



## wwPDB EM Validation Summary Report ⓘ

Jun 18, 2026 – 10:59 am BST

PDB ID : 9FSF / pdb\_00009fsf  
EMDB ID : EMD-50727  
Title : Cryo-EM structure of *Saccharolobus solfataricus* 30S initiation complex bound to Ss-MAP leaderless mRNA with h44 in up position  
Authors : Bourgeois, G.; Coureux, P.D.; Mechulam, Y.; Schmitt, E.  
Deposited on : 2024-06-21  
Resolution : 2.80 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.dev132  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

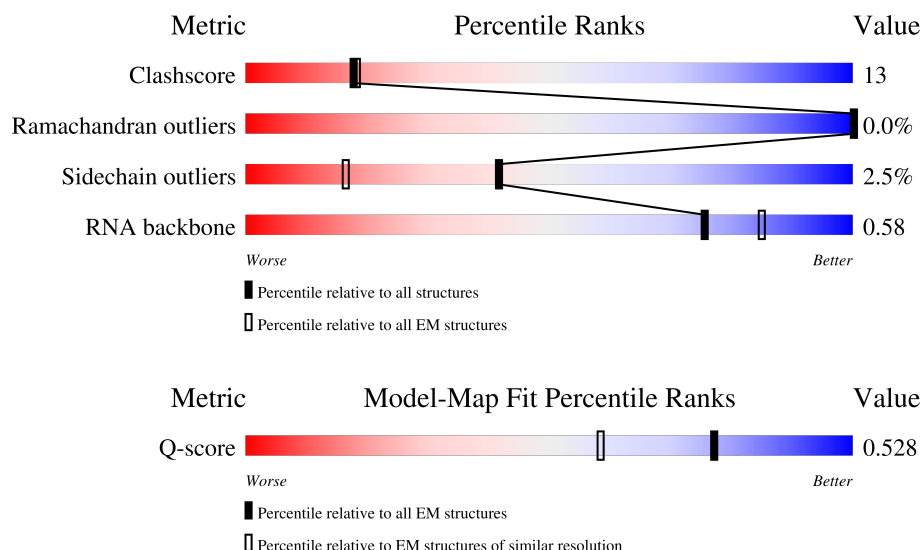
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.80 Å.

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



| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| RNA backbone          | 8273                        | 3508                        | -                                                        |
| Q-score               | -                           | 25397                       | 11806 ( 2.30 - 3.30 )                                    |

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   | 2     | 1497   |                  |
| 2   | A     | 208    |                  |
| 3   | B     | 231    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 4   | C     | 65     |                  |
| 5   | D     | 181    |                  |
| 6   | E     | 239    |                  |
| 7   | F     | 214    |                  |
| 8   | G     | 214    |                  |
| 9   | H     | 193    |                  |
| 10  | I     | 133    |                  |
| 11  | J     | 133    |                  |
| 12  | K     | 137    |                  |
| 13  | L     | 102    |                  |
| 14  | M     | 132    |                  |
| 15  | N     | 147    |                  |
| 16  | O     | 165    |                  |
| 17  | Q     | 152    |                  |
| 18  | R     | 114    |                  |
| 19  | S     | 79     |                  |
| 20  | T     | 140    |                  |
| 21  | U     | 158    |                  |
| 22  | V     | 120    |                  |
| 23  | W     | 66     |                  |
| 24  | X     | 83     |                  |
| 25  | Y     | 75     |                  |
| 26  | Z     | 229    |                  |
| 27  | 3     | 127    |                  |
| 28  | c     | 110    |                  |

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| Mol | Chain | Length | Quality of chain                                |
|-----|-------|--------|-------------------------------------------------|
| 29  | d     | 72     | <div><div></div><div>36%57%. .</div></div>      |
| 30  | e     | 52     | <div><div></div><div>60%23%17%</div></div>      |
| 31  | 5     | 14     | <div><div></div><div>14%21%57%14%7%</div></div> |
| 32  | 4     | 77     | <div><div></div><div>9%36%55%9%</div></div>     |
| 33  | s     | 15     | <div><div></div><div>20%47%33%</div></div>      |
| 34  | a     | 72     | <div><div></div><div>47%43%8%. .</div></div>    |
| 35  | P     | 54     | <div><div></div><div>63%33%. .</div></div>      |

## 2 Entry composition

There are 40 unique types of molecules in this entry. The entry contains 65754 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called rRNA 16S.

| Mol | Chain | Residues | Atoms |       |      |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|-------|
| 1   | 2     | 1451     | Total | C     | N    | O     | P    | 0       | 0     |
|     |       |          | 31215 | 13922 | 5773 | 10069 | 1451 |         |       |

There are 7 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment          | Reference     |
|-------|---------|----------|--------|------------------|---------------|
| 2     | 843     | 4AC      | C      | modified residue | GB AE006641.1 |
| 2     | 930     | C4J      | U      | modified residue | GB AE006641.1 |
| 2     | 1466    | 4AC      | C      | modified residue | GB AE006641.1 |
| 2     | 1467    | 4AC      | C      | modified residue | GB AE006641.1 |
| 2     | 1477    | 4AC      | C      | modified residue | GB AE006641.1 |
| 2     | 1478    | 4AC      | C      | modified residue | GB AE006641.1 |
| 2     | 1496    | C        | A      | conflict         | GB AE006641.1 |

- Molecule 2 is a protein called Small ribosomal subunit protein eS1.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 2   | A     | 186      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1515  | 974 | 261 | 278 | 2 |         |       |

- Molecule 3 is a protein called Small ribosomal subunit protein uS2.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 3   | B     | 215      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1698  | 1092 | 291 | 312 | 3 |         |       |

- Molecule 4 is a protein called Small zinc finger protein HVO-2753-like zinc-binding pocket domain-containing protein.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 4   | C     | 58       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 455   | 282 | 84 | 81 | 8 |         |       |

- Molecule 5 is a protein called Small ribosomal subunit protein uS4.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 5   | D     | 166      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1354  | 864 | 249 | 240 | 1 |         |       |

- Molecule 6 is a protein called Small ribosomal subunit protein eS4.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 6   | E     | 238      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1930  | 1238 | 342 | 344 | 6 |         |       |

- Molecule 7 is a protein called Small ribosomal subunit protein uS5.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 7   | F     | 210      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1625  | 1041 | 275 | 303 | 6 |         |       |

- Molecule 8 is a protein called Small ribosomal subunit protein eS6.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 8   | G     | 213      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1661  | 1052 | 292 | 315 | 2 |         |       |

- Molecule 9 is a protein called Small ribosomal subunit protein uS7.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 9   | H     | 192      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1543  | 983 | 283 | 274 | 3 |         |       |

- Molecule 10 is a protein called Small ribosomal subunit protein uS8.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 10  | I     | 132      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1050  | 675 | 187 | 182 | 6 |         |       |

- Molecule 11 is a protein called Small ribosomal subunit protein eS8.

| Mol | Chain | Residues | Atoms |     |     |     |  | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|-------|
| 11  | J     | 127      | Total | C   | N   | O   |  | 0       | 0     |
|     |       |          | 982   | 617 | 186 | 179 |  |         |       |

- Molecule 12 is a protein called Small ribosomal subunit protein uS9.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 12  | K     | 133      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1068  | 675 | 201 | 185 | 7 |         |       |

- Molecule 13 is a protein called Small ribosomal subunit protein uS10.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 13  | L     | 101      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 840   | 536 | 157 | 142 | 5 |         |       |

- Molecule 14 is a protein called Small ribosomal subunit protein uS11.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 14  | M     | 127      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 944   | 587 | 184 | 170 | 3 |         |       |

- Molecule 15 is a protein called Small ribosomal subunit protein uS12.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 15  | N     | 146      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1140  | 723 | 220 | 193 | 4 |         |       |

- Molecule 16 is a protein called Small ribosomal subunit protein uS13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 16  | O     | 140      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1124  | 708 | 210 | 202 | 4 |         |       |

- Molecule 17 is a protein called Small ribosomal subunit protein uS15.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 17  | Q     | 145      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1185  | 753 | 224 | 205 | 3 |         |       |

- Molecule 18 is a protein called Small ribosomal subunit protein uS17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 18  | R     | 113      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 901   | 570 | 166 | 161 | 4 |         |       |

- Molecule 19 is a protein called Small ribosomal subunit protein eS17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 19  | S     | 66       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 571   | 364 | 101 | 105 | 1 |         |       |

- Molecule 20 is a protein called Small ribosomal subunit protein uS19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 20  | T     | 128      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1064  | 684 | 192 | 184 | 4 |         |       |

- Molecule 21 is a protein called Small ribosomal subunit protein eS19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 21  | U     | 154      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1247  | 805 | 223 | 217 | 2 |         |       |

- Molecule 22 is a protein called Small ribosomal subunit protein eS24.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 22  | V     | 107      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 836   | 524 | 154 | 156 | 2 |         |       |

- Molecule 23 is a protein called Small ribosomal subunit protein eS27.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 23  | W     | 65       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 503   | 319 | 93 | 84 | 7 |         |       |

- Molecule 24 is a protein called Small ribosomal subunit protein eS28.

| Mol | Chain | Residues | Atoms |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---------|-------|
| 24  | X     | 67       | Total | C   | N   | O  | 0       | 0     |
|     |       |          | 535   | 335 | 103 | 97 |         |       |

- Molecule 25 is a protein called Small ribosomal subunit protein eS31.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 25  | Y     | 49       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 395   | 252 | 73 | 65 | 5 |         |       |

- Molecule 26 is a protein called Small ribosomal subunit protein uS3.



| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 26  | Z     | 196      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1561  | 1009 | 274 | 272 | 6 |         |       |

- Molecule 27 is a protein called Large ribosomal subunit protein eL8.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 27  | 3     | 117      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 893   | 567 | 149 | 175 | 2 |         |       |

- Molecule 28 is a protein called Small ribosomal subunit protein eS25.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 28  | c     | 109      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 856   | 539 | 152 | 164 | 1 |         |       |

- Molecule 29 is a protein called VapB-type antitoxin.

| Mol | Chain | Residues | Atoms |     |    |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|---|---------|-------|
| 29  | d     | 69       | Total | C   | N  | O   | S | 0       | 0     |
|     |       |          | 562   | 365 | 91 | 104 | 2 |         |       |

- Molecule 30 is a protein called LSU ribosomal protein S30E (Rps30E).

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 30  | e     | 43       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 354   | 220 | 74 | 60 |         |       |

- Molecule 31 is a RNA chain called mRNA Map.

| Mol | Chain | Residues | Atoms |     |    |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|----|---------|-------|
| 31  | 5     | 13       | Total | C   | N  | O  | P  | 0       | 0     |
|     |       |          | 283   | 126 | 54 | 90 | 13 |         |       |

- Molecule 32 is a RNA chain called tRNA Met initiator.

| Mol | Chain | Residues | Atoms |     |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---|---------|-------|
| 32  | 4     | 77       | Total | C   | N   | O   | P  | S | 0       | 0     |
|     |       |          | 1645  | 734 | 296 | 537 | 77 | 1 |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment             | Reference     |
|-------|---------|----------|--------|---------------------|---------------|
| 4     | 1       | A        | C      | engineered mutation | GB 1334604293 |
| 4     | 72      | U        | A      | engineered mutation | GB 1334604293 |

- Molecule 33 is a RNA chain called mRNA Map.

| Mol | Chain | Residues | Atoms |    |    |    |    | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|----|---------|-------|
| 33  | s     | 10       | Total | C  | N  | O  | P  | 0       | 0     |
|     |       |          | 220   | 98 | 44 | 68 | 10 |         |       |

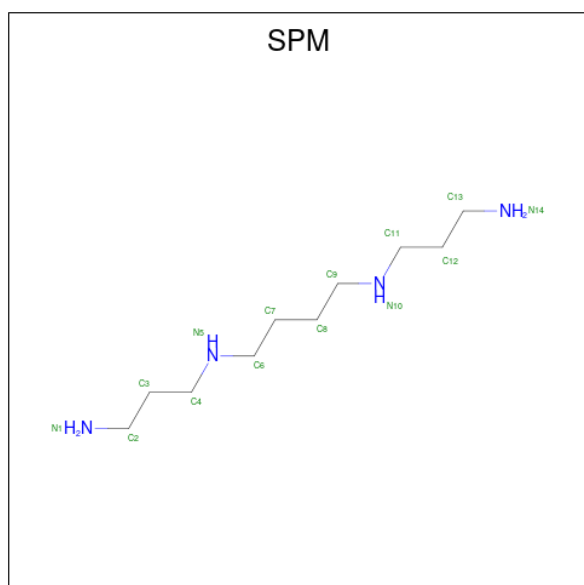
- Molecule 34 is a protein called aS34.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 34  | a     | 71       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 562   | 361 | 98 | 96 | 7 |         |       |

- Molecule 35 is a protein called Small ribosomal subunit protein uS14.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 35  | P     | 53       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 440   | 282 | 80 | 74 | 4 |         |       |

- Molecule 36 is SPERMINE (CCD ID: SPM) (formula:  $C_{10}H_{26}N_4$ ).



| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 36  | 2     | 1        | Total | C  | N | 0       |
|     |       |          | 14    | 10 | 4 |         |

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| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 36  | 2     | 1        | Total | C  | N | 0       |
|     |       |          | 14    | 10 | 4 |         |

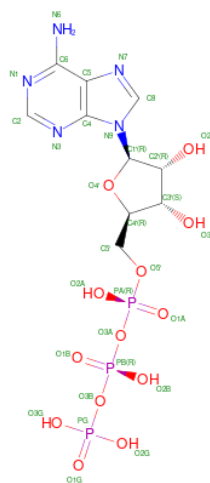
- Molecule 37 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 37  | 2     | 52       | Total | Mg | 0       |
|     |       |          | 52    | 52 |         |
| 37  | F     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 37  | R     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 37  | 5     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 37  | P     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 38 is ZINC ION (CCD ID: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 38  | C     | 2        | Total | Zn | 0       |
|     |       |          | 2     | 2  |         |
| 38  | F     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 38  | R     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 38  | W     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 38  | a     | 2        | Total | Zn | 0       |
|     |       |          | 2     | 2  |         |
| 38  | P     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 39 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).



| Mol | Chain | Residues | Atoms |    |    |    |   | AltConf |
|-----|-------|----------|-------|----|----|----|---|---------|
| 39  | 5     | 1        | Total | C  | N  | O  | P | 1       |
|     |       |          | 62    | 20 | 10 | 26 | 6 |         |

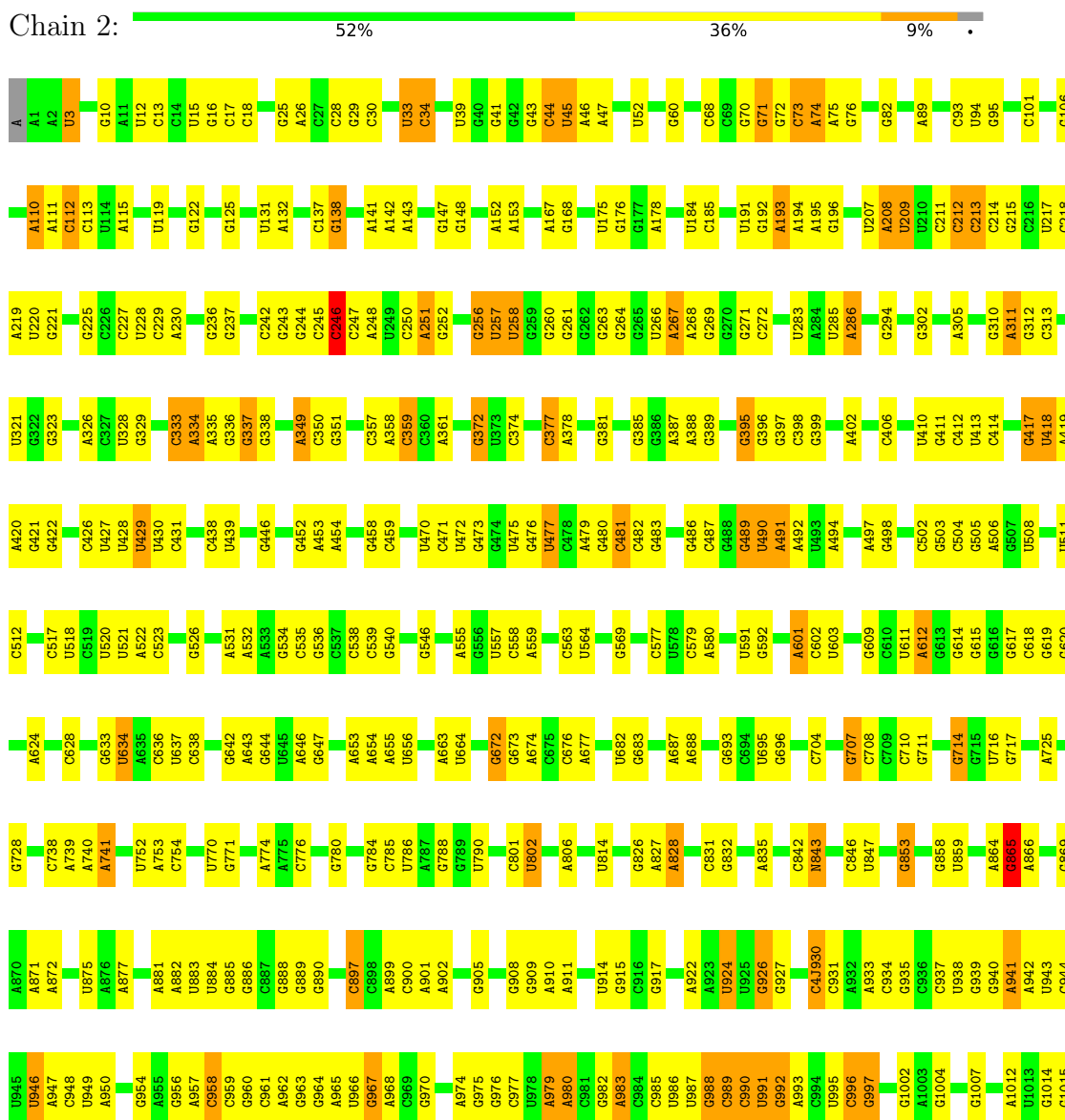
- Molecule 40 is water.

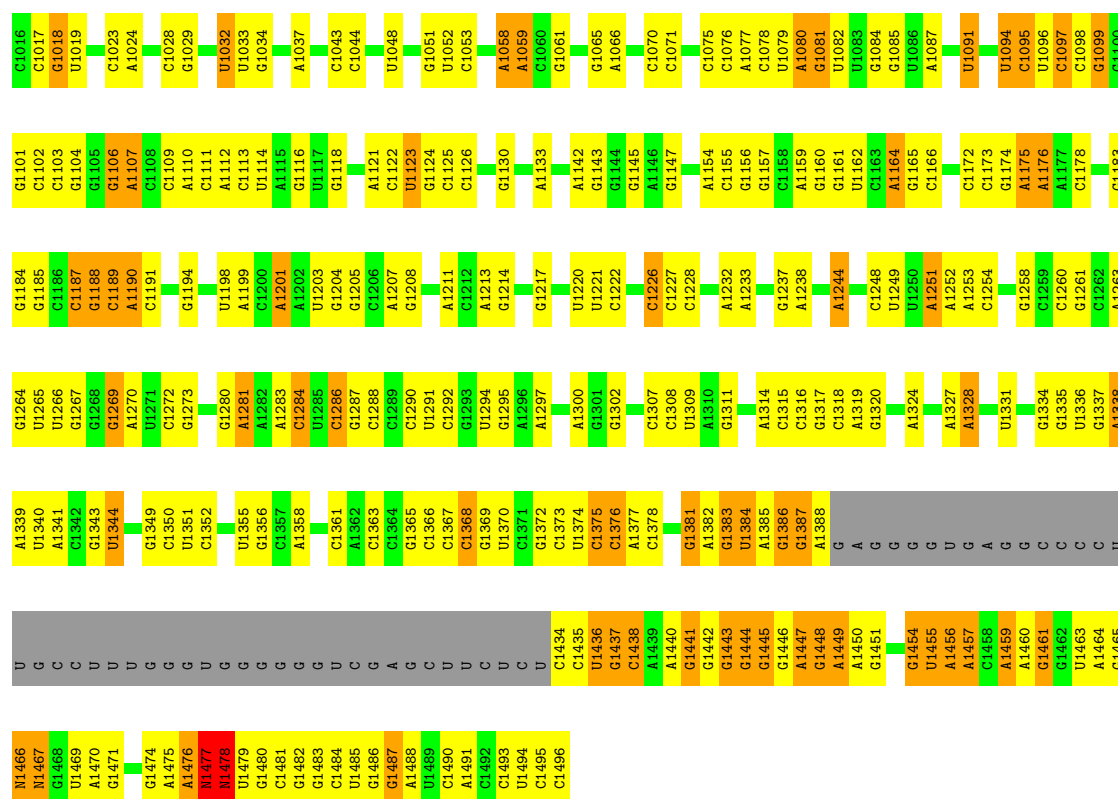
| Mol | Chain | Residues | Atoms              | AltConf |
|-----|-------|----------|--------------------|---------|
| 40  | 2     | 227      | Total O<br>227 227 | 0       |
| 40  | D     | 1        | Total O<br>1 1     | 0       |
| 40  | E     | 1        | Total O<br>1 1     | 0       |
| 40  | F     | 5        | Total O<br>5 5     | 0       |
| 40  | H     | 1        | Total O<br>1 1     | 0       |
| 40  | I     | 2        | Total O<br>2 2     | 0       |
| 40  | K     | 2        | Total O<br>2 2     | 0       |
| 40  | Q     | 2        | Total O<br>2 2     | 0       |
| 40  | R     | 2        | Total O<br>2 2     | 0       |
| 40  | 5     | 10       | Total O<br>10 10   | 0       |
| 40  | 4     | 2        | Total O<br>2 2     | 0       |

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

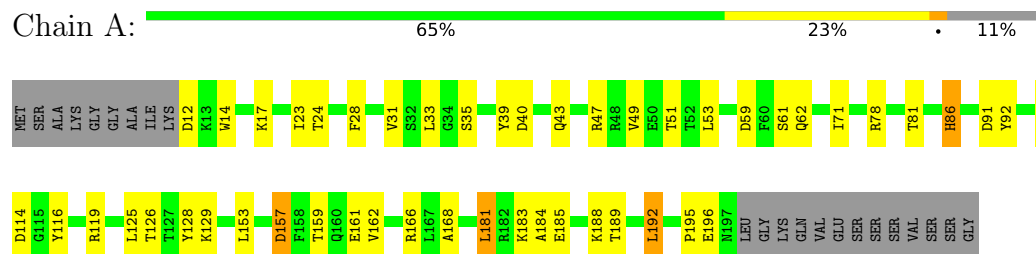
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: rRNA 16S

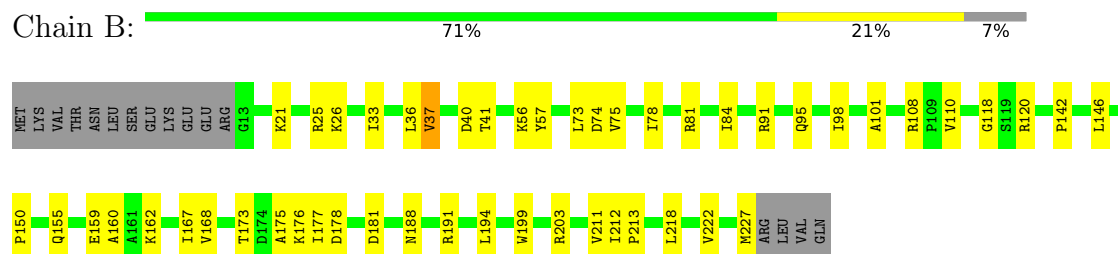




### • Molecule 2: Small ribosomal subunit protein eS1



### • Molecule 3: Small ribosomal subunit protein uS2



### • Molecule 4: Small zinc finger protein HVO-2753-like zinc-binding pocket domain-containing protein

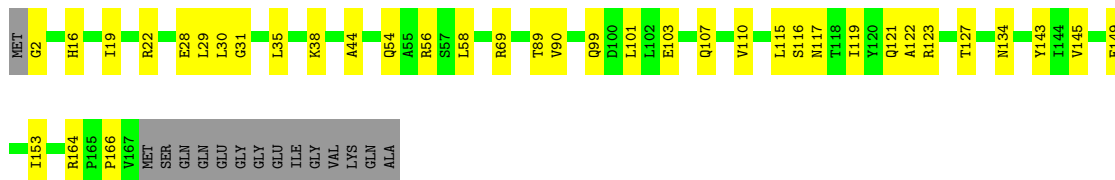






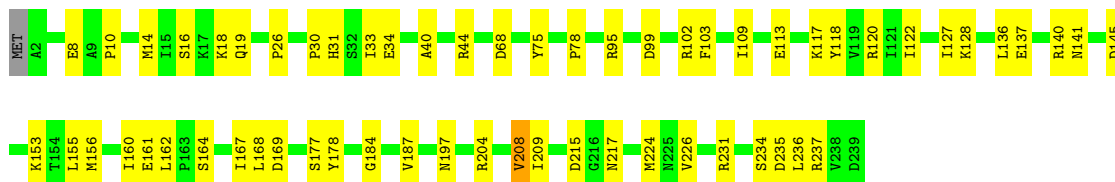
- Molecule 5: Small ribosomal subunit protein uS4

Chain D: 71% 20% 8%



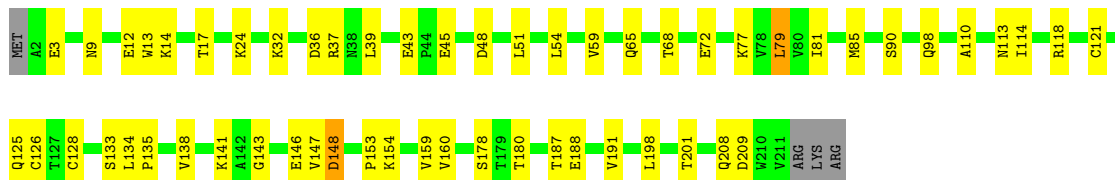
- Molecule 6: Small ribosomal subunit protein eS4

Chain E: 74% 25%



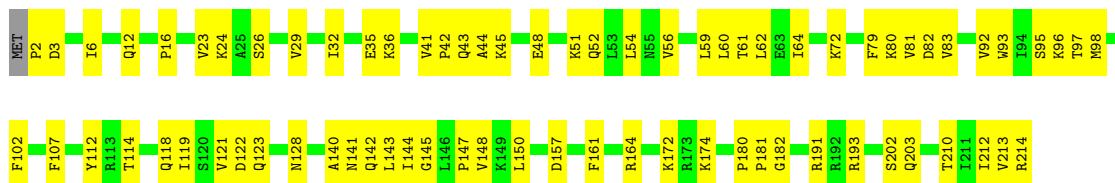
- Molecule 7: Small ribosomal subunit protein uS5

Chain F: 72% 25% ..



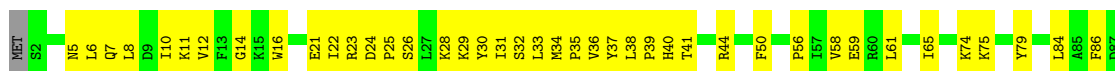
- Molecule 8: Small ribosomal subunit protein eS6

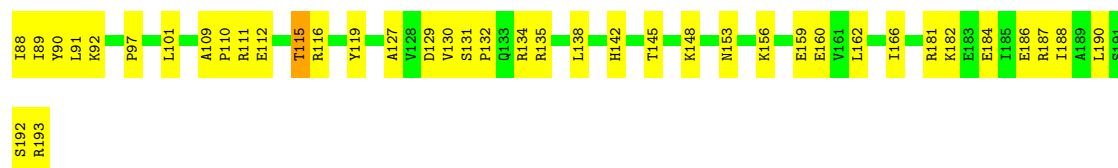
Chain G: 65% 35%



- Molecule 9: Small ribosomal subunit protein uS7

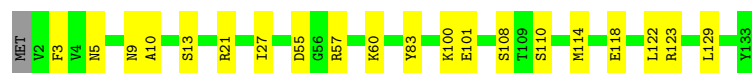
Chain H: 58% 41% ..





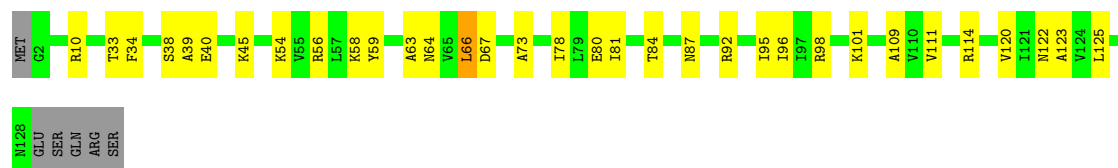
- Molecule 10: Small ribosomal subunit protein uS8

Chain I: 84% 15%



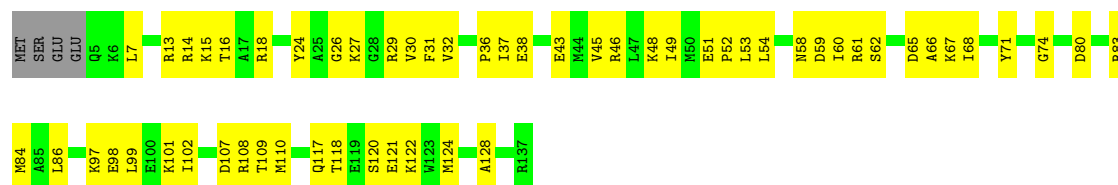
- Molecule 11: Small ribosomal subunit protein eS8

Chain J: 71% 24% 5%



- Molecule 12: Small ribosomal subunit protein uS9

Chain K: 56% 41%



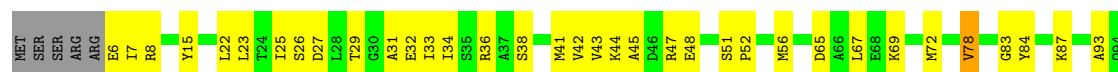
- Molecule 13: Small ribosomal subunit protein uS10

Chain L: 59% 38%



- Molecule 14: Small ribosomal subunit protein uS11

Chain M: 61% 34%





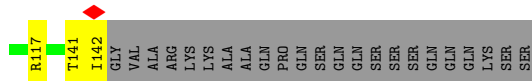
- Molecule 15: Small ribosomal subunit protein uS12

Chain N: 79% 20%



- Molecule 16: Small ribosomal subunit protein uS13

Chain O: 63% 21% 15%



- Molecule 17: Small ribosomal subunit protein uS15

Chain Q: 78% 18% 5%



- Molecule 18: Small ribosomal subunit protein uS17

Chain R: 83% 16%



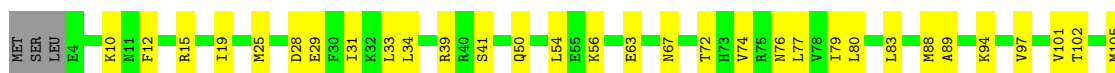
- Molecule 19: Small ribosomal subunit protein eS17

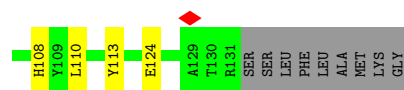
Chain S: 51% 33% 16%



- Molecule 20: Small ribosomal subunit protein uS19

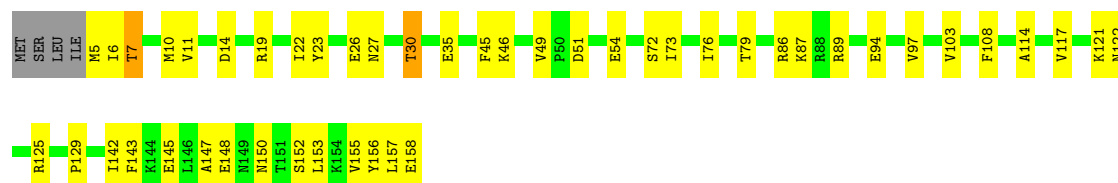
Chain T: 66% 25% 9%





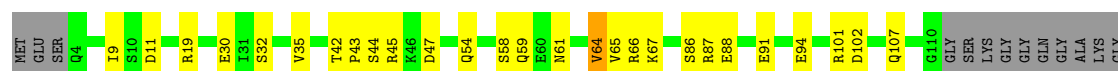
- Molecule 21: Small ribosomal subunit protein eS19

Chain U: 68% 28% . .



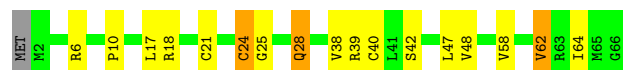
- Molecule 22: Small ribosomal subunit protein eS24

Chain V: 67% 22% . 11%



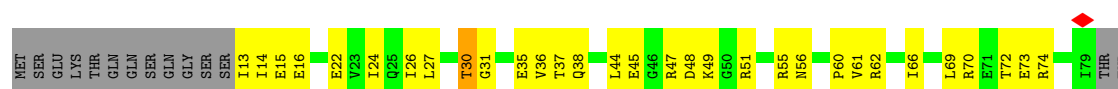
- Molecule 23: Small ribosomal subunit protein eS27

Chain W: 73% 21% 5% .



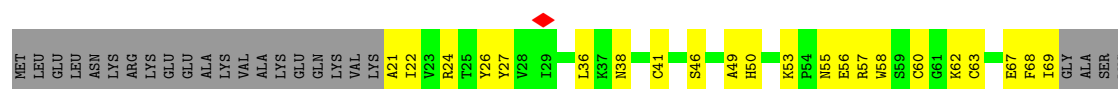
- Molecule 24: Small ribosomal subunit protein eS28

Chain X: 43% 36% . 19%



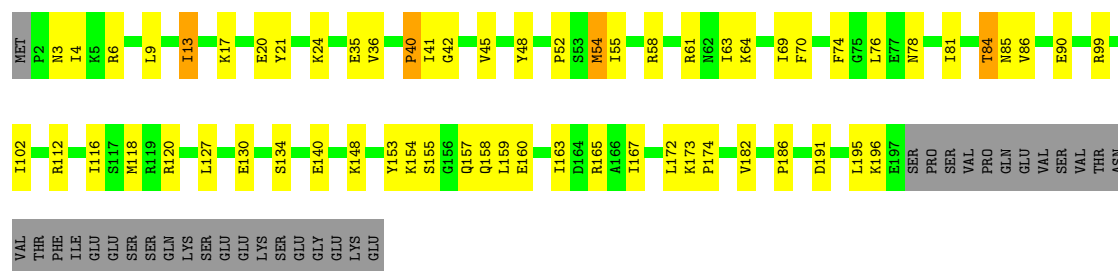
- Molecule 25: Small ribosomal subunit protein eS31

Chain Y: 36% 29% 35%



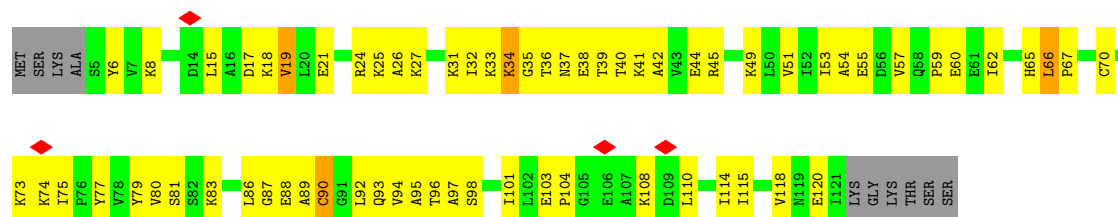
- Molecule 26: Small ribosomal subunit protein uS3

Chain Z: 



- Molecule 27: Large ribosomal subunit protein eL8

Chain 3: 

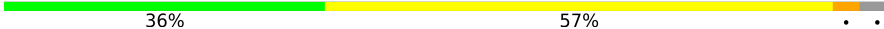


- Molecule 28: Small ribosomal subunit protein eS25

Chain c: 



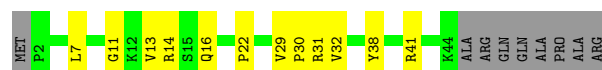
- Molecule 29: VapB-type antitoxin

Chain d: 

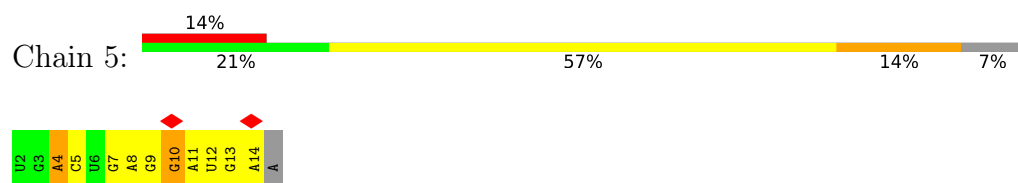


- Molecule 30: LSU ribosomal protein S30E (Rps30E)

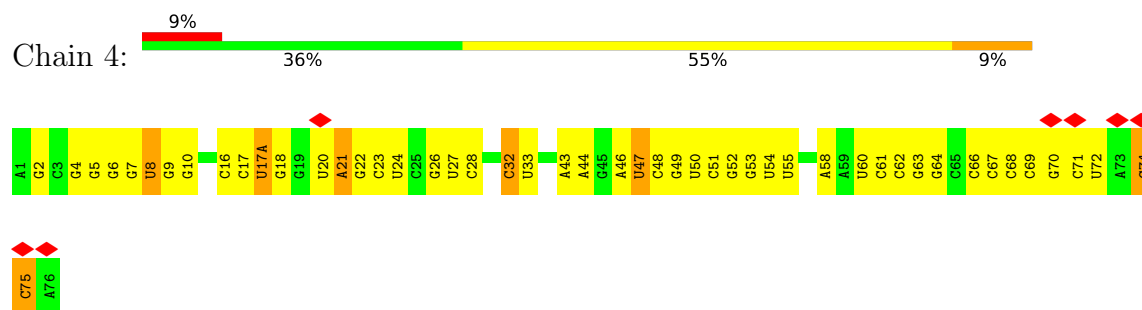
Chain e: 



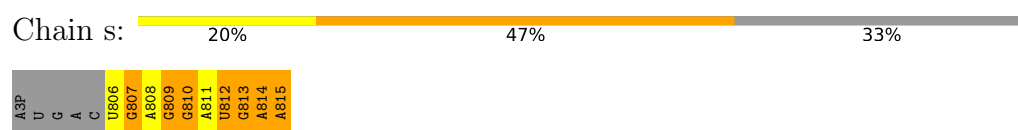
- Molecule 31: mRNA Map



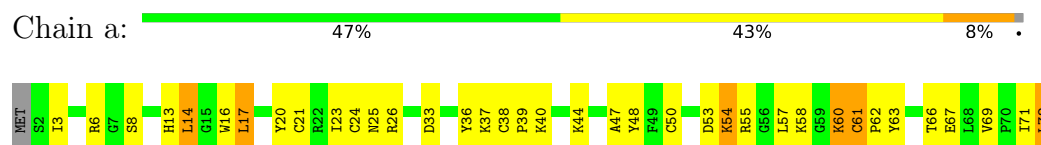
- Molecule 32: tRNA Met initiator



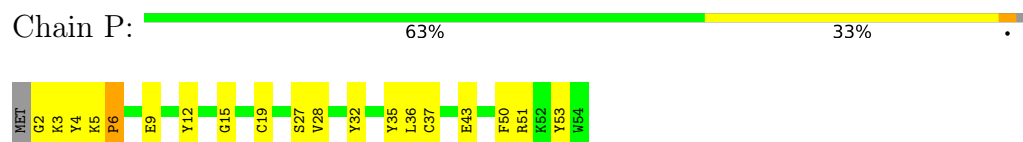
- Molecule 33: mRNA Map



- Molecule 34: aS34



- Molecule 35: Small ribosomal subunit protein uS14



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 108000                                  | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | TFS KRIOS                               | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 40                                      | Depositor |
| Minimum defocus (nm)                 | 800                                     | Depositor |
| Maximum defocus (nm)                 | 2500                                    | Depositor |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K3 BIOQUANTUM (6k x 4k)           | Depositor |
| Maximum map value                    | 0.048                                   | Depositor |
| Minimum map value                    | -0.013                                  | Depositor |
| Average map value                    | 0.000                                   | Depositor |
| Map value standard deviation         | 0.002                                   | Depositor |
| Recommended contour level            | 0.004                                   | Depositor |
| Map size (Å)                         | 365.292, 365.292, 365.292               | wwPDB     |
| Map dimensions                       | 438, 438, 438                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 0.834, 0.834, 0.834                     | Depositor |

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: OMC, 6MZ, 5MU, OMG, 4SU, PSU, MG, 5MC, OMU, SPM, H2U, C4J, ATP, ZN, A2M, MA6, 4AC

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   | 2     | 0.26         | 0/34103 | 0.28        | 0/53203       |
| 2   | A     | 0.20         | 0/1543  | 0.33        | 0/2077        |
| 3   | B     | 0.19         | 0/1731  | 0.36        | 0/2349        |
| 4   | C     | 0.25         | 0/466   | 0.42        | 0/625         |
| 5   | D     | 0.23         | 0/1380  | 0.31        | 0/1859        |
| 6   | E     | 0.22         | 0/1965  | 0.34        | 0/2644        |
| 7   | F     | 0.25         | 0/1654  | 0.37        | 0/2240        |
| 8   | G     | 0.14         | 0/1684  | 0.26        | 0/2265        |
| 9   | H     | 0.22         | 0/1571  | 0.45        | 0/2116        |
| 10  | I     | 0.26         | 0/1070  | 0.32        | 0/1444        |
| 11  | J     | 0.23         | 0/994   | 0.36        | 0/1337        |
| 12  | K     | 0.22         | 0/1084  | 0.43        | 0/1450        |
| 13  | L     | 0.23         | 0/856   | 0.50        | 0/1154        |
| 14  | M     | 0.27         | 0/960   | 0.54        | 0/1294        |
| 15  | N     | 0.25         | 0/1155  | 0.41        | 0/1540        |
| 16  | O     | 0.19         | 0/1142  | 0.37        | 0/1532        |
| 17  | Q     | 0.22         | 0/1206  | 0.34        | 0/1618        |
| 18  | R     | 0.24         | 0/918   | 0.30        | 0/1236        |
| 19  | S     | 0.23         | 0/578   | 0.44        | 0/770         |
| 20  | T     | 0.17         | 0/1087  | 0.33        | 0/1456        |
| 21  | U     | 0.21         | 0/1270  | 0.41        | 0/1710        |
| 22  | V     | 0.21         | 0/843   | 0.40        | 0/1124        |
| 23  | W     | 0.25         | 0/511   | 0.52        | 1/684 (0.1%)  |
| 24  | X     | 0.20         | 0/538   | 0.49        | 0/722         |
| 25  | Y     | 0.15         | 0/404   | 0.42        | 0/540         |
| 26  | Z     | 0.24         | 0/1584  | 0.45        | 1/2124 (0.0%) |
| 27  | 3     | 0.18         | 0/902   | 0.44        | 0/1216        |
| 28  | c     | 0.19         | 0/861   | 0.45        | 0/1143        |
| 29  | d     | 0.21         | 0/573   | 0.55        | 0/776         |
| 30  | e     | 0.19         | 0/360   | 0.41        | 0/477         |
| 31  | 5     | 0.15         | 0/317   | 0.22        | 0/493         |



| Mol | Chain | Bond lengths |                | Bond angles |                |
|-----|-------|--------------|----------------|-------------|----------------|
|     |       | RMSZ         | # Z  >5        | RMSZ        | # Z  >5        |
| 32  | 4     | 0.18         | 1/1725 (0.1%)  | 0.22        | 0/2687         |
| 33  | s     | 0.34         | 0/247          | 0.72        | 1/384 (0.3%)   |
| 34  | a     | 0.79         | 0/574          | 0.97        | 2/770 (0.3%)   |
| 35  | P     | 0.26         | 0/451          | 0.59        | 2/600 (0.3%)   |
| All | All   | 0.25         | 1/68307 (0.0%) | 0.35        | 7/99659 (0.0%) |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 32  | 4     | 8   | 4SU  | O3'-P | 5.08 | 1.61        | 1.56     |

The worst 5 of 7 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 26  | Z     | 40  | PRO  | CA-N-CD | -9.07 | 99.30       | 112.00   |
| 34  | a     | 24  | CYS  | N-CA-C  | 7.89  | 119.96      | 111.36   |
| 35  | P     | 6   | PRO  | CA-C-N  | 6.26  | 126.23      | 119.78   |
| 35  | P     | 6   | PRO  | C-N-CA  | 6.26  | 126.23      | 119.78   |
| 23  | W     | 28  | GLN  | N-CA-C  | 5.22  | 117.01      | 109.07   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | 2     | 31215 | 0        | 15795    | 573     | 0            |
| 2   | A     | 1515  | 0        | 1565     | 42      | 0            |
| 3   | B     | 1698  | 0        | 1753     | 34      | 0            |
| 4   | C     | 455   | 0        | 437      | 26      | 0            |
| 5   | D     | 1354  | 0        | 1419     | 27      | 0            |
| 6   | E     | 1930  | 0        | 2013     | 39      | 0            |
| 7   | F     | 1625  | 0        | 1689     | 43      | 0            |
| 8   | G     | 1661  | 0        | 1737     | 57      | 0            |
| 9   | H     | 1543  | 0        | 1611     | 96      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 10  | I     | 1050  | 0        | 1100     | 13      | 0            |
| 11  | J     | 982   | 0        | 1046     | 23      | 0            |
| 12  | K     | 1068  | 0        | 1125     | 59      | 0            |
| 13  | L     | 840   | 0        | 893      | 41      | 0            |
| 14  | M     | 944   | 0        | 978      | 40      | 0            |
| 15  | N     | 1140  | 0        | 1244     | 31      | 0            |
| 16  | O     | 1124  | 0        | 1162     | 34      | 0            |
| 17  | Q     | 1185  | 0        | 1260     | 26      | 0            |
| 18  | R     | 901   | 0        | 935      | 13      | 0            |
| 19  | S     | 571   | 0        | 598      | 26      | 0            |
| 20  | T     | 1064  | 0        | 1107     | 25      | 0            |
| 21  | U     | 1247  | 0        | 1329     | 48      | 0            |
| 22  | V     | 836   | 0        | 894      | 20      | 0            |
| 23  | W     | 503   | 0        | 533      | 14      | 0            |
| 24  | X     | 535   | 0        | 572      | 34      | 0            |
| 25  | Y     | 395   | 0        | 405      | 17      | 0            |
| 26  | Z     | 1561  | 0        | 1667     | 62      | 0            |
| 27  | 3     | 893   | 0        | 940      | 64      | 0            |
| 28  | c     | 856   | 0        | 941      | 69      | 0            |
| 29  | d     | 562   | 0        | 581      | 59      | 0            |
| 30  | e     | 354   | 0        | 386      | 15      | 0            |
| 31  | 5     | 283   | 0        | 141      | 6       | 0            |
| 32  | 4     | 1645  | 0        | 840      | 30      | 0            |
| 33  | s     | 220   | 0        | 109      | 10      | 0            |
| 34  | a     | 562   | 0        | 574      | 48      | 0            |
| 35  | P     | 440   | 0        | 436      | 24      | 0            |
| 36  | 2     | 616   | 0        | 1142     | 52      | 0            |
| 37  | 2     | 52    | 0        | 0        | 0       | 0            |
| 37  | 5     | 1     | 0        | 0        | 0       | 0            |
| 37  | F     | 1     | 0        | 0        | 0       | 0            |
| 37  | P     | 1     | 0        | 0        | 0       | 0            |
| 37  | R     | 1     | 0        | 0        | 0       | 0            |
| 38  | C     | 2     | 0        | 0        | 0       | 0            |
| 38  | F     | 1     | 0        | 0        | 0       | 0            |
| 38  | P     | 1     | 0        | 0        | 0       | 0            |
| 38  | R     | 1     | 0        | 0        | 0       | 0            |
| 38  | W     | 1     | 0        | 0        | 0       | 0            |
| 38  | a     | 2     | 0        | 0        | 0       | 0            |
| 39  | 5     | 62    | 0        | 22       | 0       | 0            |
| 40  | 2     | 227   | 0        | 0        | 7       | 0            |
| 40  | 4     | 2     | 0        | 0        | 0       | 0            |
| 40  | 5     | 10    | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 40  | D     | 1     | 0        | 0        | 0       | 0            |
| 40  | E     | 1     | 0        | 0        | 0       | 0            |
| 40  | F     | 5     | 0        | 0        | 0       | 0            |
| 40  | H     | 1     | 0        | 0        | 1       | 0            |
| 40  | I     | 2     | 0        | 0        | 0       | 0            |
| 40  | K     | 2     | 0        | 0        | 0       | 0            |
| 40  | Q     | 2     | 0        | 0        | 0       | 0            |
| 40  | R     | 2     | 0        | 0        | 0       | 0            |
| All | All   | 65754 | 0        | 50979    | 1546    | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

The worst 5 of 1546 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:2:476:G:H2'    | 1:2:490:U:C6     | 1.59                     | 1.37              |
| 26:Z:157:GLN:NE2 | 26:Z:160:GLU:OE1 | 1.62                     | 1.27              |
| 1:2:476:G:H2'    | 1:2:490:U:C5     | 1.71                     | 1.25              |
| 9:H:10:ILE:CG2   | 9:H:35:PRO:O     | 1.85                     | 1.25              |
| 17:Q:17:ARG:HH12 | 17:Q:63:GLN:NE2  | 1.34                     | 1.23              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 2   | A     | 184/208 (88%) | 179 (97%) | 5 (3%)  | 0        | 100         | 100 |
| 3   | B     | 213/231 (92%) | 205 (96%) | 8 (4%)  | 0        | 100         | 100 |
| 4   | C     | 56/65 (86%)   | 55 (98%)  | 1 (2%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 5   | D     | 164/181 (91%)   | 161 (98%)  | 3 (2%)   | 0        | 100         | 100 |
| 6   | E     | 236/239 (99%)   | 231 (98%)  | 5 (2%)   | 0        | 100         | 100 |
| 7   | F     | 208/214 (97%)   | 201 (97%)  | 7 (3%)   | 0        | 100         | 100 |
| 8   | G     | 211/214 (99%)   | 202 (96%)  | 9 (4%)   | 0        | 100         | 100 |
| 9   | H     | 190/193 (98%)   | 180 (95%)  | 10 (5%)  | 0        | 100         | 100 |
| 10  | I     | 130/133 (98%)   | 126 (97%)  | 4 (3%)   | 0        | 100         | 100 |
| 11  | J     | 125/133 (94%)   | 122 (98%)  | 3 (2%)   | 0        | 100         | 100 |
| 12  | K     | 131/137 (96%)   | 126 (96%)  | 5 (4%)   | 0        | 100         | 100 |
| 13  | L     | 99/102 (97%)    | 93 (94%)   | 6 (6%)   | 0        | 100         | 100 |
| 14  | M     | 125/132 (95%)   | 117 (94%)  | 8 (6%)   | 0        | 100         | 100 |
| 15  | N     | 144/147 (98%)   | 138 (96%)  | 6 (4%)   | 0        | 100         | 100 |
| 16  | O     | 138/165 (84%)   | 130 (94%)  | 8 (6%)   | 0        | 100         | 100 |
| 17  | Q     | 143/152 (94%)   | 142 (99%)  | 1 (1%)   | 0        | 100         | 100 |
| 18  | R     | 111/114 (97%)   | 109 (98%)  | 2 (2%)   | 0        | 100         | 100 |
| 19  | S     | 64/79 (81%)     | 63 (98%)   | 1 (2%)   | 0        | 100         | 100 |
| 20  | T     | 126/140 (90%)   | 125 (99%)  | 1 (1%)   | 0        | 100         | 100 |
| 21  | U     | 152/158 (96%)   | 147 (97%)  | 5 (3%)   | 0        | 100         | 100 |
| 22  | V     | 105/120 (88%)   | 103 (98%)  | 2 (2%)   | 0        | 100         | 100 |
| 23  | W     | 63/66 (96%)     | 57 (90%)   | 6 (10%)  | 0        | 100         | 100 |
| 24  | X     | 65/83 (78%)     | 59 (91%)   | 6 (9%)   | 0        | 100         | 100 |
| 25  | Y     | 47/75 (63%)     | 38 (81%)   | 9 (19%)  | 0        | 100         | 100 |
| 26  | Z     | 194/229 (85%)   | 188 (97%)  | 6 (3%)   | 0        | 100         | 100 |
| 27  | 3     | 115/127 (91%)   | 101 (88%)  | 14 (12%) | 0        | 100         | 100 |
| 28  | c     | 107/110 (97%)   | 96 (90%)   | 10 (9%)  | 1 (1%)   | 14          | 41  |
| 29  | d     | 67/72 (93%)     | 64 (96%)   | 3 (4%)   | 0        | 100         | 100 |
| 30  | e     | 41/52 (79%)     | 40 (98%)   | 1 (2%)   | 0        | 100         | 100 |
| 34  | a     | 69/72 (96%)     | 69 (100%)  | 0        | 0        | 100         | 100 |
| 35  | P     | 51/54 (94%)     | 50 (98%)   | 1 (2%)   | 0        | 100         | 100 |
| All | All   | 3874/4197 (92%) | 3717 (96%) | 156 (4%) | 1 (0%)   | 100         | 100 |

All (1) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 28  | c     | 9   | ILE  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 2   | A     | 168/184 (91%)  | 163 (97%)  | 5 (3%)   | 36          | 72  |
| 3   | B     | 182/198 (92%)  | 180 (99%)  | 2 (1%)   | 65          | 87  |
| 4   | C     | 51/58 (88%)    | 49 (96%)   | 2 (4%)   | 28          | 64  |
| 5   | D     | 147/158 (93%)  | 147 (100%) | 0        | 100         | 100 |
| 6   | E     | 214/215 (100%) | 210 (98%)  | 4 (2%)   | 50          | 81  |
| 7   | F     | 180/184 (98%)  | 177 (98%)  | 3 (2%)   | 53          | 83  |
| 8   | G     | 186/187 (100%) | 182 (98%)  | 4 (2%)   | 45          | 78  |
| 9   | H     | 166/167 (99%)  | 164 (99%)  | 2 (1%)   | 63          | 87  |
| 10  | I     | 113/114 (99%)  | 111 (98%)  | 2 (2%)   | 51          | 82  |
| 11  | J     | 104/110 (94%)  | 102 (98%)  | 2 (2%)   | 50          | 81  |
| 12  | K     | 109/113 (96%)  | 108 (99%)  | 1 (1%)   | 70          | 89  |
| 13  | L     | 93/94 (99%)    | 91 (98%)   | 2 (2%)   | 45          | 78  |
| 14  | M     | 93/98 (95%)    | 89 (96%)   | 4 (4%)   | 26          | 60  |
| 15  | N     | 122/123 (99%)  | 121 (99%)  | 1 (1%)   | 73          | 90  |
| 16  | O     | 121/142 (85%)  | 116 (96%)  | 5 (4%)   | 27          | 62  |
| 17  | Q     | 125/129 (97%)  | 125 (100%) | 0        | 100         | 100 |
| 18  | R     | 101/102 (99%)  | 101 (100%) | 0        | 100         | 100 |
| 19  | S     | 63/75 (84%)    | 62 (98%)   | 1 (2%)   | 55          | 83  |
| 20  | T     | 116/126 (92%)  | 115 (99%)  | 1 (1%)   | 70          | 89  |
| 21  | U     | 134/138 (97%)  | 128 (96%)  | 6 (4%)   | 24          | 58  |
| 22  | V     | 92/99 (93%)    | 89 (97%)   | 3 (3%)   | 33          | 69  |
| 23  | W     | 57/58 (98%)    | 54 (95%)   | 3 (5%)   | 20          | 52  |
| 24  | X     | 58/73 (80%)    | 54 (93%)   | 4 (7%)   | 14          | 41  |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 25  | Y     | 43/65 (66%)     | 43 (100%)  | 0        | 100         | 100 |
| 26  | Z     | 163/195 (84%)   | 158 (97%)  | 5 (3%)   | 35          | 70  |
| 27  | 3     | 97/105 (92%)    | 91 (94%)   | 6 (6%)   | 16          | 45  |
| 28  | c     | 95/96 (99%)     | 91 (96%)   | 4 (4%)   | 26          | 61  |
| 29  | d     | 62/65 (95%)     | 60 (97%)   | 2 (3%)   | 34          | 70  |
| 30  | e     | 40/46 (87%)     | 39 (98%)   | 1 (2%)   | 42          | 76  |
| 34  | a     | 61/62 (98%)     | 51 (84%)   | 10 (16%) | 2           | 8   |
| 35  | P     | 45/46 (98%)     | 45 (100%)  | 0        | 100         | 100 |
| All | All   | 3401/3625 (94%) | 3316 (98%) | 85 (2%)  | 42          | 76  |

5 of 85 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 26  | Z     | 13  | ILE  |
| 28  | c     | 99  | LYS  |
| 26  | Z     | 84  | THR  |
| 27  | 3     | 88  | GLU  |
| 34  | a     | 14  | LEU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 48 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 16  | O     | 121 | HIS  |
| 21  | U     | 71  | ASN  |
| 17  | Q     | 55  | GLN  |
| 18  | R     | 86  | ASN  |
| 25  | Y     | 50  | HIS  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1   | 2     | 1449/1497 (96%) | 232 (16%)         | 8 (0%)          |
| 31  | 5     | 12/14 (85%)     | 6 (50%)           | 1 (8%)          |
| 32  | 4     | 76/77 (98%)     | 14 (18%)          | 1 (1%)          |
| 33  | s     | 9/15 (60%)      | 8 (88%)           | 0               |
| All | All   | 1546/1603 (96%) | 260 (16%)         | 10 (0%)         |

5 of 260 RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 2     | 3   | U    |
| 1   | 2     | 33  | U    |
| 1   | 2     | 34  | C    |
| 1   | 2     | 43  | G    |
| 1   | 2     | 45  | U    |

5 of 10 RNA pucker outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 2     | 1477 | 4AC  |
| 31  | 5     | 12   | U    |
| 32  | 4     | 74   | C    |
| 1   | 2     | 1188 | G    |
| 1   | 2     | 1436 | U    |

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

38 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 | $\# Z  > 2$ |
| 32  | 5MU  | 4     | 54   | 32   | 19,22,23     | 1.39 | 5 (26%)     | 28,32,35    | 2.06 | 7 (25%)     |
| 1   | 4AC  | 2     | 1478 | 1    | 21,24,25     | 1.01 | 2 (9%)      | 29,34,37    | 1.31 | 4 (13%)     |
| 1   | OMG  | 2     | 399  | 1    | 23,26,27     | 1.21 | 3 (13%)     | 33,38,41    | 1.95 | 6 (18%)     |
| 1   | OMG  | 2     | 1018 | 1    | 23,26,27     | 1.22 | 3 (13%)     | 33,38,41    | 1.96 | 6 (18%)     |
| 1   | OMC  | 2     | 481  | 1    | 19,22,23     | 0.94 | 1 (5%)      | 26,31,34    | 1.45 | 4 (15%)     |
| 1   | OMG  | 2     | 865  | 1    | 23,26,27     | 1.22 | 3 (13%)     | 33,38,41    | 1.94 | 6 (18%)     |
| 1   | OMU  | 2     | 1344 | 1    | 19,22,23     | 1.22 | 3 (15%)     | 26,31,34    | 1.70 | 6 (23%)     |
| 1   | OMC  | 2     | 246  | 1    | 19,22,23     | 0.85 | 0           | 26,31,34    | 0.97 | 1 (3%)      |
| 1   | OMC  | 2     | 313  | 1    | 19,22,23     | 0.85 | 0           | 26,31,34    | 0.91 | 1 (3%)      |
| 1   | OMG  | 2     | 926  | 1    | 23,26,27     | 1.21 | 3 (13%)     | 33,38,41    | 1.96 | 6 (18%)     |
| 1   | A2M  | 2     | 494  | 1    | 22,25,26     | 1.46 | 4 (18%)     | 31,36,39    | 2.11 | 9 (29%)     |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 1   | OMU  | 2     | 15   | 1    | 19,22,23     | 1.27 | 3 (15%)  | 26,31,34    | 1.79 | 5 (19%)  |
| 1   | OMC  | 2     | 1366 | 1    | 19,22,23     | 0.81 | 0        | 26,31,34    | 0.79 | 0        |
| 1   | 4AC  | 2     | 1467 | 1    | 21,24,25     | 1.01 | 2 (9%)   | 29,34,37    | 1.31 | 4 (13%)  |
| 1   | OMC  | 2     | 512  | 1    | 19,22,23     | 0.82 | 0        | 26,31,34    | 0.81 | 0        |
| 1   | OMC  | 2     | 113  | 1    | 19,22,23     | 0.82 | 0        | 26,31,34    | 0.82 | 0        |
| 1   | OMG  | 2     | 1194 | 1    | 23,26,27     | 1.22 | 3 (13%)  | 33,38,41    | 2.00 | 7 (21%)  |
| 1   | OMG  | 2     | 905  | 1    | 23,26,27     | 1.23 | 3 (13%)  | 33,38,41    | 1.97 | 7 (21%)  |
| 32  | OMC  | 4     | 32   | 32   | 19,22,23     | 0.85 | 0        | 26,31,34    | 0.99 | 2 (7%)   |
| 1   | 4AC  | 2     | 1466 | 1    | 21,24,25     | 1.01 | 2 (9%)   | 29,34,37    | 1.31 | 4 (13%)  |
| 1   | OMC  | 2     | 710  | 1    | 19,22,23     | 0.84 | 0        | 26,31,34    | 0.86 | 1 (3%)   |
| 1   | OMG  | 2     | 337  | 1    | 23,26,27     | 1.22 | 3 (13%)  | 33,38,41    | 1.94 | 6 (18%)  |
| 1   | OMC  | 2     | 1060 | 1    | 19,22,23     | 0.84 | 0        | 26,31,34    | 0.75 | 0        |
| 1   | C4J  | 2     | 930  | 1    | 24,29,30     | 0.65 | 1 (4%)   | 29,42,45    | 0.51 | 0        |
| 1   | 6MZ  | 2     | 1457 | 1,37 | 22,25,26     | 1.66 | 4 (18%)  | 30,36,39    | 2.24 | 14 (46%) |
| 1   | OMC  | 2     | 538  | 1    | 19,22,23     | 0.83 | 0        | 26,31,34    | 0.81 | 0        |
| 1   | OMG  | 2     | 1061 | 1    | 23,26,27     | 1.22 | 3 (13%)  | 33,38,41    | 1.95 | 6 (18%)  |
| 32  | 4SU  | 4     | 8    | 32   | 18,21,22     | 0.27 | 0        | 26,30,33    | 0.36 | 0        |
| 1   | 4AC  | 2     | 843  | 1    | 21,24,25     | 1.05 | 2 (9%)   | 29,34,37    | 1.39 | 5 (17%)  |
| 1   | 4AC  | 2     | 1477 | 1    | 21,24,25     | 1.08 | 2 (9%)   | 29,34,37    | 1.52 | 5 (17%)  |
| 1   | OMU  | 2     | 1032 | 1    | 19,22,23     | 1.25 | 3 (15%)  | 26,31,34    | 1.74 | 4 (15%)  |
| 32  | PSU  | 4     | 55   | 32   | 18,21,22     | 1.30 | 2 (11%)  | 22,30,33    | 1.87 | 3 (13%)  |
| 1   | OMU  | 2     | 52   | 1    | 19,22,23     | 1.25 | 3 (15%)  | 26,31,34    | 1.76 | 4 (15%)  |
| 1   | MA6  | 2     | 1475 | 1    | 23,26,27     | 1.45 | 4 (17%)  | 34,38,41    | 2.11 | 10 (29%) |
| 1   | 5MC  | 2     | 1368 | 1    | 18,22,23     | 0.90 | 2 (11%)  | 26,32,35    | 1.06 | 2 (7%)   |
| 1   | OMG  | 2     | 672  | 1    | 23,26,27     | 1.23 | 3 (13%)  | 33,38,41    | 1.95 | 6 (18%)  |
| 1   | OMG  | 2     | 546  | 1    | 23,26,27     | 1.21 | 3 (13%)  | 33,38,41    | 1.93 | 6 (18%)  |
| 32  | H2U  | 4     | 20   | 32   | 18,21,22     | 0.29 | 0        | 21,30,33    | 0.43 | 0        |

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

| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|------|------|---------|------------|---------|
| 32  | 5MU  | 4     | 54   | 32   | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | 4AC  | 2     | 1478 | 1    | -       | 0/11/29/30 | 0/2/2/2 |
| 1   | OMG  | 2     | 399  | 1    | -       | 0/9/27/28  | 0/3/3/3 |
| 1   | OMG  | 2     | 1018 | 1    | -       | 0/9/27/28  | 0/3/3/3 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|------|------|---------|------------|---------|
| 1   | OMC  | 2     | 481  | 1    | -       | 1/9/27/28  | 0/2/2/2 |
| 1   | OMG  | 2     | 865  | 1    | -       | 3/9/27/28  | 0/3/3/3 |
| 1   | OMU  | 2     | 1344 | 1    | -       | 0/9/27/28  | 0/2/2/2 |
| 1   | OMC  | 2     | 246  | 1    | -       | 3/9/27/28  | 0/2/2/2 |
| 1   | OMC  | 2     | 313  | 1    | -       | 1/9/27/28  | 0/2/2/2 |
| 1   | OMG  | 2     | 926  | 1    | -       | 0/9/27/28  | 0/3/3/3 |
| 1   | A2M  | 2     | 494  | 1    | -       | 1/9/27/28  | 0/3/3/3 |
| 1   | OMU  | 2     | 15   | 1    | -       | 0/9/27/28  | 0/2/2/2 |
| 1   | OMC  | 2     | 1366 | 1    | -       | 0/9/27/28  | 0/2/2/2 |
| 1   | 4AC  | 2     | 1467 | 1    | -       | 0/11/29/30 | 0/2/2/2 |
| 1   | OMC  | 2     | 512  | 1    | -       | 0/9/27/28  | 0/2/2/2 |
| 1   | OMC  | 2     | 113  | 1    | -       | 0/9/27/28  | 0/2/2/2 |
| 1   | OMG  | 2     | 1194 | 1    | -       | 0/9/27/28  | 0/3/3/3 |
| 1   | OMG  | 2     | 905  | 1    | -       | 0/9/27/28  | 0/3/3/3 |
| 32  | OMC  | 4     | 32   | 32   | -       | 3/9/27/28  | 0/2/2/2 |
| 1   | 4AC  | 2     | 1466 | 1    | -       | 0/11/29/30 | 0/2/2/2 |
| 1   | OMC  | 2     | 710  | 1    | -       | 0/9/27/28  | 0/2/2/2 |
| 1   | OMG  | 2     | 337  | 1    | -       | 1/9/27/28  | 0/3/3/3 |
| 1   | OMC  | 2     | 1060 | 1    | -       | 0/9/27/28  | 0/2/2/2 |
| 1   | C4J  | 2     | 930  | 1    | -       | 3/16/34/35 | 0/2/2/2 |
| 1   | 6MZ  | 2     | 1457 | 1,37 | -       | 0/9/27/28  | 0/3/3/3 |
| 1   | OMC  | 2     | 538  | 1    | -       | 0/9/27/28  | 0/2/2/2 |
| 1   | OMG  | 2     | 1061 | 1    | -       | 0/9/27/28  | 0/3/3/3 |
| 32  | 4SU  | 4     | 8    | 32   | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | 4AC  | 2     | 843  | 1    | -       | 0/11/29/30 | 0/2/2/2 |
| 1   | 4AC  | 2     | 1477 | 1    | -       | 1/11/29/30 | 0/2/2/2 |
| 1   | OMU  | 2     | 1032 | 1    | -       | 2/9/27/28  | 0/2/2/2 |
| 32  | PSU  | 4     | 55   | 32   | -       | 2/7/25/26  | 0/2/2/2 |
| 1   | OMU  | 2     | 52   | 1    | -       | 0/9/27/28  | 0/2/2/2 |
| 1   | MA6  | 2     | 1475 | 1    | -       | 0/11/29/30 | 0/3/3/3 |
| 1   | 5MC  | 2     | 1368 | 1    | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | OMG  | 2     | 672  | 1    | -       | 0/9/27/28  | 0/3/3/3 |
| 1   | OMG  | 2     | 546  | 1    | -       | 1/9/27/28  | 0/3/3/3 |
| 32  | H2U  | 4     | 20   | 32   | -       | 3/7/38/39  | 0/2/2/2 |

The worst 5 of 75 bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 1   | 2     | 1457 | 6MZ  | C5-C4 | 4.50 | 1.47        | 1.39     |
| 1   | 2     | 494  | A2M  | C5-C4 | 4.44 | 1.47        | 1.39     |
| 1   | 2     | 1475 | MA6  | C5-C4 | 4.42 | 1.47        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 1   | 2     | 1457 | 6MZ  | C5-N7 | -3.51 | 1.32        | 1.39     |
| 32  | 4     | 55   | PSU  | C6-C5 | 3.02  | 1.38        | 1.35     |

The worst 5 of 157 bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 1   | 2     | 672  | OMG  | C5-C4-N3 | -6.23 | 118.35      | 128.46   |
| 1   | 2     | 1194 | OMG  | C5-C4-N3 | -6.20 | 118.39      | 128.46   |
| 1   | 2     | 926  | OMG  | C5-C4-N3 | -6.16 | 118.46      | 128.46   |
| 1   | 2     | 494  | A2M  | C5-C4-N3 | -6.16 | 118.71      | 126.75   |
| 1   | 2     | 1018 | OMG  | C5-C4-N3 | -6.16 | 118.47      | 128.46   |

There are no chirality outliers.

5 of 25 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 1   | 2     | 246 | OMC  | C3'-C4'-C5'-O5' |
| 1   | 2     | 246 | OMC  | O4'-C4'-C5'-O5' |
| 32  | 4     | 20  | H2U  | O4'-C1'-N1-C6   |
| 1   | 2     | 930 | C4J  | C4'-C5'-O5'-P   |
| 32  | 4     | 20  | H2U  | O4'-C1'-N1-C2   |

There are no ring outliers.

21 monomers are involved in 32 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 1   | 2     | 1478 | 4AC  | 3       | 0            |
| 1   | 2     | 1018 | OMG  | 2       | 0            |
| 1   | 2     | 481  | OMC  | 2       | 0            |
| 1   | 2     | 865  | OMG  | 1       | 0            |
| 1   | 2     | 1344 | OMU  | 2       | 0            |
| 1   | 2     | 246  | OMC  | 2       | 0            |
| 1   | 2     | 926  | OMG  | 1       | 0            |
| 1   | 2     | 1366 | OMC  | 2       | 0            |
| 1   | 2     | 1467 | 4AC  | 1       | 0            |
| 1   | 2     | 512  | OMC  | 1       | 0            |
| 1   | 2     | 113  | OMC  | 1       | 0            |
| 32  | 4     | 32   | OMC  | 1       | 0            |
| 1   | 2     | 1466 | 4AC  | 2       | 0            |
| 1   | 2     | 337  | OMG  | 1       | 0            |
| 1   | 2     | 1457 | 6MZ  | 1       | 0            |

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| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 1   | 2     | 538  | OMC  | 2       | 0            |
| 1   | 2     | 843  | 4AC  | 2       | 0            |
| 1   | 2     | 1477 | 4AC  | 4       | 0            |
| 1   | 2     | 1032 | OMU  | 2       | 0            |
| 1   | 2     | 1368 | 5MC  | 1       | 0            |
| 1   | 2     | 672  | OMG  | 1       | 0            |

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 110 ligands modelled in this entry, 64 are monoatomic - leaving 46 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 | $\# Z  > 2$ |
| 36  | SPM  | 2     | 1521   | 1    | 13,13,13     | 0.09 | 0           | 12,12,12    | 0.11 | 0           |
| 36  | SPM  | 2     | 1530   | -    | 13,13,13     | 0.11 | 0           | 12,12,12    | 0.07 | 0           |
| 36  | SPM  | 2     | 1540   | -    | 13,13,13     | 0.12 | 0           | 12,12,12    | 0.09 | 0           |
| 36  | SPM  | 2     | 1541   | 1    | 13,13,13     | 0.09 | 0           | 12,12,12    | 0.16 | 0           |
| 36  | SPM  | 2     | 1537   | -    | 13,13,13     | 0.11 | 0           | 12,12,12    | 0.08 | 0           |
| 36  | SPM  | 2     | 1533   | -    | 13,13,13     | 0.10 | 0           | 12,12,12    | 0.10 | 0           |
| 36  | SPM  | 2     | 1538   | -    | 13,13,13     | 0.09 | 0           | 12,12,12    | 0.10 | 0           |
| 36  | SPM  | 2     | 1522   | -    | 13,13,13     | 0.10 | 0           | 12,12,12    | 0.07 | 0           |
| 36  | SPM  | 2     | 1527   | -    | 13,13,13     | 0.10 | 0           | 12,12,12    | 0.08 | 0           |
| 36  | SPM  | 2     | 1542   | -    | 13,13,13     | 0.10 | 0           | 12,12,12    | 0.06 | 0           |
| 36  | SPM  | 2     | 1514   | -    | 13,13,13     | 0.10 | 0           | 12,12,12    | 0.08 | 0           |
| 36  | SPM  | 2     | 1529   | -    | 13,13,13     | 0.10 | 0           | 12,12,12    | 0.07 | 0           |
| 36  | SPM  | 2     | 1506   | -    | 13,13,13     | 0.07 | 0           | 12,12,12    | 0.13 | 0           |
| 36  | SPM  | 2     | 1523   | -    | 13,13,13     | 0.10 | 0           | 12,12,12    | 0.09 | 0           |
| 36  | SPM  | 2     | 1508   | -    | 13,13,13     | 0.08 | 0           | 12,12,12    | 0.09 | 0           |
| 36  | SPM  | 2     | 1531   | -    | 13,13,13     | 0.10 | 0           | 12,12,12    | 0.06 | 0           |
| 39  | ATP  | 5     | 102[B] | 31   | 29,33,33     | 0.30 | 0           | 44,52,52    | 0.46 | 1 (2%)      |

| Mol | Type | Chain | Res    | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|--------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |        |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 36  | SPM  | 2     | 1503   | -    | 13,13,13     | 0.09 | 0        | 12,12,12    | 0.13 | 0        |
| 36  | SPM  | 2     | 1509   | -    | 13,13,13     | 0.07 | 0        | 12,12,12    | 0.12 | 0        |
| 39  | ATP  | 5     | 102[A] | 31   | 29,33,33     | 0.31 | 0        | 44,52,52    | 0.47 | 1 (2%)   |
| 36  | SPM  | 2     | 1517   | -    | 13,13,13     | 0.07 | 0        | 12,12,12    | 0.15 | 0        |
| 36  | SPM  | 2     | 1512   | -    | 13,13,13     | 0.10 | 0        | 12,12,12    | 0.08 | 0        |
| 36  | SPM  | 2     | 1504   | -    | 13,13,13     | 0.11 | 0        | 12,12,12    | 0.07 | 0        |
| 36  | SPM  | 2     | 1511   | -    | 13,13,13     | 0.09 | 0        | 12,12,12    | 0.09 | 0        |
| 36  | SPM  | 2     | 1516   | -    | 13,13,13     | 0.06 | 0        | 12,12,12    | 0.12 | 0        |
| 36  | SPM  | 2     | 1528   | -    | 13,13,13     | 0.08 | 0        | 12,12,12    | 0.09 | 0        |
| 36  | SPM  | 2     | 1505   | -    | 13,13,13     | 0.06 | 0        | 12,12,12    | 0.13 | 0        |
| 36  | SPM  | 2     | 1501   | -    | 13,13,13     | 0.07 | 0        | 12,12,12    | 0.13 | 0        |
| 36  | SPM  | 2     | 1513   | -    | 13,13,13     | 0.09 | 0        | 12,12,12    | 0.15 | 0        |
| 36  | SPM  | 2     | 1524   | -    | 13,13,13     | 0.08 | 0        | 12,12,12    | 0.09 | 0        |
| 36  | SPM  | 2     | 1543   | -    | 13,13,13     | 0.09 | 0        | 12,12,12    | 0.16 | 0        |
| 36  | SPM  | 2     | 1515   | -    | 13,13,13     | 0.09 | 0        | 12,12,12    | 0.08 | 0        |
| 36  | SPM  | 2     | 1525   | -    | 13,13,13     | 0.11 | 0        | 12,12,12    | 0.10 | 0        |
| 36  | SPM  | 2     | 1502   | -    | 13,13,13     | 0.13 | 0        | 12,12,12    | 0.09 | 0        |
| 36  | SPM  | 2     | 1510   | -    | 13,13,13     | 0.08 | 0        | 12,12,12    | 0.08 | 0        |
| 36  | SPM  | 2     | 1534   | -    | 13,13,13     | 0.09 | 0        | 12,12,12    | 0.10 | 0        |
| 36  | SPM  | 2     | 1535   | -    | 13,13,13     | 0.11 | 0        | 12,12,12    | 0.10 | 0        |
| 36  | SPM  | 2     | 1520   | -    | 13,13,13     | 0.10 | 0        | 12,12,12    | 0.12 | 0        |
| 36  | SPM  | 2     | 1507   | -    | 13,13,13     | 0.08 | 0        | 12,12,12    | 0.11 | 0        |
| 36  | SPM  | 2     | 1544   | -    | 13,13,13     | 0.11 | 0        | 12,12,12    | 0.10 | 0        |
| 36  | SPM  | 2     | 1532   | -    | 13,13,13     | 0.10 | 0        | 12,12,12    | 0.07 | 0        |
| 36  | SPM  | 2     | 1539   | -    | 13,13,13     | 0.11 | 0        | 12,12,12    | 0.08 | 0        |
| 36  | SPM  | 2     | 1526   | -    | 13,13,13     | 0.10 | 0        | 12,12,12    | 0.08 | 0        |
| 36  | SPM  | 2     | 1519   | -    | 13,13,13     | 0.11 | 0        | 12,12,12    | 0.06 | 0        |
| 36  | SPM  | 2     | 1518   | -    | 13,13,13     | 0.07 | 0        | 12,12,12    | 0.11 | 0        |
| 36  | SPM  | 2     | 1536   | -    | 13,13,13     | 0.09 | 0        | 12,12,12    | 0.08 | 0        |

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

| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings |
|-----|------|-------|------|------|---------|------------|-------|
| 36  | SPM  | 2     | 1521 | 1    | -       | 2/11/11/11 | -     |
| 36  | SPM  | 2     | 1530 | -    | -       | 4/11/11/11 | -     |
| 36  | SPM  | 2     | 1540 | -    | -       | 2/11/11/11 | -     |
| 36  | SPM  | 2     | 1541 | 1    | -       | 4/11/11/11 | -     |
| 36  | SPM  | 2     | 1537 | -    | -       | 2/11/11/11 | -     |

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| Mol | Type | Chain | Res    | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|--------|------|---------|------------|---------|
| 36  | SPM  | 2     | 1533   | -    | -       | 2/11/11/11 | -       |
| 36  | SPM  | 2     | 1538   | -    | -       | 1/11/11/11 | -       |
| 36  | SPM  | 2     | 1522   | -    | -       | 2/11/11/11 | -       |
| 36  | SPM  | 2     | 1527   | -    | -       | 3/11/11/11 | -       |
| 36  | SPM  | 2     | 1542   | -    | -       | 4/11/11/11 | -       |
| 36  | SPM  | 2     | 1514   | -    | -       | 3/11/11/11 | -       |
| 36  | SPM  | 2     | 1529   | -    | -       | 2/11/11/11 | -       |
| 36  | SPM  | 2     | 1506   | -    | -       | 4/11/11/11 | -       |
| 36  | SPM  | 2     | 1523   | -    | -       | 4/11/11/11 | -       |
| 36  | SPM  | 2     | 1508   | -    | -       | 1/11/11/11 | -       |
| 36  | SPM  | 2     | 1531   | -    | -       | 2/11/11/11 | -       |
| 39  | ATP  | 5     | 102[B] | 31   | -       | 6/22/38/38 | 0/3/3/3 |
| 36  | SPM  | 2     | 1503   | -    | -       | 3/11/11/11 | -       |
| 36  | SPM  | 2     | 1509   | -    | -       | 2/11/11/11 | -       |
| 39  | ATP  | 5     | 102[A] | 31   | -       | 5/22/38/38 | 0/3/3/3 |
| 36  | SPM  | 2     | 1517   | -    | -       | 5/11/11/11 | -       |
| 36  | SPM  | 2     | 1512   | -    | -       | 3/11/11/11 | -       |
| 36  | SPM  | 2     | 1504   | -    | -       | 1/11/11/11 | -       |
| 36  | SPM  | 2     | 1511   | -    | -       | 2/11/11/11 | -       |
| 36  | SPM  | 2     | 1516   | -    | -       | 2/11/11/11 | -       |
| 36  | SPM  | 2     | 1528   | -    | -       | 3/11/11/11 | -       |
| 36  | SPM  | 2     | 1505   | -    | -       | 2/11/11/11 | -       |
| 36  | SPM  | 2     | 1501   | -    | -       | 2/11/11/11 | -       |
| 36  | SPM  | 2     | 1513   | -    | -       | 0/11/11/11 | -       |
| 36  | SPM  | 2     | 1524   | -    | -       | 3/11/11/11 | -       |
| 36  | SPM  | 2     | 1543   | -    | -       | 4/11/11/11 | -       |
| 36  | SPM  | 2     | 1515   | -    | -       | 2/11/11/11 | -       |
| 36  | SPM  | 2     | 1525   | -    | -       | 3/11/11/11 | -       |
| 36  | SPM  | 2     | 1502   | -    | -       | 3/11/11/11 | -       |
| 36  | SPM  | 2     | 1510   | -    | -       | 1/11/11/11 | -       |
| 36  | SPM  | 2     | 1534   | -    | -       | 3/11/11/11 | -       |
| 36  | SPM  | 2     | 1535   | -    | -       | 3/11/11/11 | -       |
| 36  | SPM  | 2     | 1520   | -    | -       | 4/11/11/11 | -       |
| 36  | SPM  | 2     | 1507   | -    | -       | 4/11/11/11 | -       |
| 36  | SPM  | 2     | 1544   | -    | -       | 2/11/11/11 | -       |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings |
|-----|------|-------|------|------|---------|------------|-------|
| 36  | SPM  | 2     | 1532 | -    | -       | 4/11/11/11 | -     |
| 36  | SPM  | 2     | 1539 | -    | -       | 2/11/11/11 | -     |
| 36  | SPM  | 2     | 1526 | -    | -       | 1/11/11/11 | -     |
| 36  | SPM  | 2     | 1519 | -    | -       | 2/11/11/11 | -     |
| 36  | SPM  | 2     | 1518 | -    | -       | 2/11/11/11 | -     |
| 36  | SPM  | 2     | 1536 | -    | -       | 3/11/11/11 | -     |

There are no bond length outliers.

All (2) bond angle outliers are listed below:

| Mol | Chain | Res    | Type | Atoms     | Z    | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|------|-------------|----------|
| 39  | 5     | 102[B] | ATP  | PB-O3B-PG | 2.02 | 139.75      | 132.83   |
| 39  | 5     | 102[A] | ATP  | PB-O3B-PG | 2.00 | 139.69      | 132.83   |

There are no chirality outliers.

5 of 124 torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms          |
|-----|-------|------|------|----------------|
| 36  | 2     | 1509 | SPM  | C12-C11-N10-C9 |
| 36  | 2     | 1518 | SPM  | C7-C6-N5-C4    |
| 36  | 2     | 1520 | SPM  | C12-C11-N10-C9 |
| 36  | 2     | 1521 | SPM  | C3-C4-N5-C6    |
| 36  | 2     | 1523 | SPM  | C7-C6-N5-C4    |

There are no ring outliers.

30 monomers are involved in 52 short contacts:

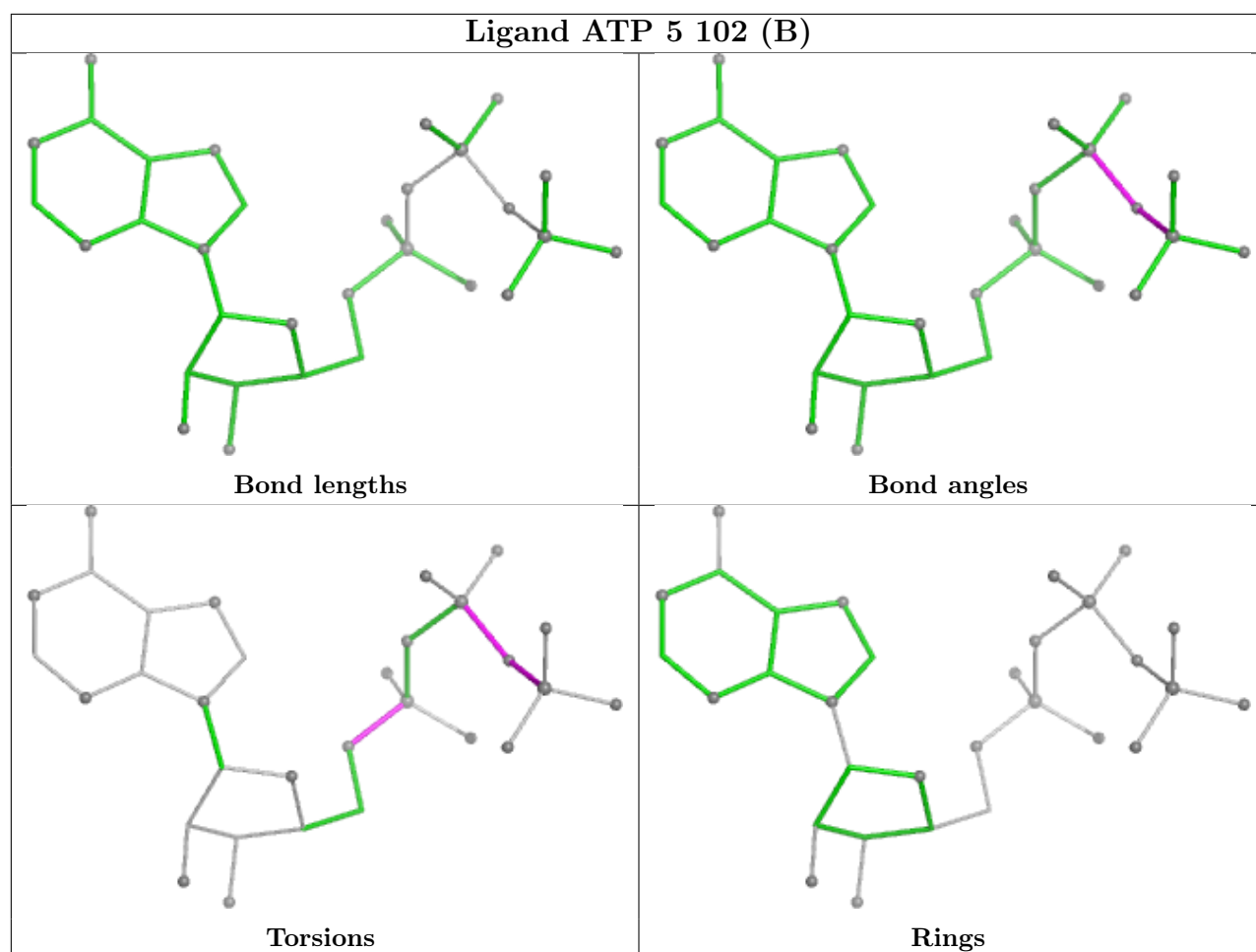
| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 36  | 2     | 1521 | SPM  | 1       | 0            |
| 36  | 2     | 1530 | SPM  | 1       | 0            |
| 36  | 2     | 1540 | SPM  | 2       | 0            |
| 36  | 2     | 1541 | SPM  | 5       | 0            |
| 36  | 2     | 1537 | SPM  | 3       | 0            |
| 36  | 2     | 1533 | SPM  | 2       | 0            |
| 36  | 2     | 1522 | SPM  | 1       | 0            |
| 36  | 2     | 1527 | SPM  | 1       | 0            |
| 36  | 2     | 1514 | SPM  | 3       | 0            |
| 36  | 2     | 1523 | SPM  | 1       | 0            |
| 36  | 2     | 1508 | SPM  | 1       | 0            |
| 36  | 2     | 1509 | SPM  | 2       | 0            |

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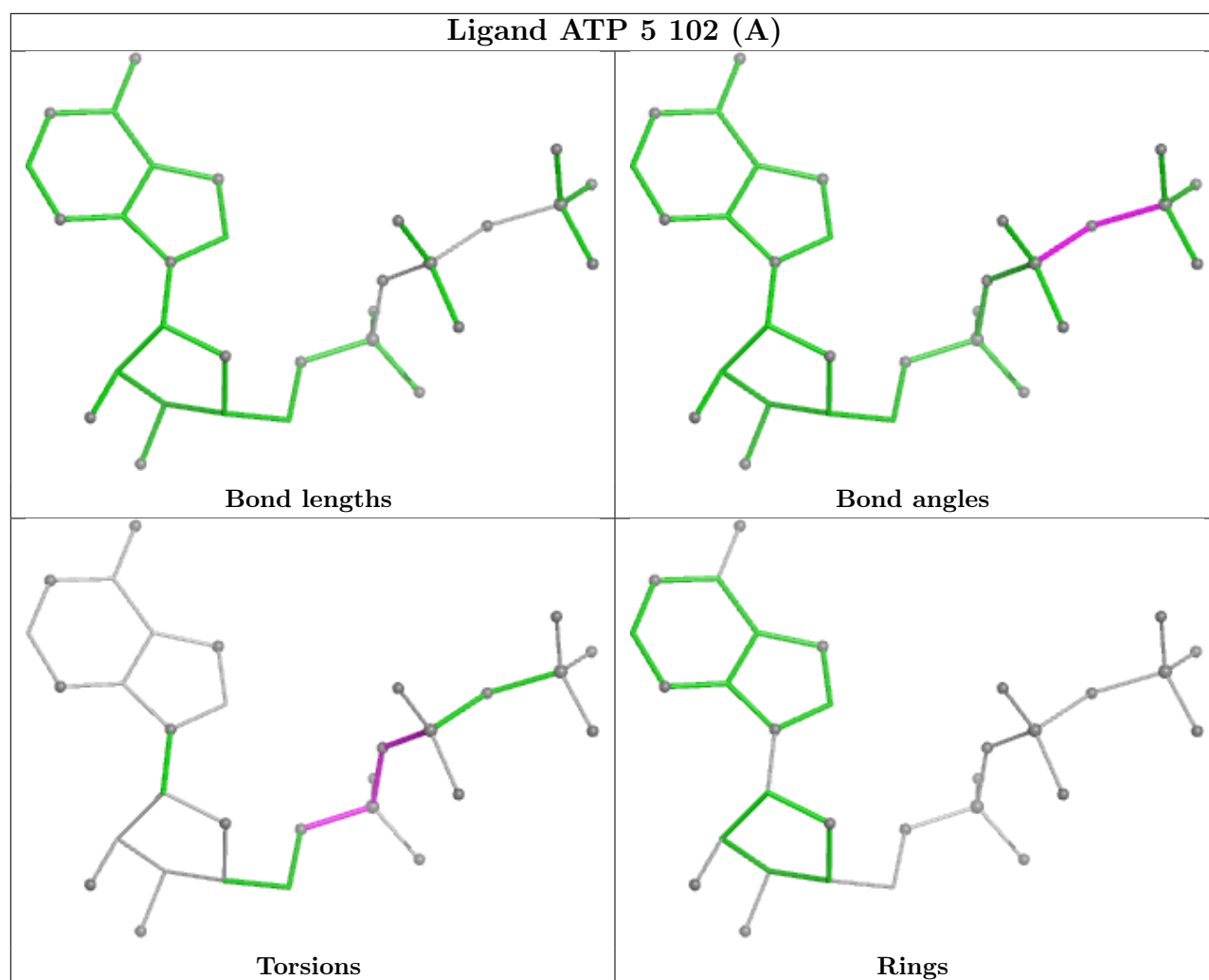
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| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 36  | 2     | 1517 | SPM  | 2       | 0            |
| 36  | 2     | 1516 | SPM  | 3       | 0            |
| 36  | 2     | 1528 | SPM  | 1       | 0            |
| 36  | 2     | 1501 | SPM  | 2       | 0            |
| 36  | 2     | 1513 | SPM  | 2       | 0            |
| 36  | 2     | 1524 | SPM  | 1       | 0            |
| 36  | 2     | 1543 | SPM  | 2       | 0            |
| 36  | 2     | 1515 | SPM  | 2       | 0            |
| 36  | 2     | 1525 | SPM  | 1       | 0            |
| 36  | 2     | 1502 | SPM  | 1       | 0            |
| 36  | 2     | 1534 | SPM  | 1       | 0            |
| 36  | 2     | 1535 | SPM  | 1       | 0            |
| 36  | 2     | 1520 | SPM  | 3       | 0            |
| 36  | 2     | 1507 | SPM  | 2       | 0            |
| 36  | 2     | 1544 | SPM  | 1       | 0            |
| 36  | 2     | 1532 | SPM  | 1       | 0            |
| 36  | 2     | 1526 | SPM  | 2       | 0            |
| 36  | 2     | 1518 | SPM  | 2       | 0            |

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







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

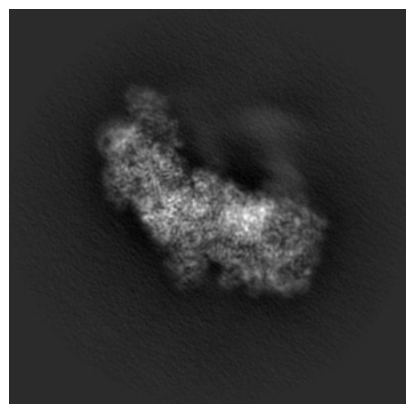
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-50727. These allow visual inspection of the internal detail of the map and identification of artifacts.

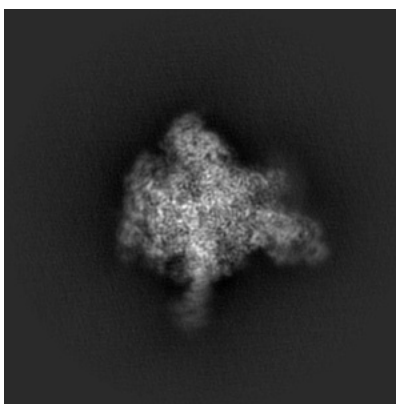
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

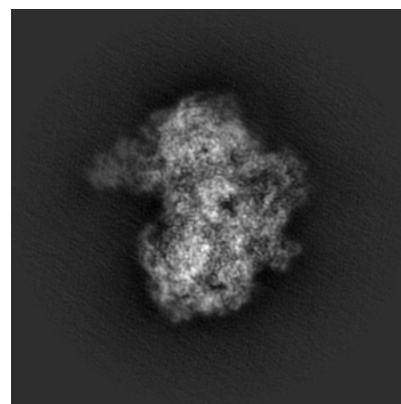
#### 6.1.1 Primary map



X

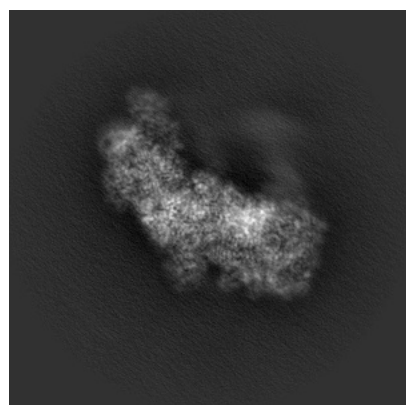


Y

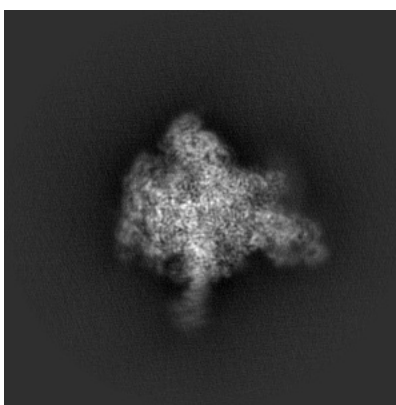


Z

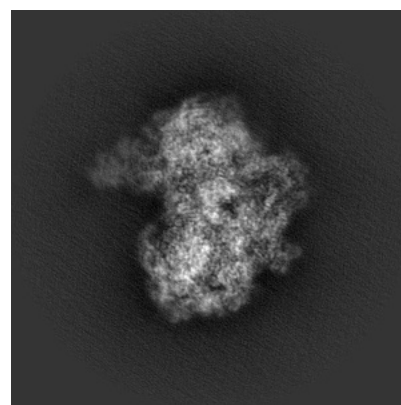
#### 6.1.2 Raw map



X



Y

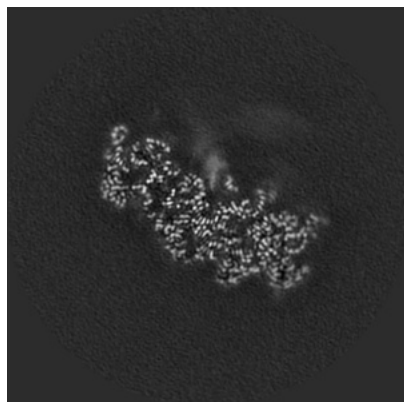


Z

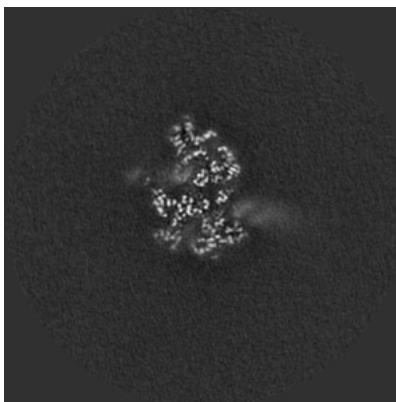
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

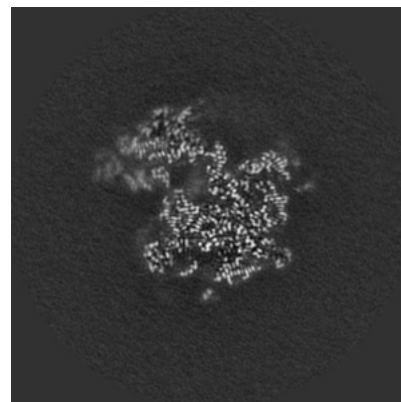
### 6.2.1 Primary map



X Index: 219

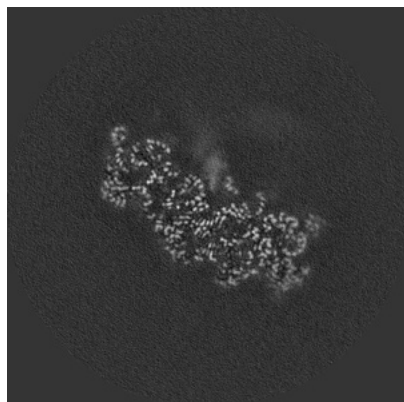


Y Index: 219

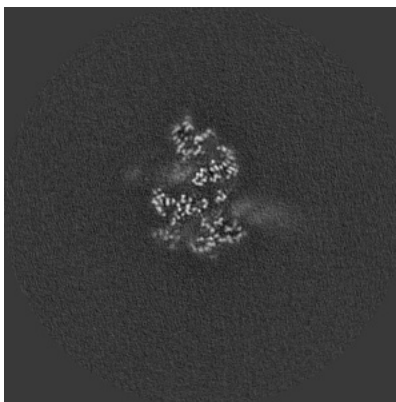


Z Index: 219

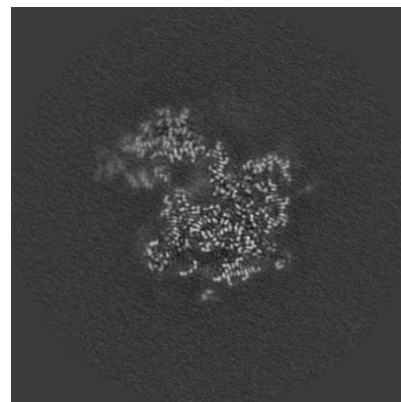
### 6.2.2 Raw map



X Index: 219



Y Index: 219

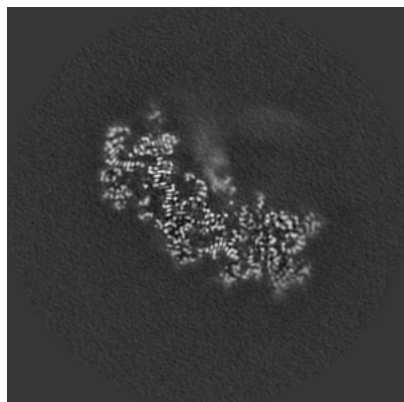


Z Index: 219

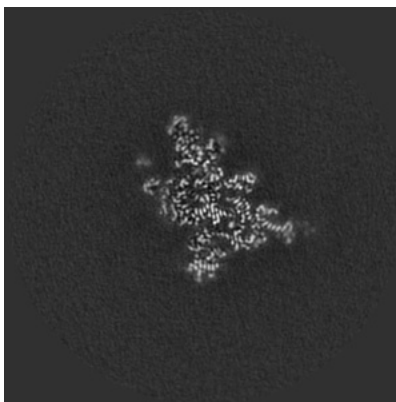
The images above show central slices of the map in three orthogonal directions.

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

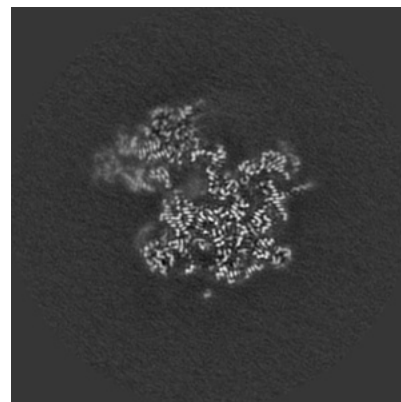
### 6.3.1 Primary map



X Index: 214

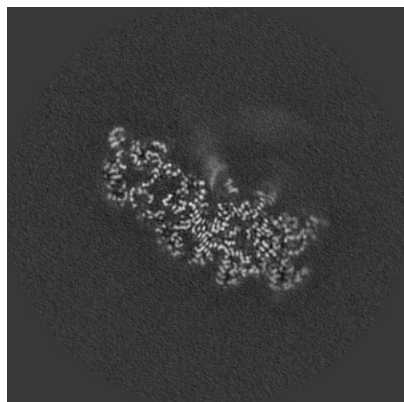


Y Index: 176

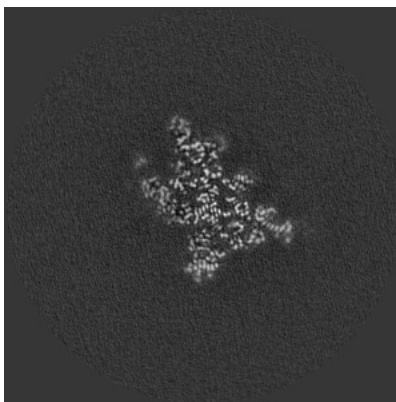


Z Index: 217

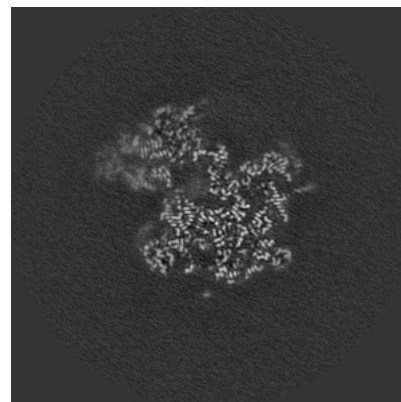
### 6.3.2 Raw map



X Index: 222



Y Index: 178



Z Index: 216

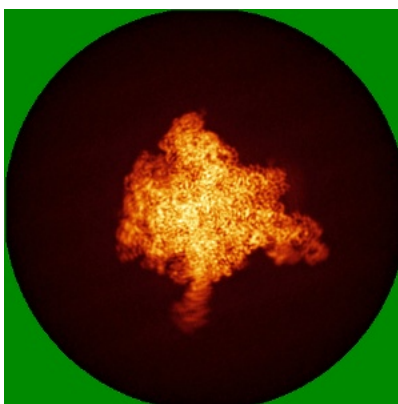
The images above show the largest variance slices of the map in three orthogonal directions.

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

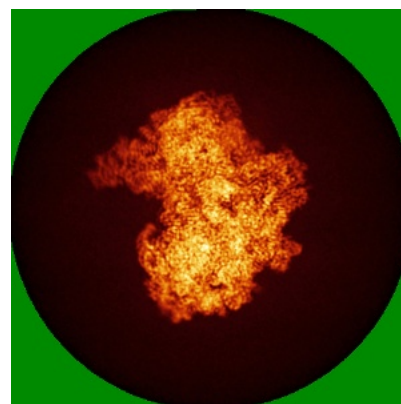
### 6.4.1 Primary map



X

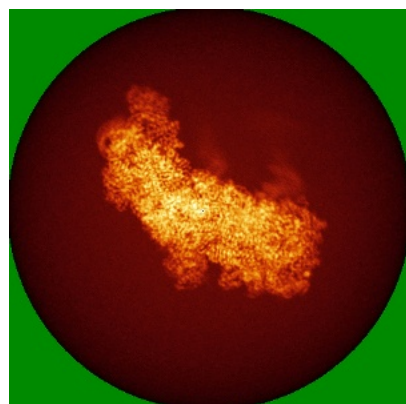


Y

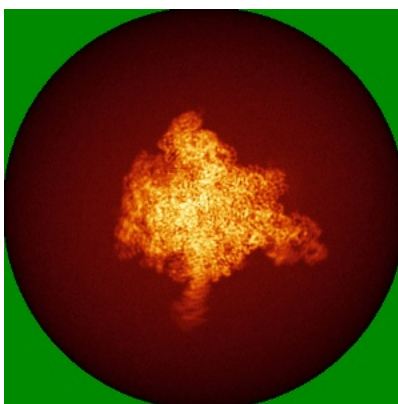


Z

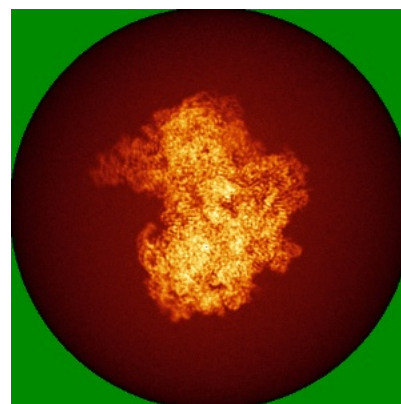
### 6.4.2 Raw map



X



Y



Z

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



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

### 6.5.1 Primary map



X



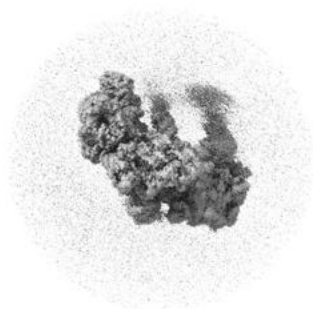
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.004. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



X



Y



Z

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

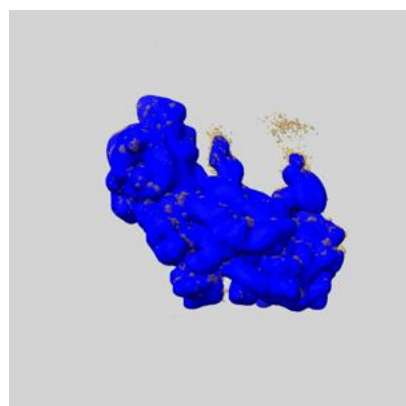
## 6.6 Mask visualisation [i](#)

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

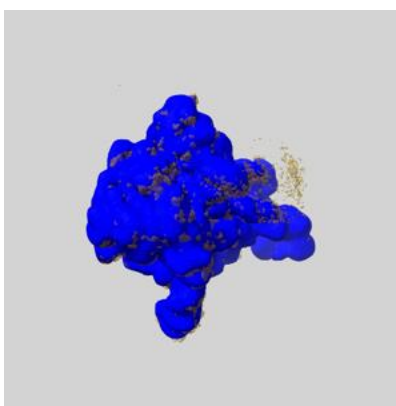
A mask typically either:

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

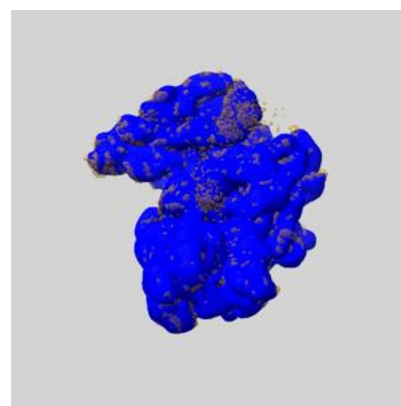
### 6.6.1 emd\_50727\_msk\_1.map [i](#)



X



Y

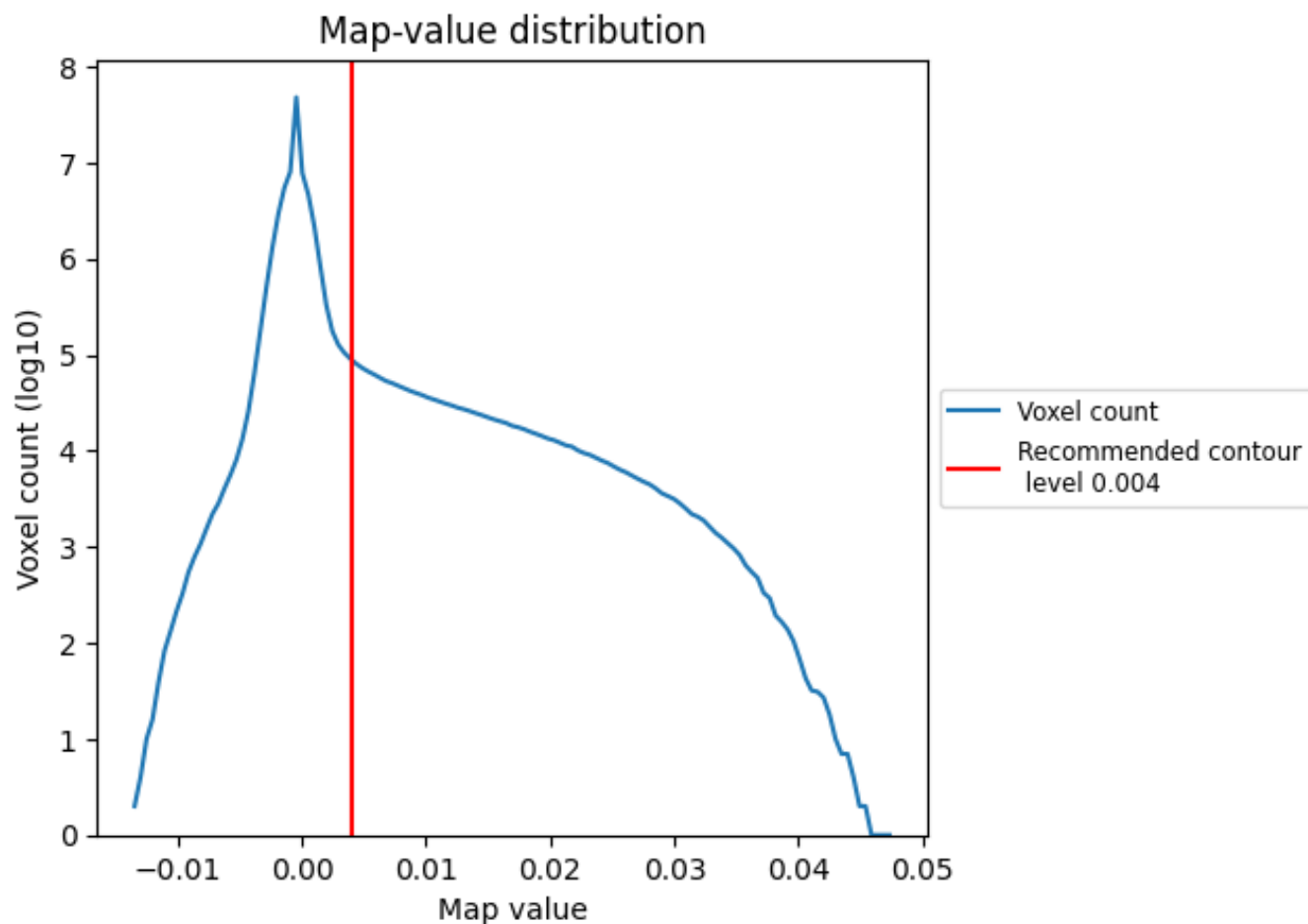


Z

## 7 Map analysis [i](#)

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

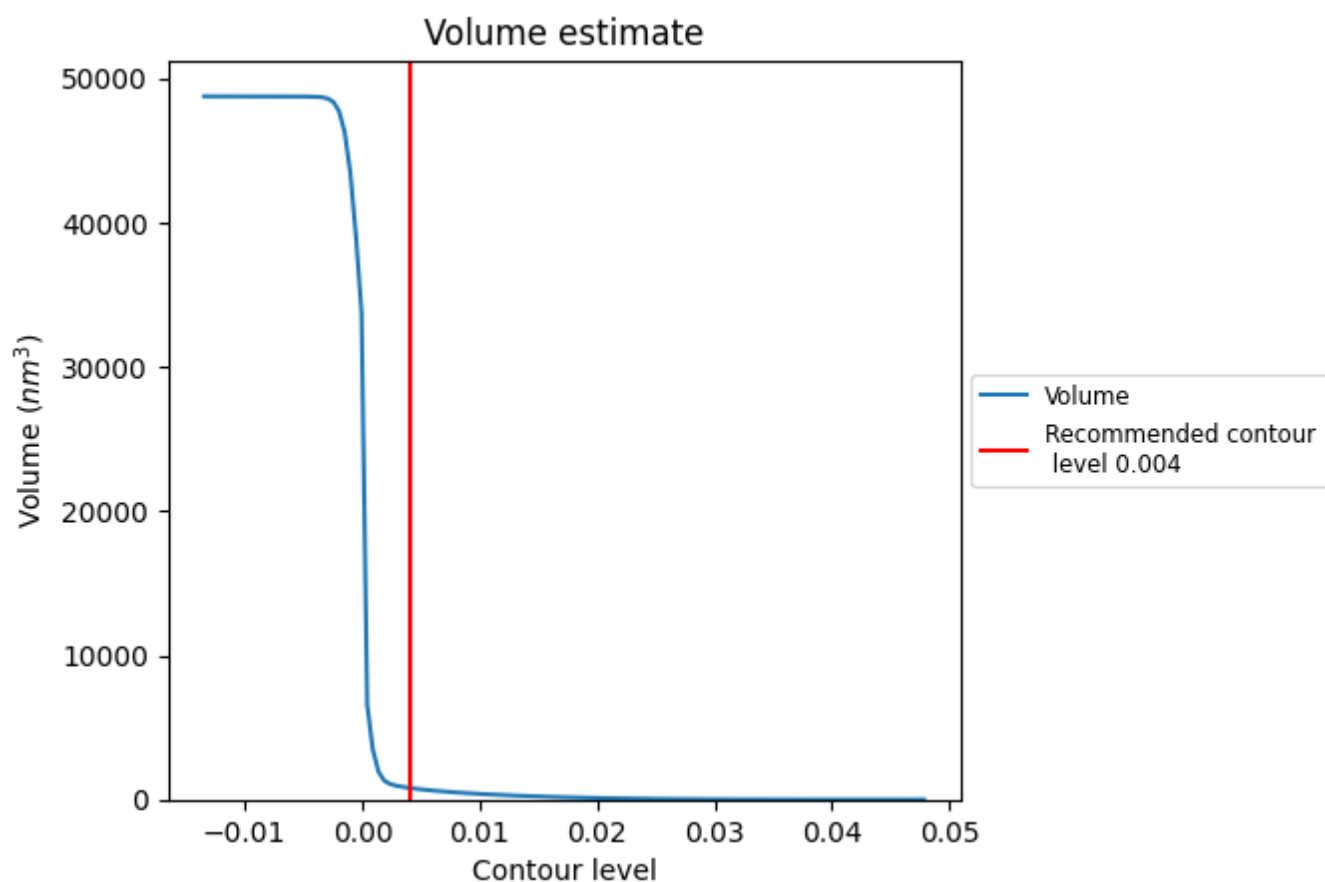
### 7.1 Map-value distribution [i](#)



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



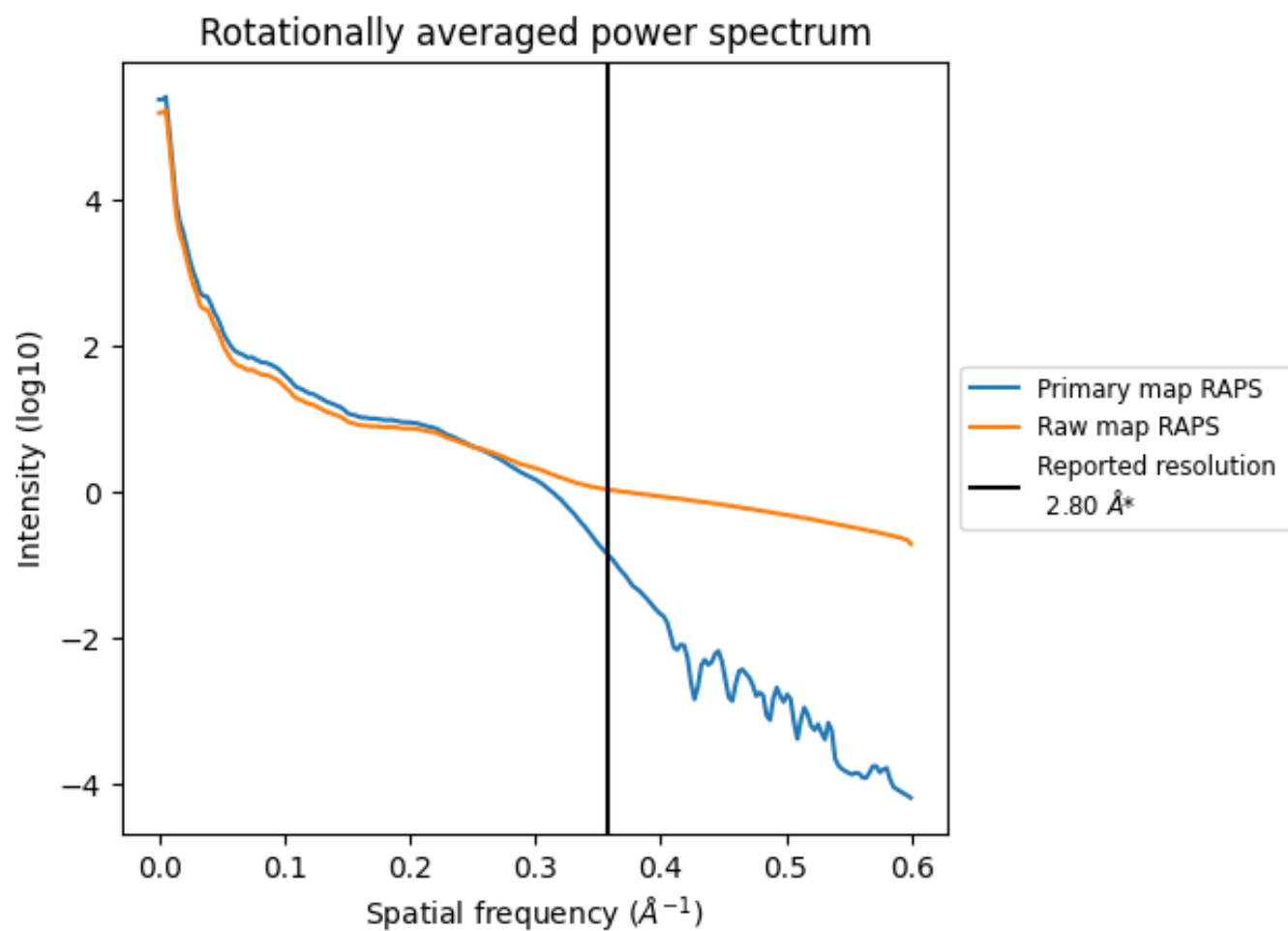
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 808  $\text{nm}^3$ ; this corresponds to an approximate mass of 730 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 ⓘ

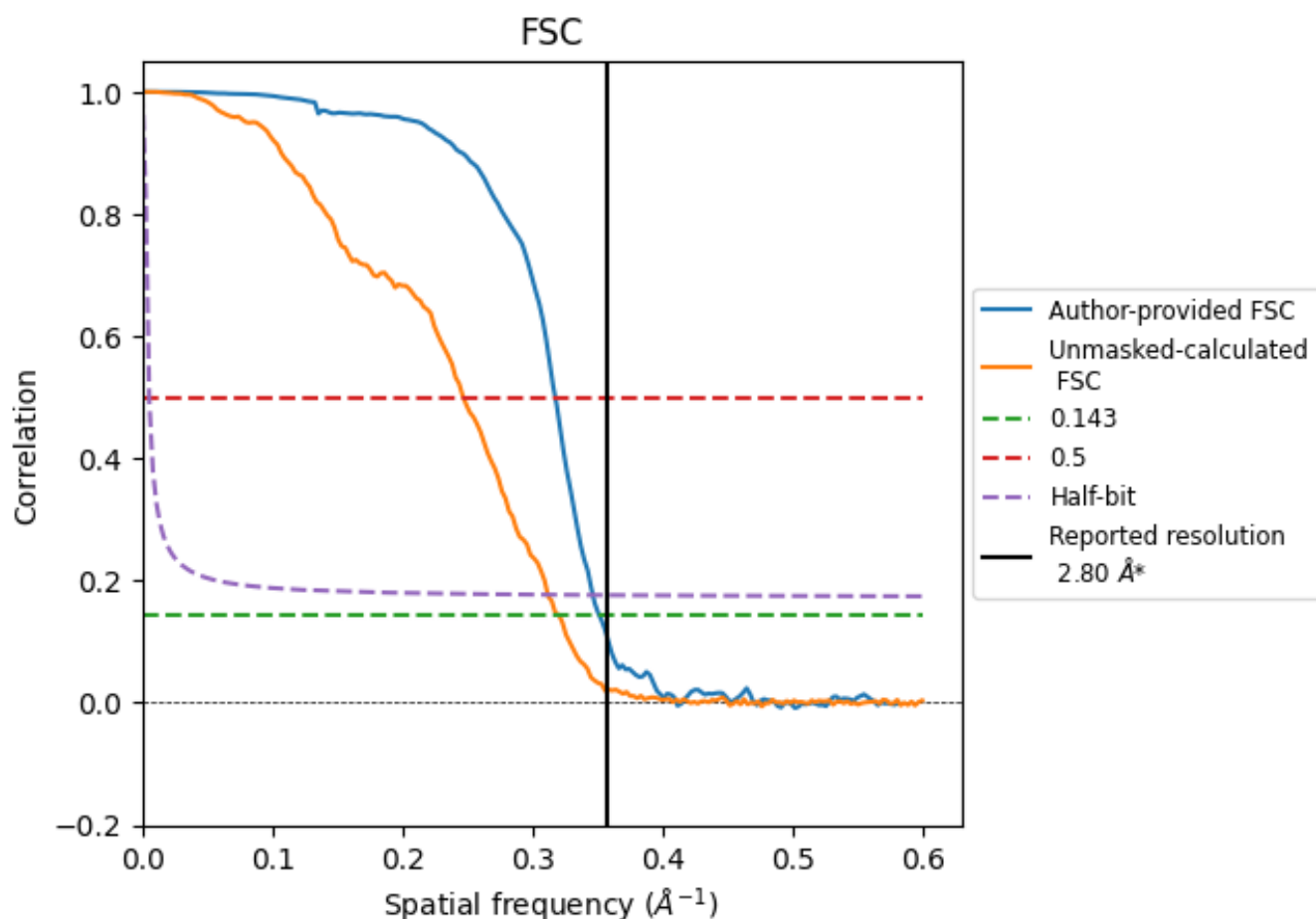


\*Reported resolution corresponds to spatial frequency of 0.357 Å<sup>-1</sup>

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.357 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

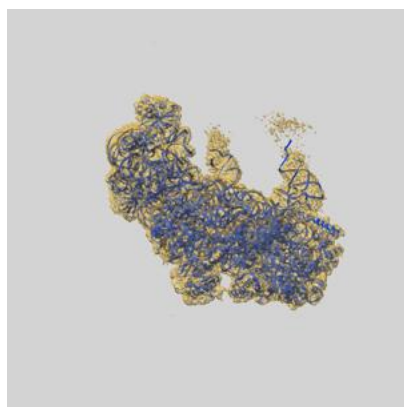
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 2.80                               | -    | -        |
| Author-provided FSC curve | 2.85                               | 3.15 | 2.89     |
| Unmasked-calculated*      | 3.12                               | 4.05 | 3.21     |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.12 differs from the reported value 2.8 by more than 10 %

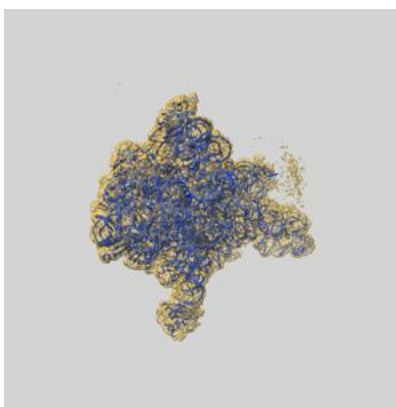
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-50727 and PDB model 9FSF. Per-residue inclusion information can be found in section [3](#) on page [15](#).

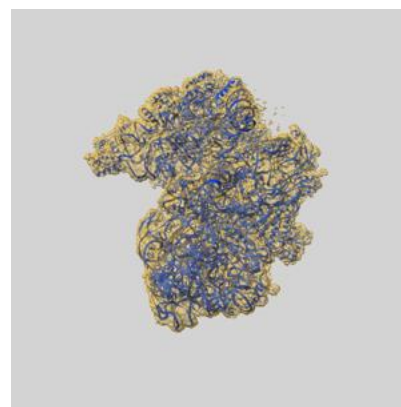
### 9.1 Map-model overlay [i](#)



X



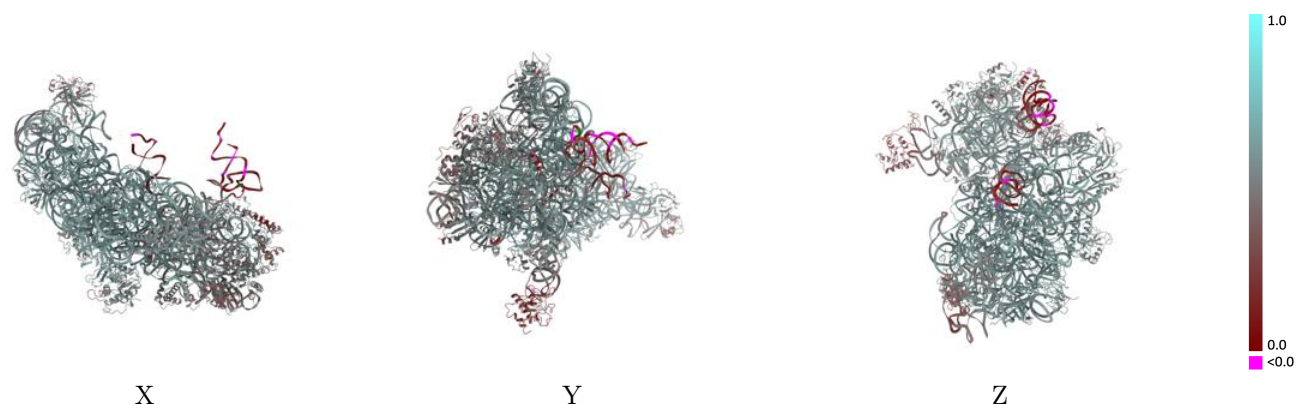
Y



Z

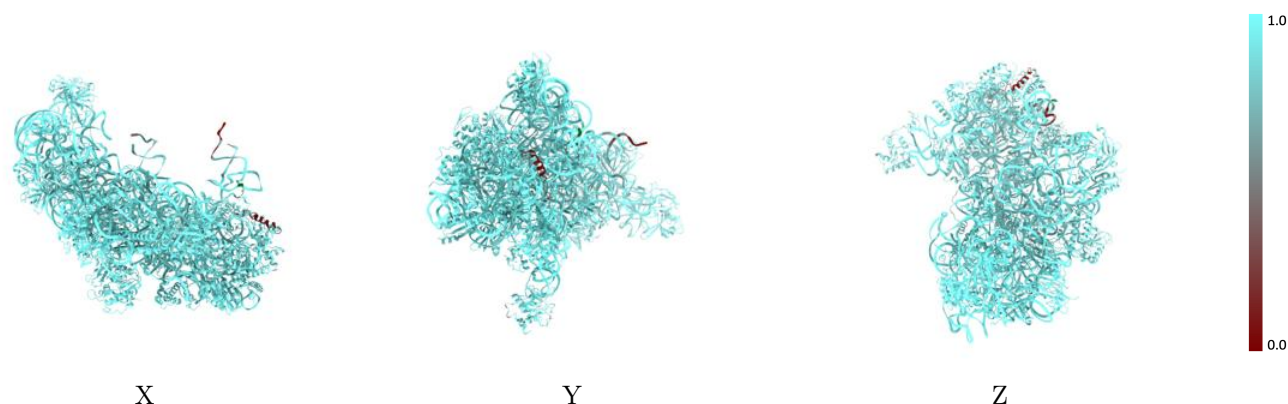
The images above show the 3D surface view of the map at the recommended contour level 0.004 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



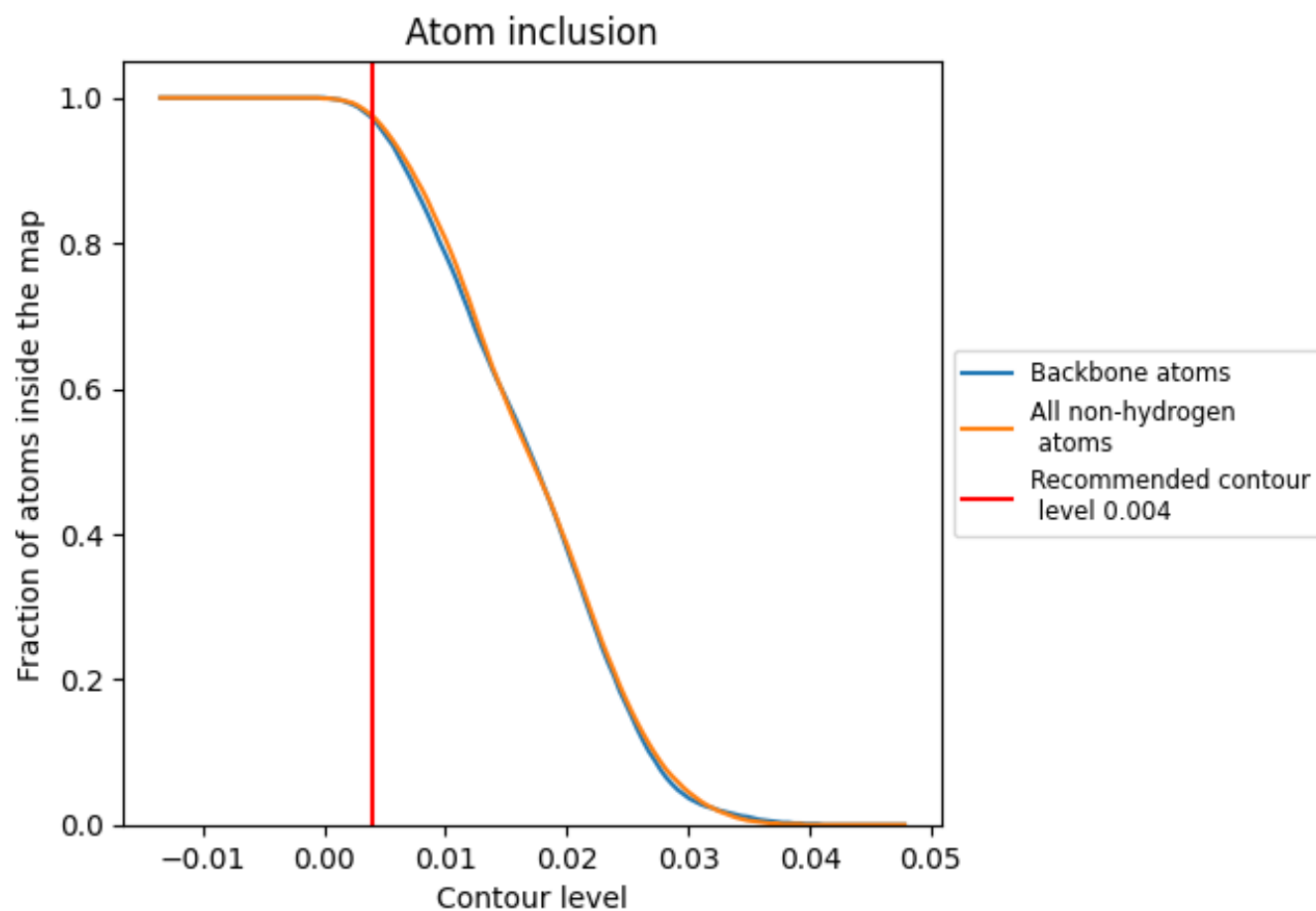
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.004).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 98% 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 (0.004) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.9750   |  0.5280   |
| 2     |  0.9940   |  0.5580   |
| 3     |  0.8800   |  0.2190   |
| 4     |  0.8670   |  0.2380   |
| 5     |  0.7840   |  0.3620   |
| A     |  0.9780   |  0.5220   |
| B     |  0.9650   |  0.5310   |
| C     |  0.9750   |  0.5650   |
| D     |  0.9890   |  0.5760   |
| E     |  0.9920   |  0.5750   |
| F     |  0.9880   |  0.5860   |
| G     |  0.9760   |  0.4500   |
| H     |  0.9570   |  0.4820   |
| I     |  0.9890   |  0.5960   |
| J     |  0.9950  |  0.5620  |
| K     |  0.9830 |  0.5140 |
| L     |  0.9640 |  0.4930 |
| M     |  0.9710 |  0.5210 |
| N     |  0.9880 |  0.5760 |
| O     |  0.9840 |  0.5190 |
| P     |  0.9860 |  0.5660 |
| Q     |  0.9880 |  0.5580 |
| R     |  0.9870 |  0.5900 |
| S     |  0.9800 |  0.5070 |
| T     |  0.9650 |  0.5070 |
| U     |  0.9830 |  0.5170 |
| V     |  0.9600 |  0.5420 |
| W     |  0.9920 |  0.5540 |
| X     |  0.9550 |  0.4400 |
| Y     |  0.8860 |  0.2320 |
| Z     |  0.9720 |  0.5330 |
| a     |  0.9710 |  0.5070 |
| c     |  0.6820 |  0.3630 |
| d     |  0.9550 |  0.3860 |
| e     |  0.8540 |  0.5430 |
| s     |  0.9320 |  0.2950 |

