358 Å<sup>-1</sup>



## 8.2 Resolution estimates [i](#)

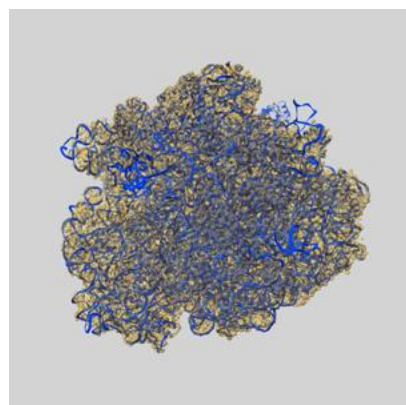
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 2.79                               | -    | -        |
| Author-provided FSC curve | 2.78                               | 3.08 | 2.82     |
| Unmasked-calculated*      | -                                  | -    | -        |

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

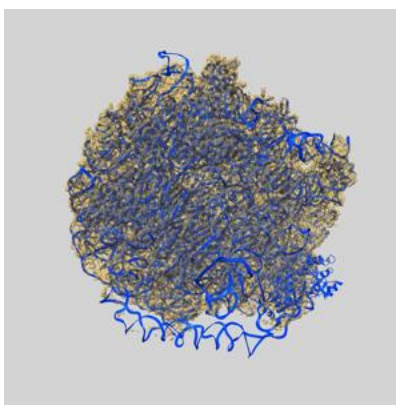
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-23969 and PDB model 7MSM. Per-residue inclusion information can be found in section [3](#) on page [16](#).

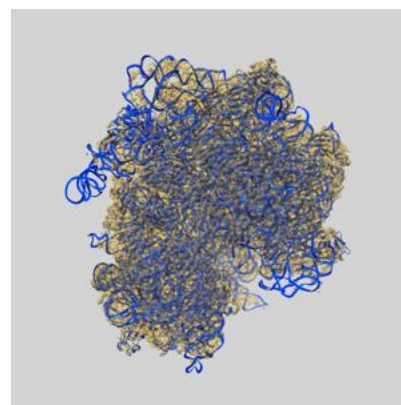
### 9.1 Map-model overlay [i](#)



X



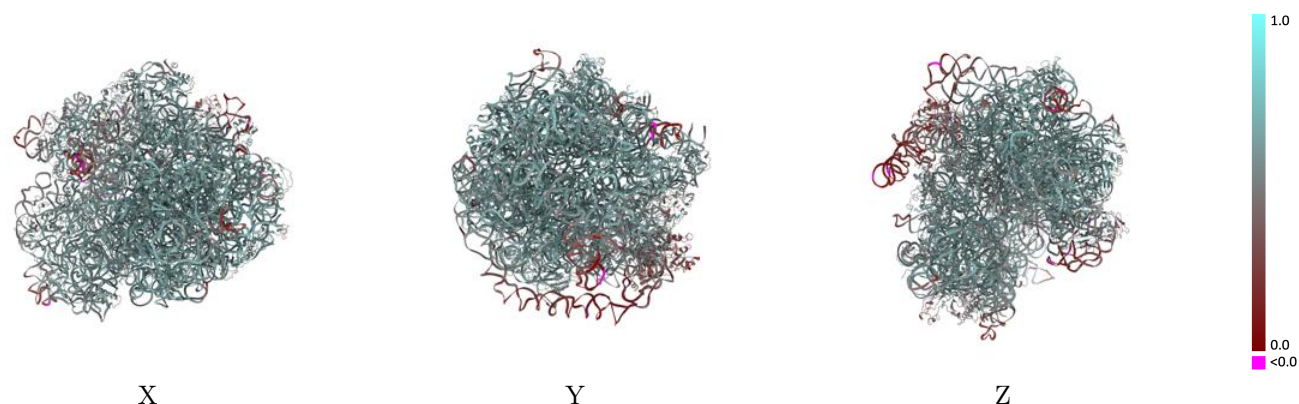
Y



Z

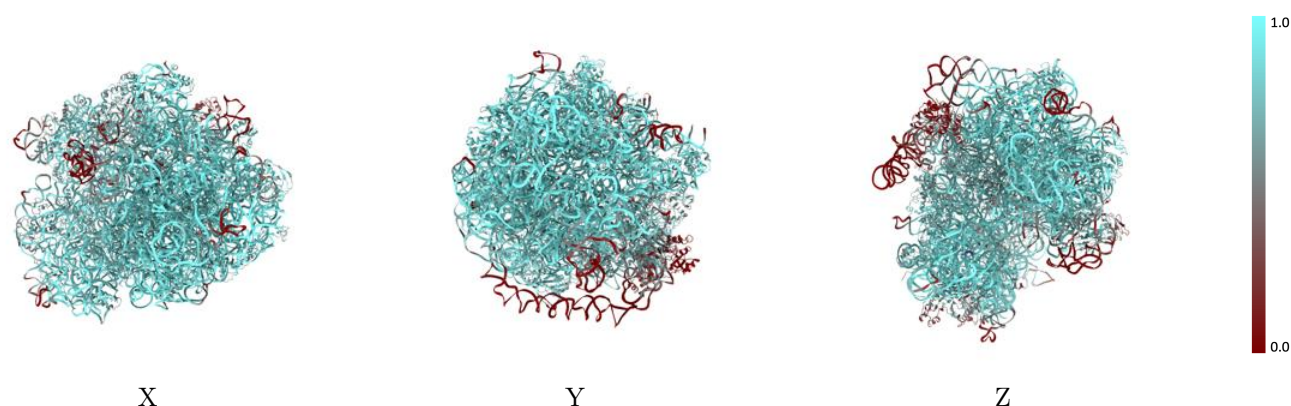
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



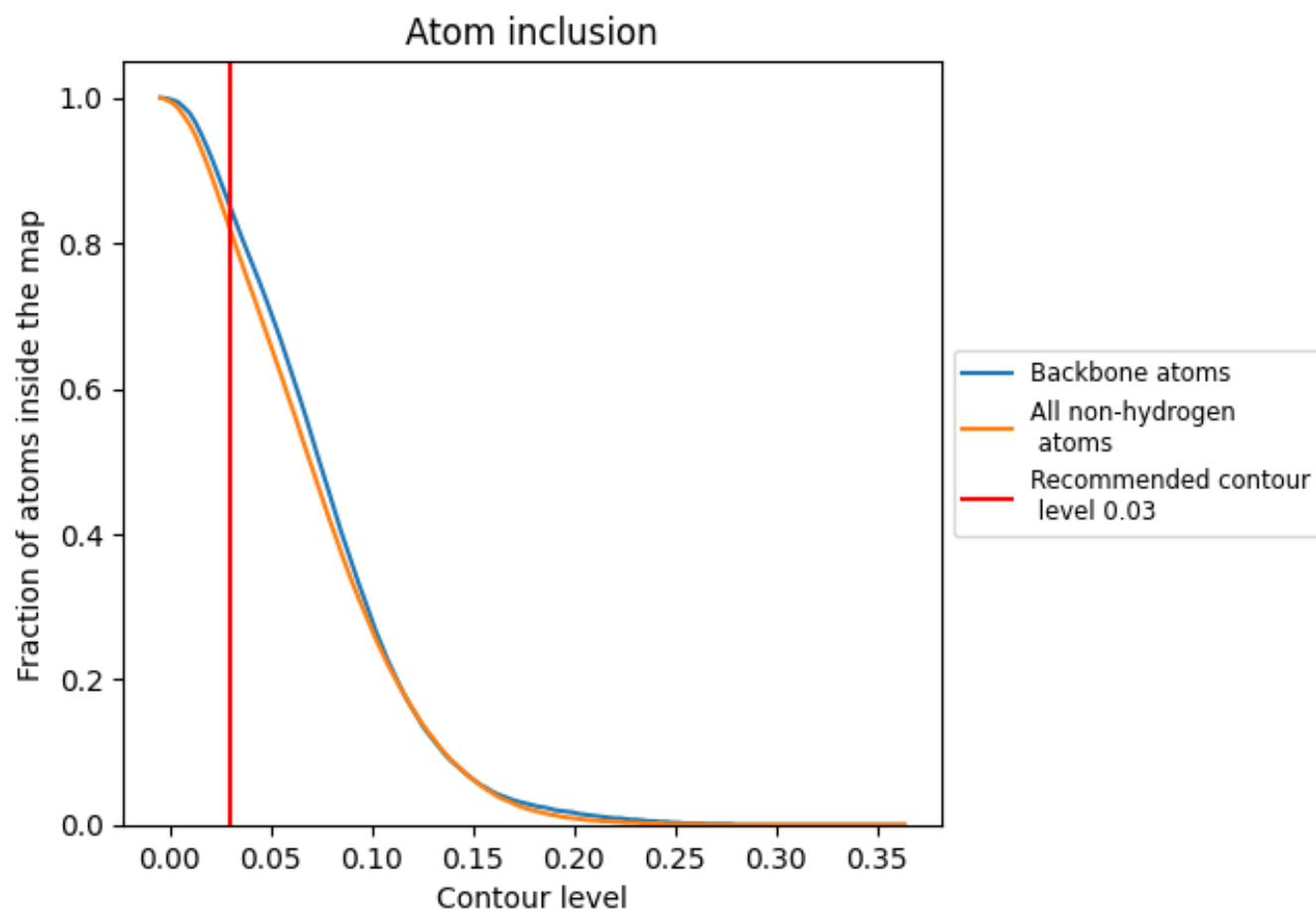
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 85% of all backbone atoms, 82% 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   |  0.8160   |  0.5610   |
| 0     |  0.8270   |  0.5960   |
| 1     |  0.8380   |  0.5820   |
| 2     |  0.9130   |  0.6210   |
| 3     |  0.8920   |  0.6260   |
| 4     |  0.8190   |  0.5980   |
| 6     |  0.6910   |  0.4870   |
| 7     |  0.3600   |  0.5600   |
| 8     |  0.1840   |  0.3420   |
| A     |  0.8430   |  0.5690   |
| B     |  0.8790   |  0.5690   |
| C     |  0.8750   |  0.6140   |
| D     |  0.8500   |  0.5880   |
| E     |  0.8560   |  0.5890   |
| F     |  0.6910  |  0.5120  |
| G     |  0.5870 |  0.4840 |
| H     |  0.3470 |  0.4670 |
| J     |  0.8520 |  0.5950 |
| K     |  0.8570 |  0.5920 |
| L     |  0.8370 |  0.5900 |
| M     |  0.7990 |  0.5810 |
| N     |  0.8710 |  0.6020 |
| O     |  0.8000 |  0.5690 |
| P     |  0.8290 |  0.5800 |
| Q     |  0.8840 |  0.6090 |
| R     |  0.8410 |  0.5900 |
| S     |  0.8770 |  0.5970 |
| T     |  0.8070 |  0.5640 |
| U     |  0.7870 |  0.5450 |
| V     |  0.5300 |  0.4760 |
| W     |  0.8680 |  0.5790 |
| X     |  0.8880 |  0.6000 |
| Y     |  0.7580 |  0.5390 |
| Z     |  0.8480 |  0.5850 |
| a     |  0.8840 |  0.5740 |



*Continued on next page...*

*Continued from previous page...*

| Chain | Atom inclusion   | Q-score  |
|-------|--|--|
| c     |  0.6650   |  0.5010   |
| d     |  0.6000   |  0.4660   |
| e     |  0.7580   |  0.5530   |
| f     |  0.7220   |  0.5430   |
| g     |  0.7440   |  0.5440   |
| h     |  0.8020   |  0.5630   |
| i     |  0.7100   |  0.5190   |
| j     |  0.5550   |  0.4460   |
| k     |  0.7560   |  0.5450   |
| l     |  0.7460   |  0.5210   |
| m     |  0.7060   |  0.5240   |
| n     |  0.8290   |  0.5700   |
| o     |  0.7810   |  0.5540   |
| p     |  0.6790   |  0.5100   |
| q     |  0.7350   |  0.5190   |
| r     |  0.7640   |  0.5470   |
| s     |  0.7110   |  0.5310   |
| t     |  0.7320  |  0.5400  |
| x     |  0.6020 |  0.4980 |
| y     |  0.8440 |  0.5730 |
| z     |  0.7520 |  0.5010 |