# wwPDB EM Validation Summary Report (i)

Jul 14, 2026 – 06:11 pm BST

| | | |
|---|---|---|
| PDB ID | : | 9TEX / pdb_00009tex |
| EMDB ID | : | EMD-55845 |
| Title | : | Dal2 bound to the Escherichia coli 70S ribosome |
| Authors | : | Berger, M.J.; Safdari, H.A.; Wilson, D.N. |
| Deposited on | : | 2025-11-26 |
| Resolution | : | 2.54 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

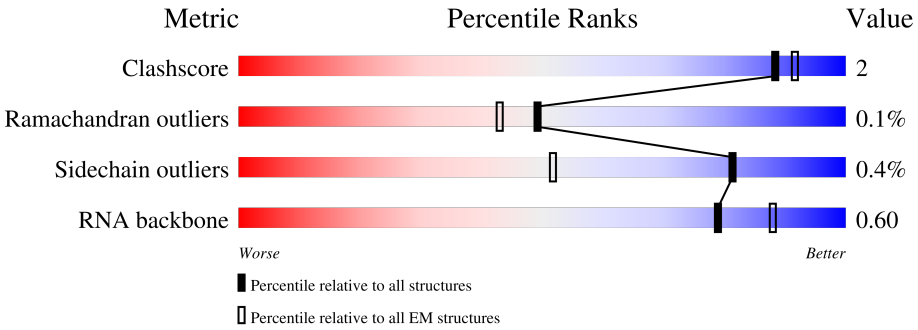
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev133 |
| Mogul | : | 1.8.4, CSD as541be (2020) |
| MolProbity | : | 4-5-2 with Phenix2.0 |
| Percentile statistics | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| EM percentile statistics | : | 202505.v01 (Using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

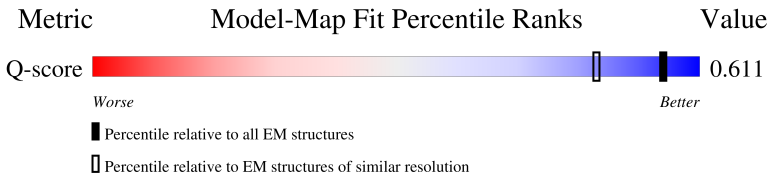
# 1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.54 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 (#Entries) | EM structures (#Entries) | Similar EM resolution (#Entries, resolution range(Å)) |
|---|---|---|---|
| Clashscore | 229148 | 23984 | - |
| Ramachandran outliers | 224038 | 23583 | - |
| Sidechain outliers | 223484 | 23102 | - |
| RNA backbone | 8273 | 3508 | - |
| Q-score | - | 25397 | 7403 ( 2.04 - 3.04 ) |

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 >=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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | a | 2904 | 5% 78% 15% • 5% |
| 2 | A | 1542 | 7% 77% 20% •• |
| 3 | 3 | 38 | 8% 87% 13% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 4 | 4 | 70 | 67% 74% 10% 16% |
| 5 | K | 129 | 12% 81% 9% 9% |
| 6 | L | 124 | 14% 89% 10% |
| 7 | d | 209 | 5% 92% 8% |
| 8 | l | 136 | 86% 14% |
| 9 | 0 | 55 | 7% 82% 7% 11% |
| 10 | 1 | 46 | 93% |
| 11 | 2 | 65 | 85% 14% |
| 12 | B | 241 | 48% 83% 10% 7% |
| 13 | C | 233 | 27% 83% 5% 12% |
| 14 | D | 206 | 29% 84% 15% |
| 15 | E | 167 | 8% 87% 6% 7% |
| 16 | F | 135 | 19% 67% 10% 24% |
| 17 | G | 179 | 35% 77% 6% 18% |
| 18 | H | 130 | 9% 94% 5% |
| 19 | I | 130 | 36% 90% 6% |
| 20 | J | 103 | 57% 81% 15% 5% |
| 21 | M | 118 | 44% 84% 14% |
| 22 | N | 101 | 24% 96% |
| 23 | O | 89 | 16% 96% |
| 24 | P | 82 | 21% 88% 11% |
| 25 | Q | 84 | 32% 76% 15% 8% |
| 26 | R | 75 | 11% 64% 9% 27% |
| 27 | S | 92 | 45% 82% 10% 9% |
| 28 | T | 87 | 17% 92% 6% |

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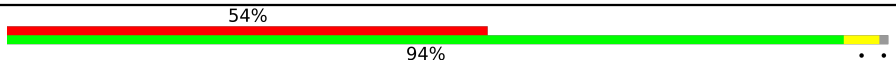
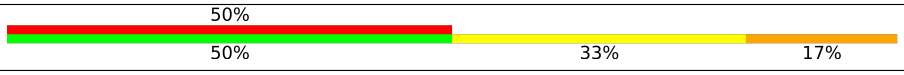
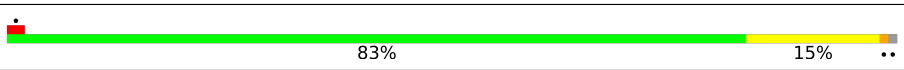
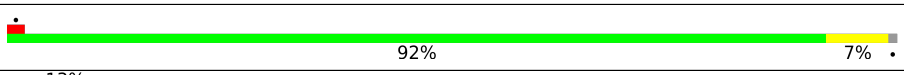
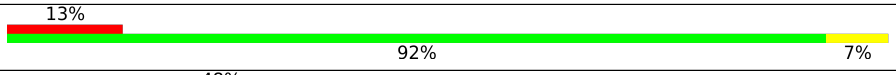
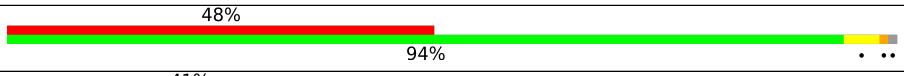
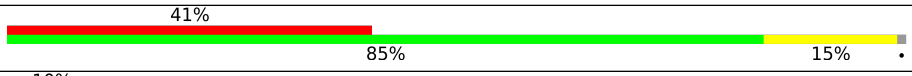
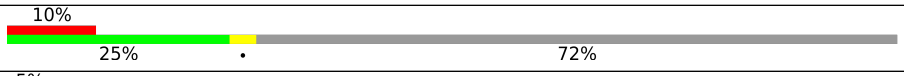
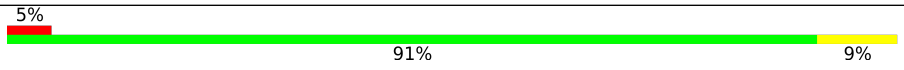
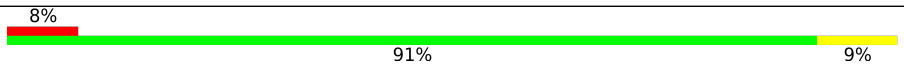
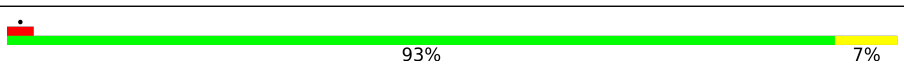
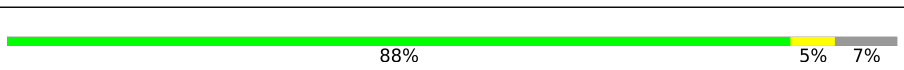
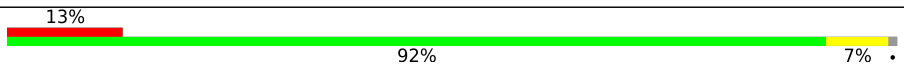
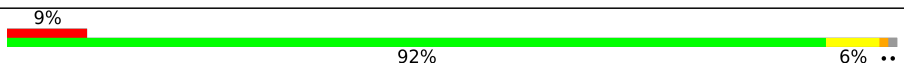
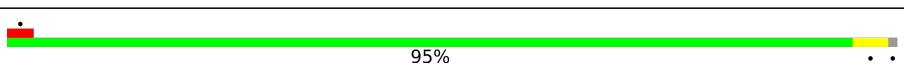
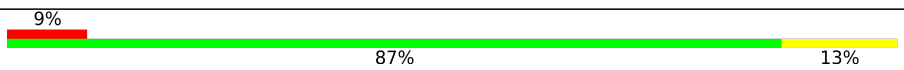
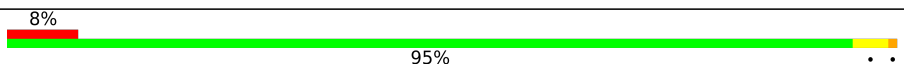
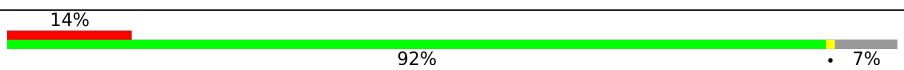
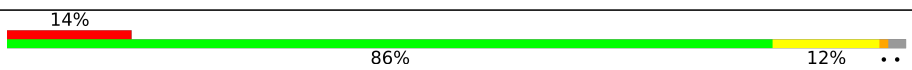
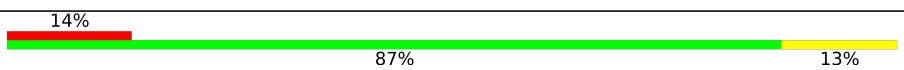
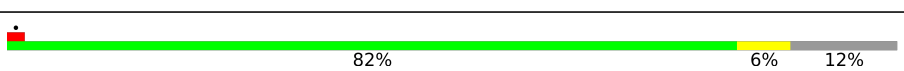
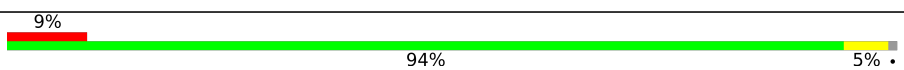
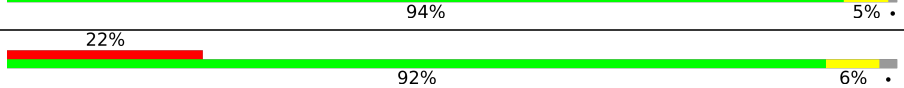
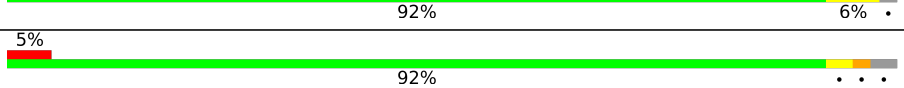
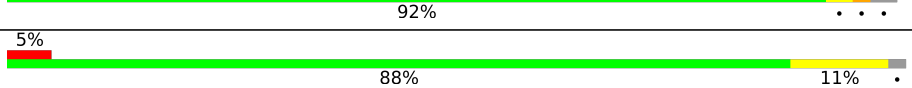
| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 29 | U | 71 |   |
| 30 | X | 6 |   |
| 31 | b | 120 |   |
| 32 | c | 273 |   |
| 33 | e | 201 |   |
| 34 | f | 179 |   |
| 35 | g | 177 |   |
| 36 | h | 149 |   |
| 37 | i | 142 |   |
| 38 | j | 123 |   |
| 39 | k | 144 |   |
| 40 | m | 127 |   |
| 41 | n | 117 |   |
| 42 | o | 115 |   |
| 43 | p | 118 |   |
| 44 | q | 103 |   |
| 45 | r | 110 |   |
| 46 | s | 100 |   |
| 47 | t | 104 |   |
| 48 | u | 94 |   |
| 49 | v | 85 |   |
| 50 | w | 78 |   |
| 51 | x | 63 |   |
| 52 | y | 59 |   |
| 53 | z | 57 |   |

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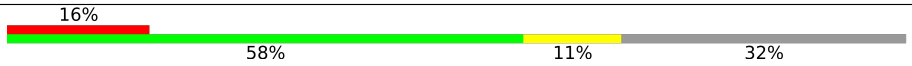
| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 54 | Z | 77 |   |
| 55 | 8 | 19 |   |

# 2 Entry composition (i)

There are 56 unique types of molecules in this entry. The entry contains 139733 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 1 | a | 2753 | 59130 | 26384 | 10897 | 19096 | 2753 | 0 | 0 |

- Molecule 2 is a RNA chain called 16S rRNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 2 | A | 1519 | 32612 | 14552 | 5986 | 10555 | 1519 | 0 | 0 |

- Molecule 3 is a protein called Large ribosomal subunit protein bL36A.

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

- Molecule 4 is a protein called Large ribosomal subunit protein bL31A.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 4 | 4 | 59 | 472 | 293 | 89 | 84 | 6 | 0 | 0 |

- Molecule 5 is a protein called Small ribosomal subunit protein uS11.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 5 | K | 117 | 877 | 540 | 173 | 161 | 3 | 0 | 0 |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| K | 119 | IAS | ASN | variant | UNP P0A7R9 |

- Molecule 6 is a protein called Small ribosomal subunit protein uS12.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 6 | L | 123 | Total | C | N | O | S | 0 | 0 |
| | | | 957 | 591 | 196 | 165 | 5 | | |

- Molecule 7 is a protein called Large ribosomal subunit protein uL3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 7 | d | 209 | Total | C | N | O | S | 0 | 0 |
| | | | 1566 | 980 | 288 | 294 | 4 | | |

- Molecule 8 is a protein called Large ribosomal subunit protein uL16.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 8 | l | 136 | Total | C | N | O | S | 0 | 0 |
| | | | 1075 | 686 | 205 | 177 | 7 | | |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| l | 82 | MS6 | MET | variant | UNP P0ADY7 |

- Molecule 9 is a protein called Large ribosomal subunit protein bL33.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 9 | 0 | 49 | Total | C | N | O | 0 | 0 |
| | | | 405 | 261 | 74 | 70 | | |

- Molecule 10 is a protein called Large ribosomal subunit protein bL34.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 10 | 1 | 45 | Total | C | N | O | S | 0 | 0 |
| | | | 367 | 222 | 88 | 55 | 2 | | |

- Molecule 11 is a protein called Large ribosomal subunit protein bL35.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 11 | 2 | 64 | Total | C | N | O | S | 0 | 0 |
| | | | 504 | 323 | 105 | 74 | 2 | | |

- Molecule 12 is a protein called 30S ribosomal protein S2.

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

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

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

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

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

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

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

- Molecule 16 is a protein called 30S ribosomal protein S6, fully modified isoform.

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

- Molecule 17 is a protein called 30S ribosomal protein S7.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 17 | G | 147 | Total | C | N | O | S | 0 | 0 |
| | | | 1164 | 728 | 222 | 210 | 4 | | |

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

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

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

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

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

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

- Molecule 21 is a protein called Small ribosomal subunit protein uS13.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 21 | M | 115 | Total | C | N | O | S | 0 | 0 |
| | | | 891 | 552 | 179 | 157 | 3 | | |

- Molecule 22 is a protein called Small ribosomal subunit protein uS14.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 22 | N | 100 | Total | C | N | O | S | 0 | 0 |
| | | | 805 | 499 | 164 | 139 | 3 | | |

- Molecule 23 is a protein called Small ribosomal subunit protein uS15.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 23 | O | 88 | Total | C | N | O | S | 0 | 0 |
| | | | 714 | 439 | 144 | 130 | 1 | | |

- Molecule 24 is a protein called 30S ribosomal protein S16.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 24 | P | 81 | Total | C | N | O | S | 0 | 0 |
| | | | 643 | 403 | 127 | 112 | 1 | | |

- Molecule 25 is a protein called Small ribosomal subunit protein uS17.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 25 | Q | 77 | Total | C | N | O | S | 0 | 0 |
| | | | 624 | 394 | 117 | 110 | 3 | | |

- Molecule 26 is a protein called Small ribosomal subunit protein bS18.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 26 | R | 55 | Total | C | N | O | 0 | 0 |
| | | | 455 | 288 | 86 | 81 | | |

- Molecule 27 is a protein called Small ribosomal subunit protein uS19.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 27 | S | 84 | Total | C | N | O | S | 0 | 0 |
| | | | 668 | 427 | 127 | 112 | 2 | | |

- Molecule 28 is a protein called 30S ribosomal protein S20.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 28 | T | 86 | Total | C | N | O | S | 0 | 0 |
| | | | 670 | 414 | 138 | 115 | 3 | | |

- Molecule 29 is a protein called Small ribosomal subunit protein bS21.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 29 | U | 70 | Total | C | N | O | S | 0 | 0 |
| | | | 589 | 366 | 125 | 97 | 1 | | |

- Molecule 30 is a RNA chain called mRNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 30 | X | 6 | Total | C | N | O | P | 0 | 0 |
| | | | 131 | 59 | 27 | 39 | 6 | | |

- Molecule 31 is a RNA chain called 5S rRNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 31 | b | 119 | Total | C | N | O | P | 0 | 0 |
| | | | 2549 | 1135 | 466 | 829 | 119 | | |

- Molecule 32 is a protein called Large ribosomal subunit protein uL2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 32 | c | 271 | Total | C | N | O | S | 0 | 0 |
| | | | 2082 | 1288 | 423 | 364 | 7 | | |

- Molecule 33 is a protein called Large ribosomal subunit protein uL4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 33 | e | 201 | Total | C | N | O | S | 0 | 0 |
| | | | 1552 | 974 | 283 | 290 | 5 | | |

- Molecule 34 is a protein called Large ribosomal subunit protein uL5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 34 | f | 177 | Total | C | N | O | S | 0 | 0 |
| | | | 1410 | 899 | 249 | 256 | 6 | | |

- Molecule 35 is a protein called Large ribosomal subunit protein uL6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 35 | g | 176 | Total | C | N | O | S | 0 | 0 |
| | | | 1323 | 832 | 243 | 246 | 2 | | |

- Molecule 36 is a protein called Large ribosomal subunit protein bL9.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 36 | h | 41 | Total | C | N | O | S | 0 | 0 |
| | | | 303 | 194 | 54 | 54 | 1 | | |

- Molecule 37 is a protein called Large ribosomal subunit protein uL13.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 37 | i | 142 | Total | C | N | O | S | 0 | 0 |
| | | | 1129 | 714 | 212 | 199 | 4 | | |

- Molecule 38 is a protein called Large ribosomal subunit protein uL14.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 38 | j | 123 | Total | C | N | O | S | 0 | 0 |
| | | | 946 | 593 | 181 | 166 | 6 | | |

- Molecule 39 is a protein called 50S ribosomal protein L15.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 39 | k | 144 | Total | C | N | O | S | 0 | 0 |
| | | | 1053 | 654 | 207 | 190 | 2 | | |

- Molecule 40 is a protein called Large ribosomal subunit protein bL17.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 40 | m | 118 | Total<br>945 | C<br>585 | N<br>194 | O<br>161 | S<br>5 | 0 | 0 |

- Molecule 41 is a protein called Large ribosomal subunit protein uL18.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 41 | n | 116 | Total<br>892 | C<br>552 | N<br>178 | O<br>162 | 0 | 0 |

- Molecule 42 is a protein called Large ribosomal subunit protein bL19.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 42 | o | 114 | Total<br>917 | C<br>574 | N<br>179 | O<br>163 | S<br>1 | 0 | 0 |

- Molecule 43 is a protein called Large ribosomal subunit protein bL20.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 43 | p | 117 | Total<br>947 | C<br>604 | N<br>192 | O<br>151 | 0 | 0 |

- Molecule 44 is a protein called Large ribosomal subunit protein bL21.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 44 | q | 103 | Total<br>816 | C<br>516 | N<br>153 | O<br>145 | S<br>2 | 0 | 0 |

- Molecule 45 is a protein called Large ribosomal subunit protein uL22.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 45 | r | 110 | Total<br>857 | C<br>532 | N<br>166 | O<br>156 | S<br>3 | 0 | 0 |

- Molecule 46 is a protein called Large ribosomal subunit protein uL23.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 46 | s | 93 | Total<br>738 | C<br>466 | N<br>139 | O<br>131 | S<br>2 | 0 | 0 |

- Molecule 47 is a protein called Large ribosomal subunit protein uL24.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 47 | t | 102 | Total<br>779 | C<br>492 | N<br>146 | O<br>141 | 0 | 0 |

- Molecule 48 is a protein called 50S ribosomal protein L25.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 48 | u | 94 | Total<br>753 | C<br>479 | N<br>137 | O<br>134 | S<br>3 | 0 | 0 |

- Molecule 49 is a protein called Large ribosomal subunit protein bL27.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 49 | v | 75 | Total<br>569 | C<br>353 | N<br>113 | O<br>102 | S<br>1 | 0 | 0 |

- Molecule 50 is a protein called Large ribosomal subunit protein bL28.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 50 | w | 77 | Total<br>625 | C<br>388 | N<br>129 | O<br>106 | S<br>2 | 0 | 0 |

- Molecule 51 is a protein called Large ribosomal subunit protein uL29.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 51 | x | 62 | Total<br>501 | C<br>308 | N<br>98 | O<br>94 | S<br>1 | 0 | 0 |

- Molecule 52 is a protein called Large ribosomal subunit protein uL30.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 52 | y | 57 | Total<br>444 | C<br>278 | N<br>86 | O<br>78 | S<br>2 | 0 | 0 |

- Molecule 53 is a protein called Large ribosomal subunit protein bL32.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 53 | z | 56 | Total<br>444 | C<br>269 | N<br>94 | O<br>80 | S<br>1 | 0 | 0 |

- Molecule 54 is a RNA chain called fMet-Initiator P-tRNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 54 | Z | 76 | Total | C | N | O | P | 0 | 0 |
| | | | 1623 | 723 | 294 | 530 | 76 | | |

- Molecule 55 is a protein called Dal2.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 55 | 8 | 13 | Total | C | N | O | 0 | 0 |
| | | | 115 | 76 | 22 | 17 | | |

- Molecule 56 is ZINC ION (CCD ID: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | | AltConf |
|---|---|---|---|---|---|
| 56 | 3 | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |
| 56 | 4 | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |

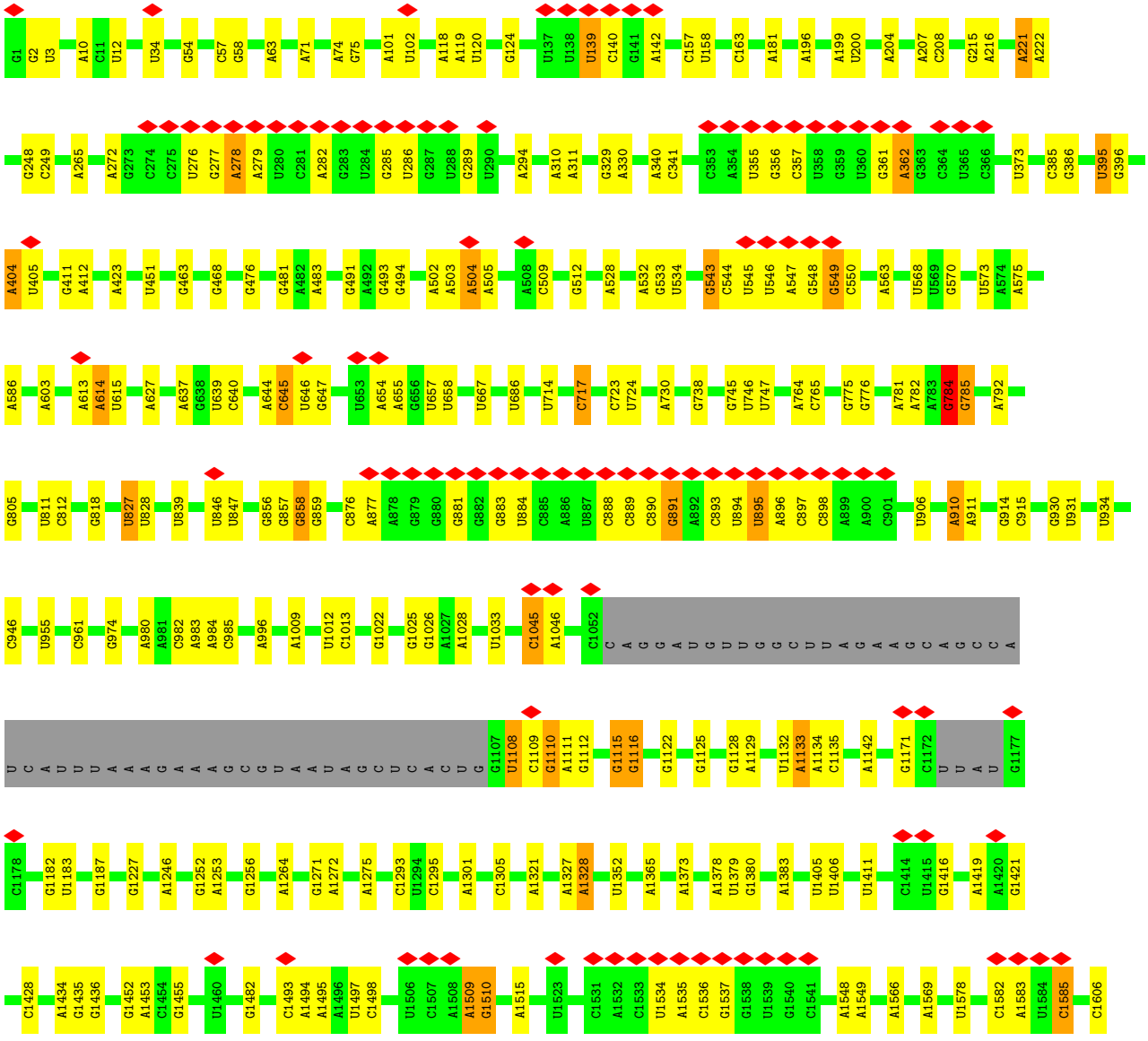
# 3 Residue-property plots (i)

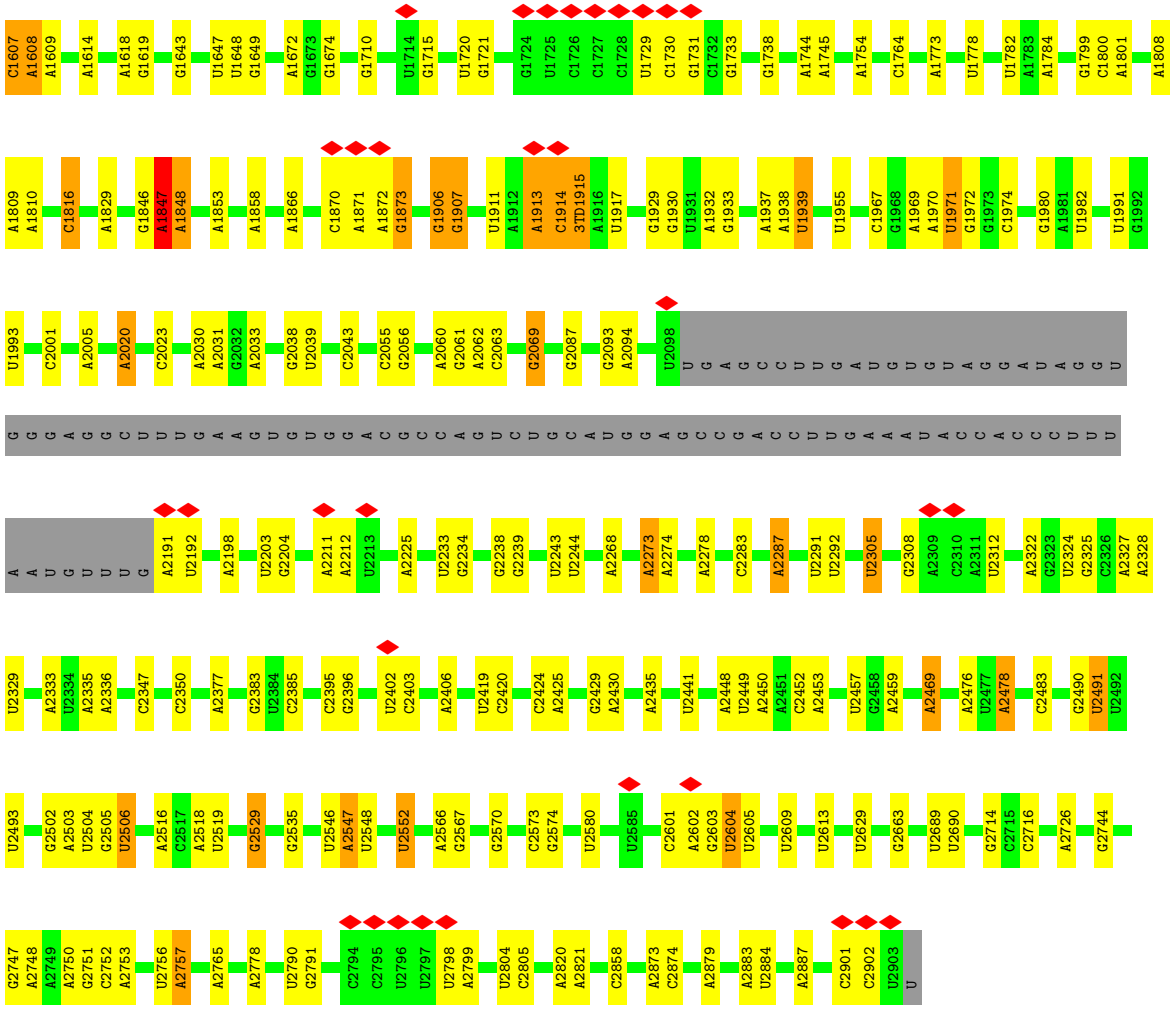
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: 23S rRNA

Chain a:



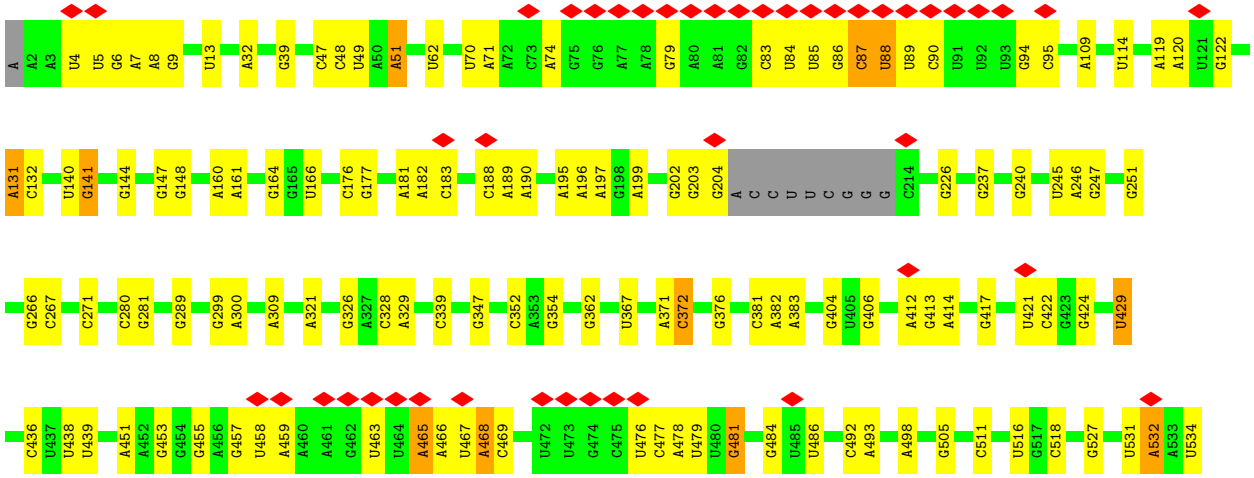



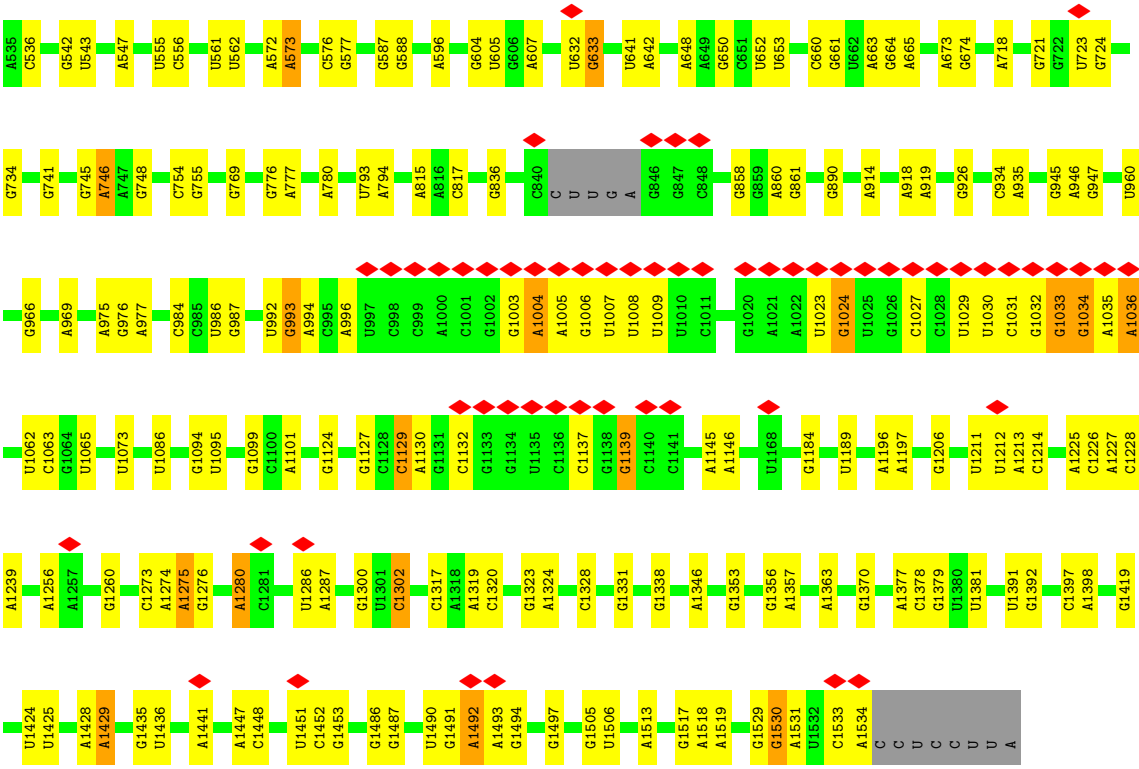


• Molecule 2: 16S rRNA

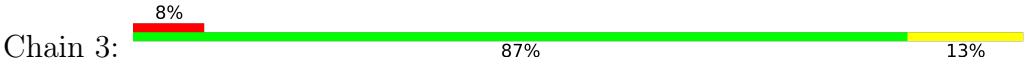
Chain A:

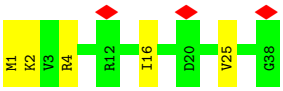




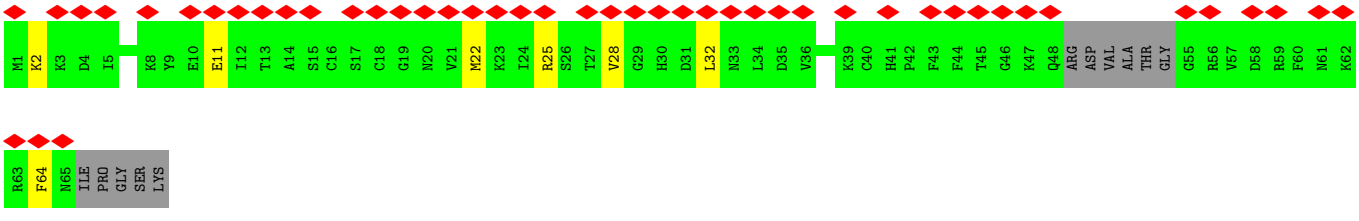

• Molecule 3: Large ribosomal subunit protein bL36A



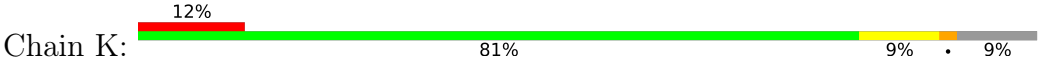



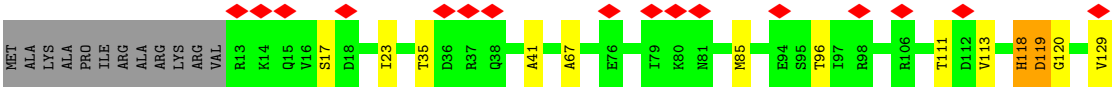

• Molecule 4: Large ribosomal subunit protein bL31A




• Molecule 5: Small ribosomal subunit protein uS11

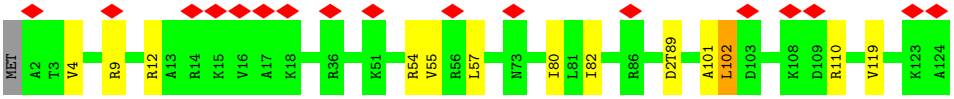



• Molecule 6: Small ribosomal subunit protein uS12

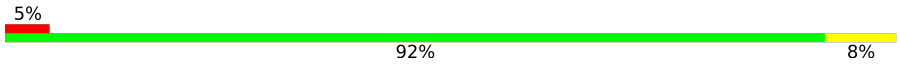
Chain L:

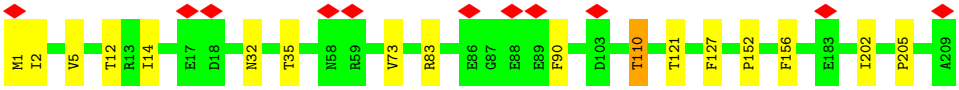



• Molecule 7: Large ribosomal subunit protein uL3

Chain d:

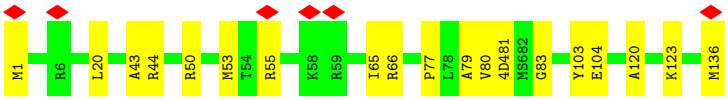



• Molecule 8: Large ribosomal subunit protein uL16

Chain l:

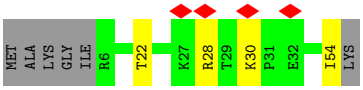



• Molecule 9: Large ribosomal subunit protein bL33

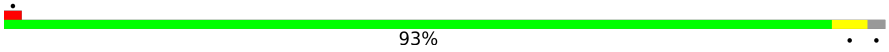
Chain 0:

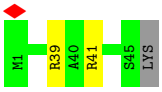



• Molecule 10: Large ribosomal subunit protein bL34

Chain 1:




• Molecule 11: Large ribosomal subunit protein bL35

Chain 2:



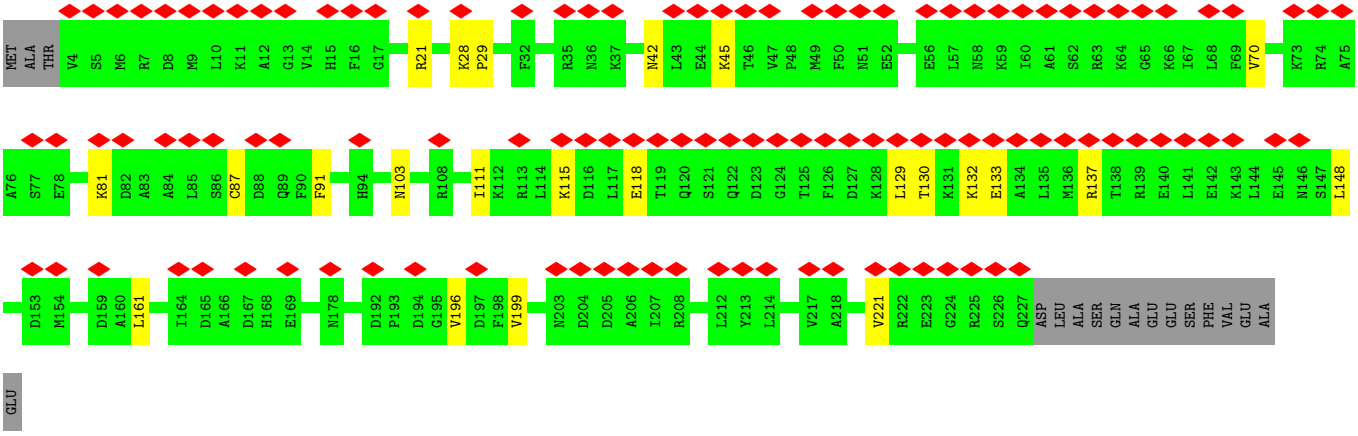




• Molecule 12: 30S ribosomal protein S2

Chain B:

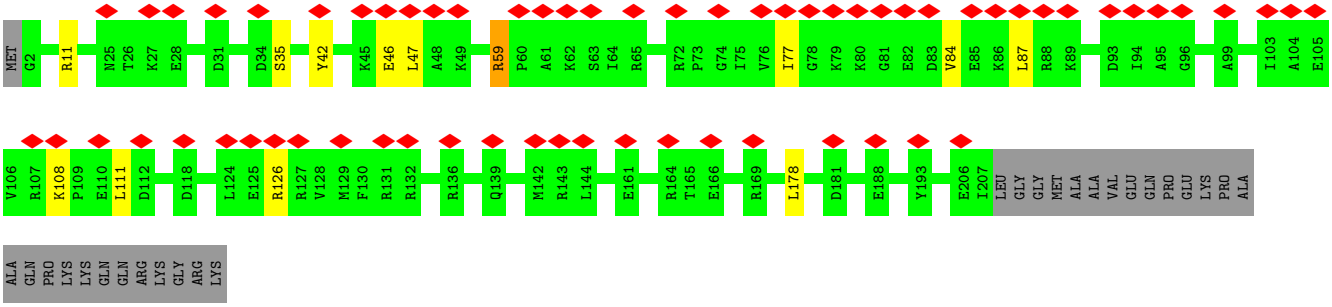




• Molecule 13: Small ribosomal subunit protein uS3

Chain C:

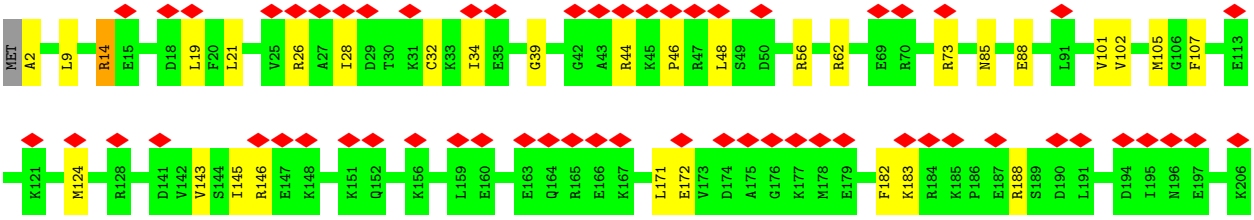


• Molecule 14: Small ribosomal subunit protein uS4

Chain D:

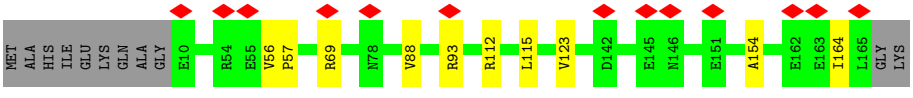


• Molecule 15: Small ribosomal subunit protein uS5

Chain E:

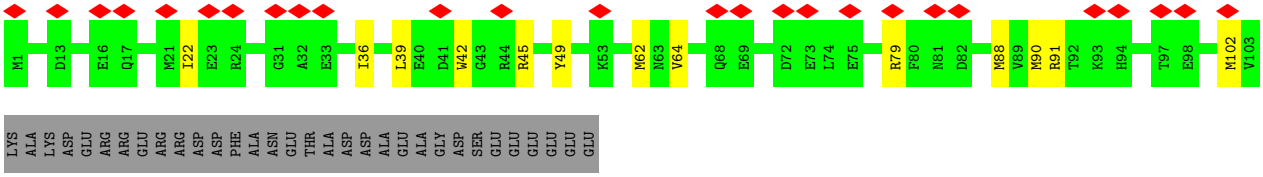


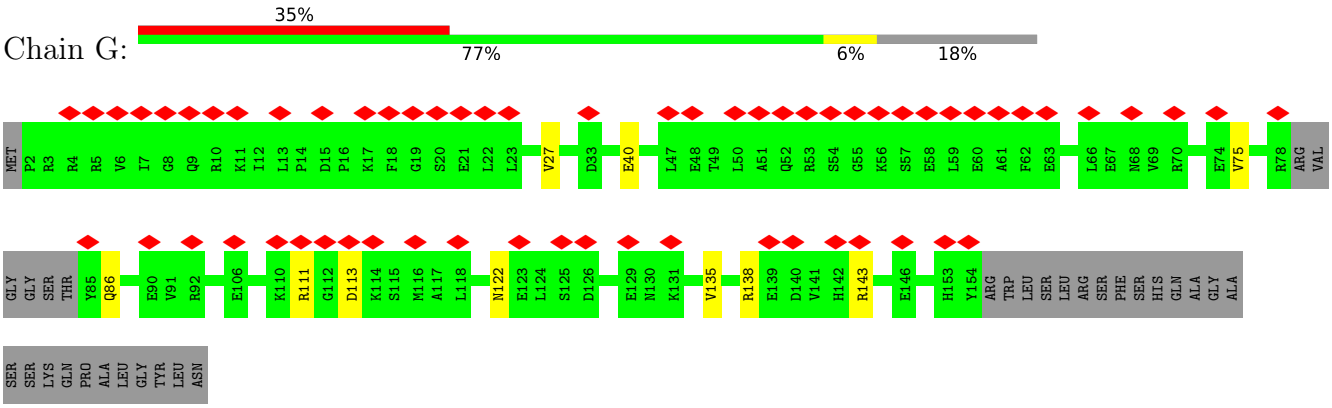
• Molecule 16: 30S ribosomal protein S6, fully modified isoform

Chain F:

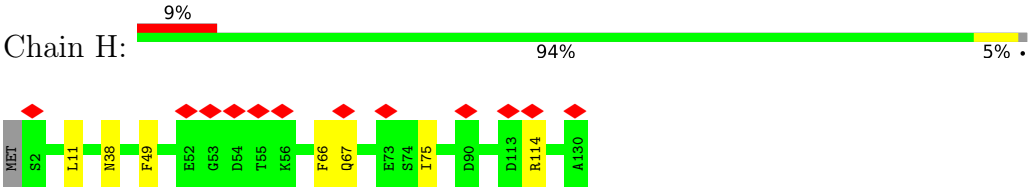




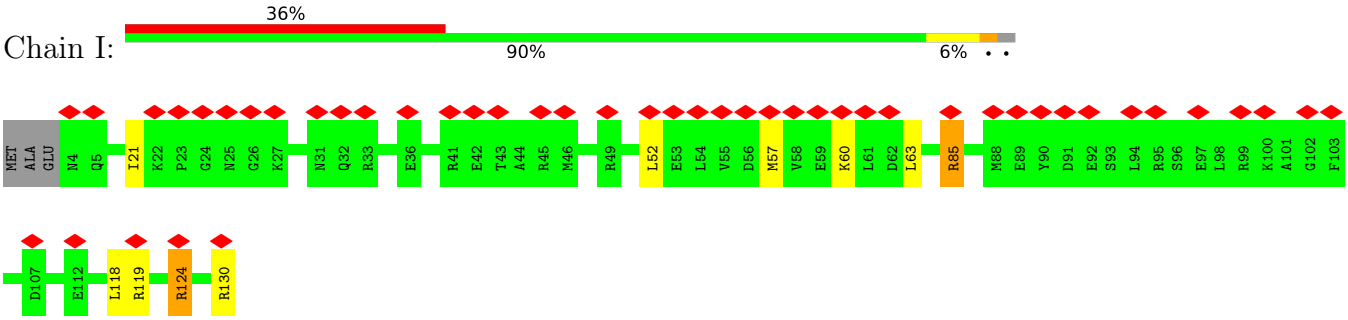

• Molecule 17: 30S ribosomal protein S7



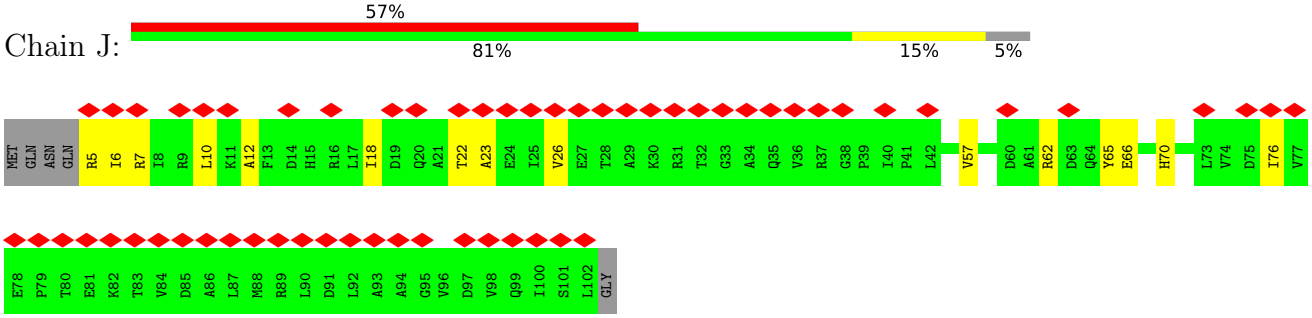

• Molecule 18: Small ribosomal subunit protein uS8




• Molecule 19: Small ribosomal subunit protein uS9



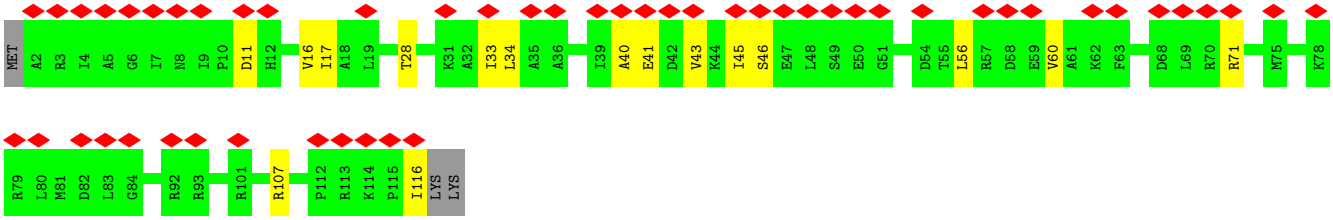

• Molecule 20: Small ribosomal subunit protein uS10



• Molecule 21: Small ribosomal subunit protein uS13

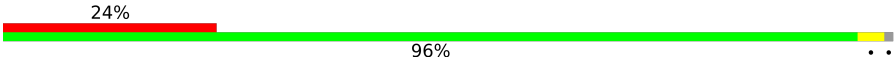
Chain M:

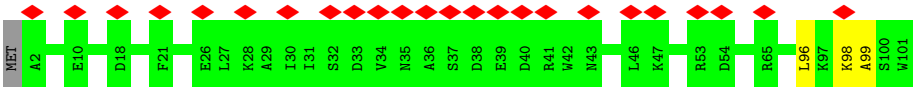



• Molecule 22: Small ribosomal subunit protein uS14

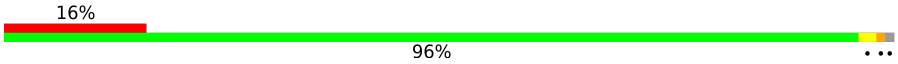
Chain N:

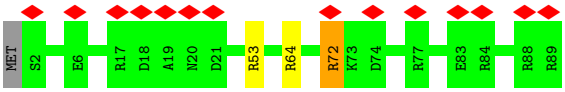



• Molecule 23: Small ribosomal subunit protein uS15

Chain O:

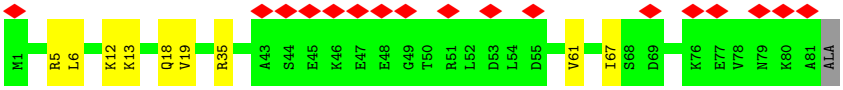



• Molecule 24: 30S ribosomal protein S16

Chain P:

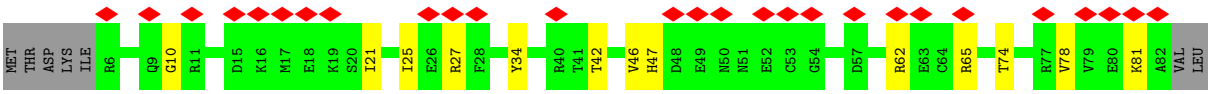



• Molecule 25: Small ribosomal subunit protein uS17

Chain Q:

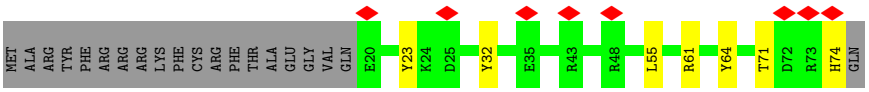



• Molecule 26: Small ribosomal subunit protein bS18

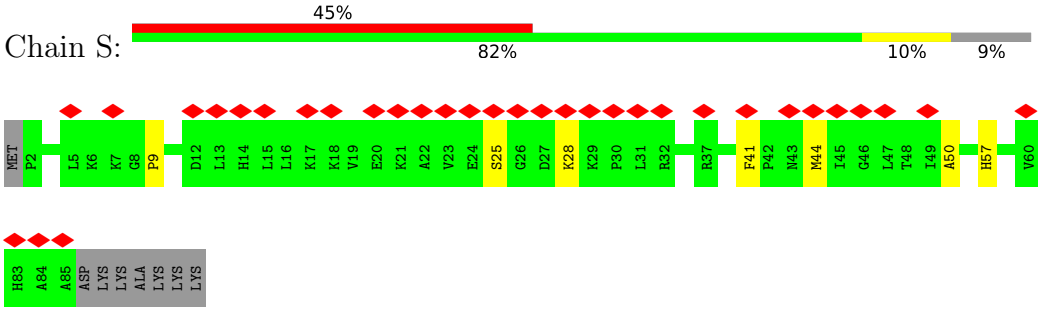
Chain R:



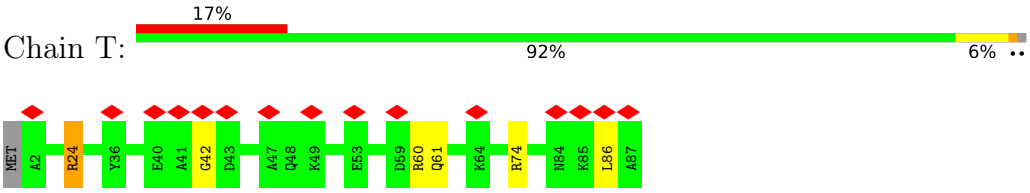

• Molecule 27: Small ribosomal subunit protein uS19

Chain S:



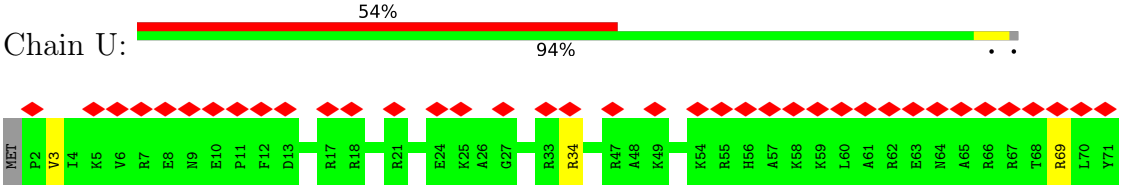

• Molecule 28: 30S ribosomal protein S20

Chain T:



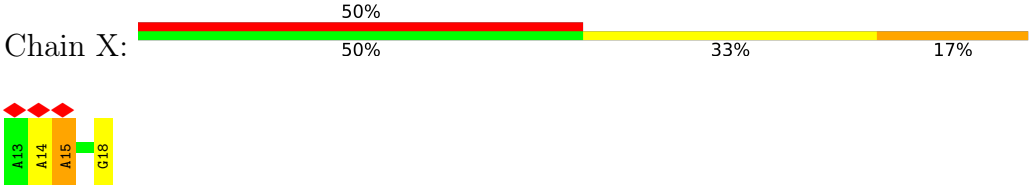

• Molecule 29: Small ribosomal subunit protein bS21

Chain U:



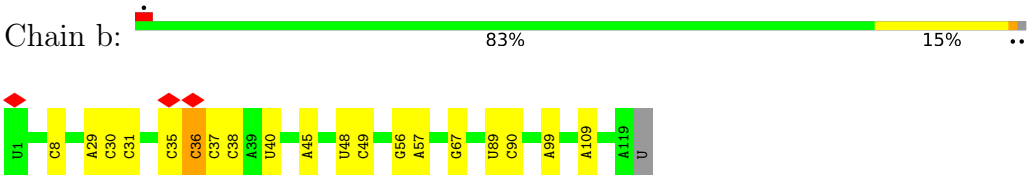

• Molecule 30: mRNA

Chain X:



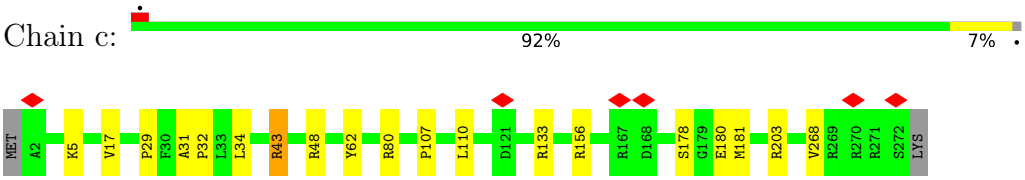

• Molecule 31: 5S rRNA

Chain b:



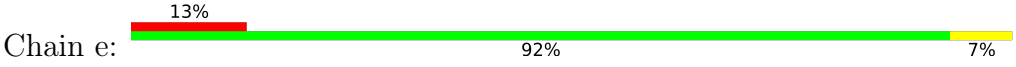

• Molecule 32: Large ribosomal subunit protein uL2

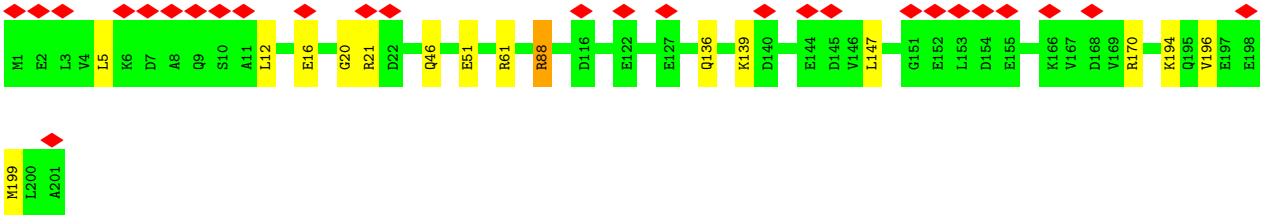
Chain c:




• Molecule 33: Large ribosomal subunit protein uL4

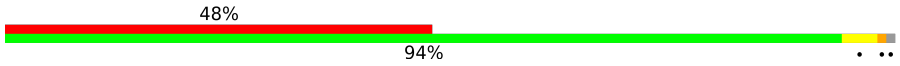
Chain e:

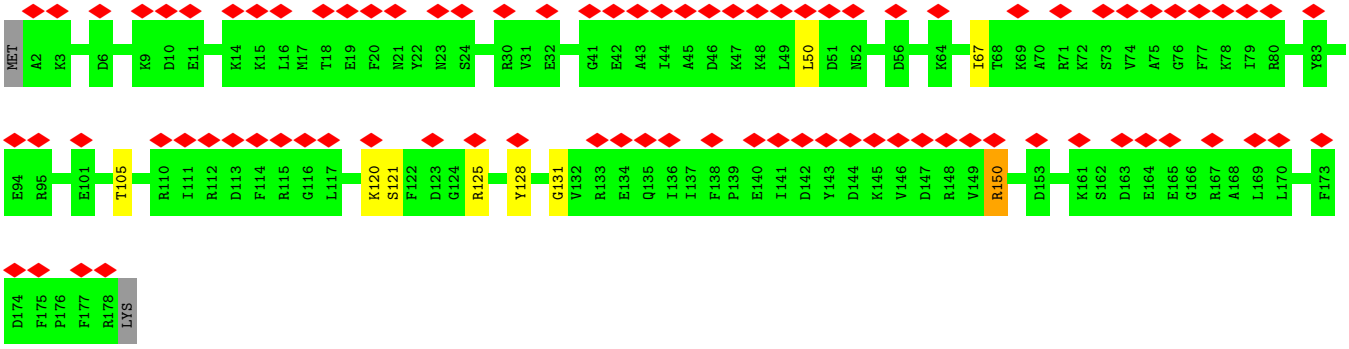





• Molecule 34: Large ribosomal subunit protein uL5

Chain f:

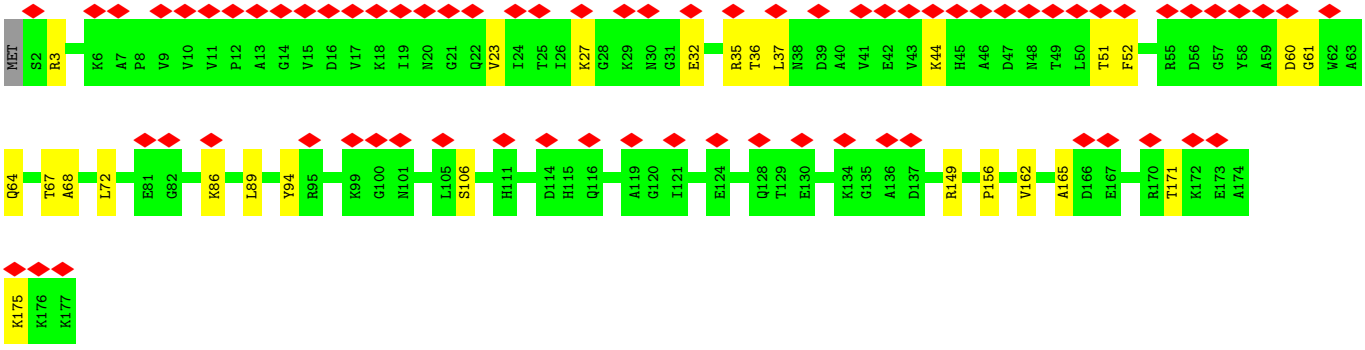



• Molecule 35: Large ribosomal subunit protein uL6

Chain g:

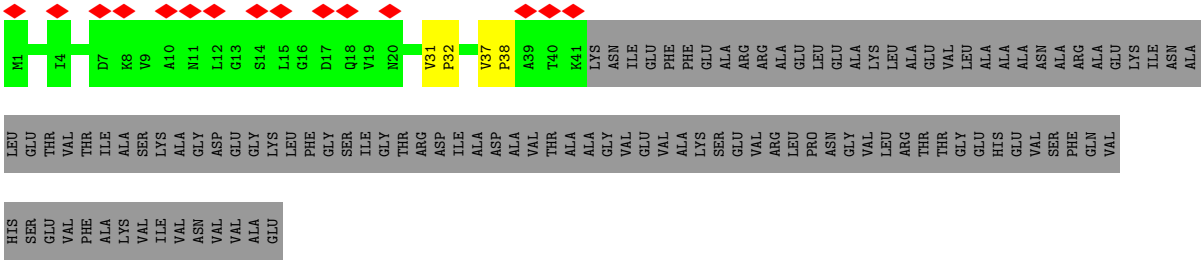



• Molecule 36: Large ribosomal subunit protein bL9

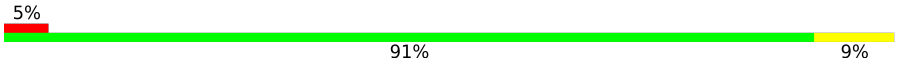
Chain h:

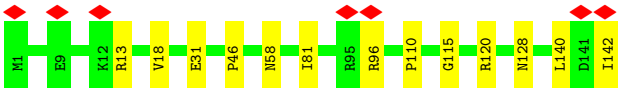



• Molecule 37: Large ribosomal subunit protein uL13

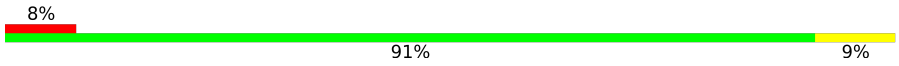
Chain i:

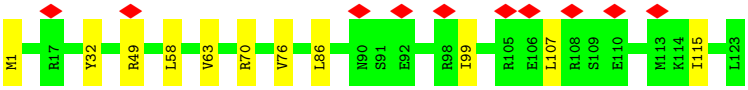



• Molecule 38: Large ribosomal subunit protein uL14

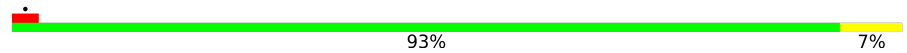
Chain j:

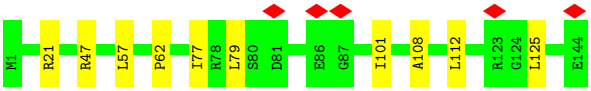



• Molecule 39: 50S ribosomal protein L15

Chain k:




• Molecule 40: Large ribosomal subunit protein bL17

Chain m:

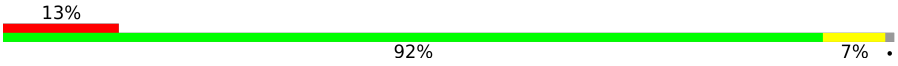


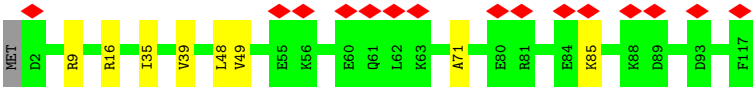




• Molecule 41: Large ribosomal subunit protein uL18

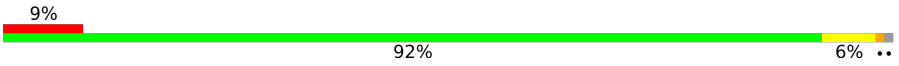
Chain n:

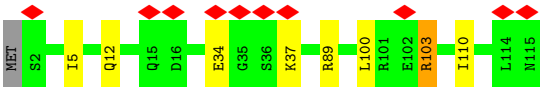



• Molecule 42: Large ribosomal subunit protein bL19

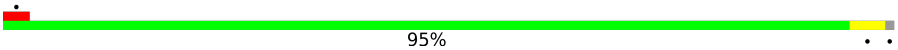
Chain o:

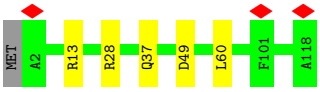



• Molecule 43: Large ribosomal subunit protein bL20

Chain p:

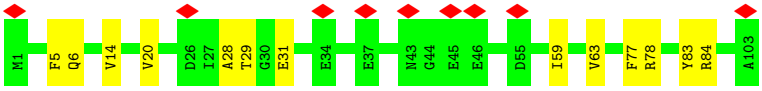


• Molecule 44: Large ribosomal subunit protein bL21

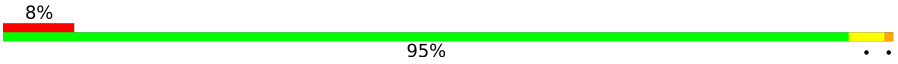
Chain q:

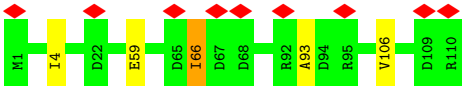



• Molecule 45: Large ribosomal subunit protein uL22

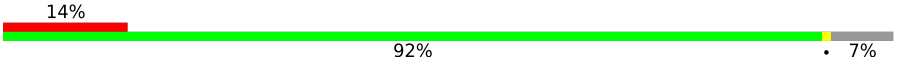
Chain r:

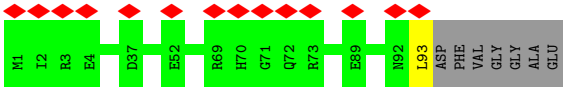



• Molecule 46: Large ribosomal subunit protein uL23

Chain s:

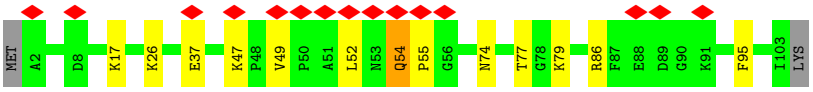



• Molecule 47: Large ribosomal subunit protein uL24

Chain t:

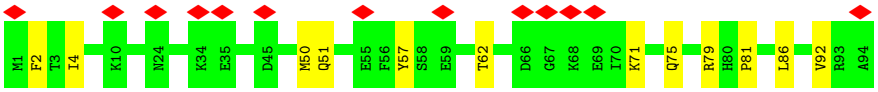



• Molecule 48: 50S ribosomal protein L25

Chain u:

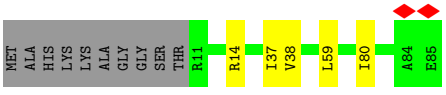



• Molecule 49: Large ribosomal subunit protein bL27

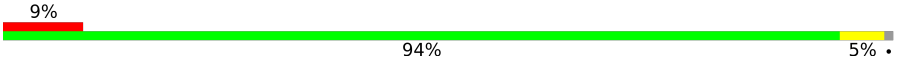
Chain v:

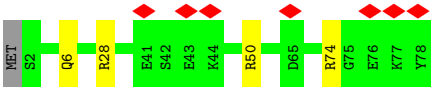


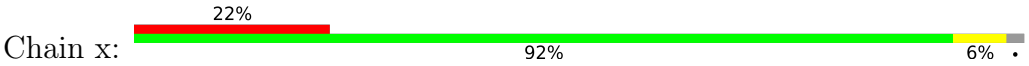

• Molecule 50: Large ribosomal subunit protein bL28

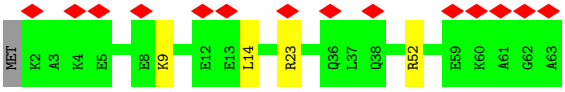
Chain w:



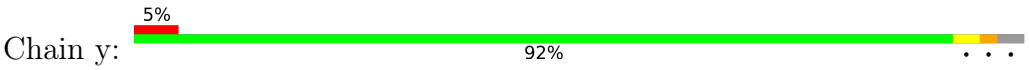


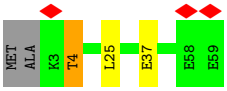

• Molecule 51: Large ribosomal subunit protein uL29



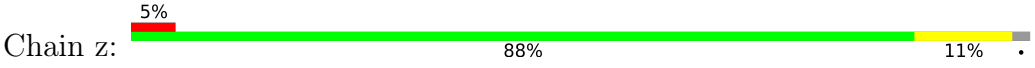




• Molecule 52: Large ribosomal subunit protein uL30




• Molecule 53: Large ribosomal subunit protein bL32

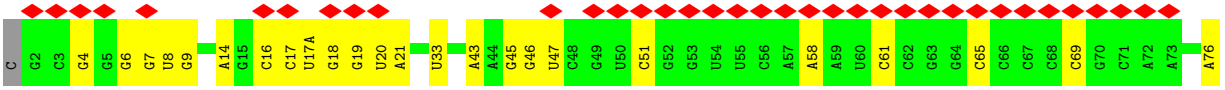






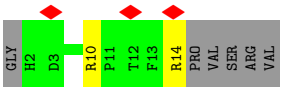
• Molecule 54: fMet-Initiator P-tRNA




• Molecule 55: Dal2



# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 334003 | 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 ($e^-/Å^2$) | 1.14 | Depositor |
| Minimum defocus (nm) | 300 | Depositor |
| Maximum defocus (nm) | 900 | Depositor |
| Magnification | Not provided | |
| Image detector | GATAN K3 BIOQUANTUM (6k x 4k) | Depositor |
| Maximum map value | 0.054 | Depositor |
| Minimum map value | -0.018 | Depositor |
| Average map value | 0.000 | Depositor |
| Map value standard deviation | 0.002 | Depositor |
| Recommended contour level | 0.01 | Depositor |
| Map size (Å) | 346.112, 346.112, 346.112 | wwPDB |
| Map dimensions | 416, 416, 416 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 0.832, 0.832, 0.832 | Depositor |

# 5 Model quality

## 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: G7M, PSU, 4OC, 2MA, ZN, OMG, MS6, D2T, 3TD, 5MU, 2MG, OMU, 4D4, 6MZ, IAS, MEQ, 5MC, OMC, 1MG, H2U, UR3, MA6

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

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | $\#\|Z\| > 5$ | RMSZ | $\#\|Z\| > 5$ |
| 1 | a | 0.55 | 2/65651 (0.0%) | 0.90 | 43/102413 (0.0%) |
| 2 | A | 0.51 | 0/36236 | 0.85 | 8/56520 (0.0%) |
| 3 | 3 | 0.62 | 0/303 | 0.78 | 0/397 |
| 4 | 4 | 0.58 | 0/480 | 0.90 | 0/638 |
| 5 | K | 0.85 | 1/884 (0.1%) | 0.86 | 0/1191 |
| 6 | L | 0.57 | 0/960 | 0.80 | 0/1286 |
| 7 | d | 0.66 | 0/1576 | 0.85 | 0/2119 |
| 8 | l | 0.67 | 2/1073 (0.2%) | 0.88 | 0/1433 |
| 9 | 0 | 0.57 | 0/412 | 0.87 | 0/549 |
| 10 | 1 | 0.80 | 0/370 | 0.90 | 0/487 |
| 11 | 2 | 0.78 | 0/513 | 0.90 | 0/676 |
| 12 | B | 0.55 | 0/1784 | 0.94 | 0/2403 |
| 13 | C | 0.55 | 0/1651 | 0.84 | 0/2225 |
| 14 | D | 0.53 | 0/1665 | 0.92 | 0/2227 |
| 15 | E | 0.60 | 0/1165 | 0.88 | 0/1568 |
| 16 | F | 0.53 | 0/858 | 0.87 | 0/1160 |
| 17 | G | 0.56 | 0/1179 | 0.92 | 0/1580 |
| 18 | H | 0.56 | 0/989 | 0.84 | 0/1326 |
| 19 | I | 0.55 | 0/1034 | 0.87 | 0/1375 |
| 20 | J | 0.59 | 0/796 | 0.87 | 0/1077 |
| 21 | M | 0.57 | 0/900 | 0.94 | 0/1204 |
| 22 | N | 0.55 | 0/817 | 0.91 | 0/1088 |
| 23 | O | 0.56 | 0/722 | 0.94 | 0/964 |
| 24 | P | 0.54 | 0/653 | 0.83 | 0/877 |
| 25 | Q | 0.54 | 0/633 | 0.80 | 0/849 |
| 26 | R | 0.57 | 0/462 | 0.90 | 0/621 |
| 27 | S | 0.60 | 0/685 | 0.88 | 0/922 |
| 28 | T | 0.55 | 0/676 | 0.95 | 0/895 |
| 29 | U | 0.57 | 0/597 | 0.95 | 0/792 |
| 30 | X | 0.59 | 0/147 | 0.89 | 0/227 |
| 31 | b | 0.51 | 0/2850 | 0.84 | 1/4444 (0.0%) |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 32 | c | 0.70 | 0/2121 | 0.87 | 0/2852 |
| 33 | e | 0.65 | 0/1571 | 0.89 | 0/2113 |
| 34 | f | 0.54 | 0/1434 | 0.93 | 0/1926 |
| 35 | g | 0.57 | 0/1343 | 0.90 | 0/1816 |
| 36 | h | 0.56 | 0/306 | 0.92 | 0/413 |
| 37 | i | 0.64 | 0/1152 | 0.84 | 0/1551 |
| 38 | j | 0.61 | 0/955 | 0.87 | 0/1279 |
| 39 | k | 0.69 | 0/1062 | 0.85 | 0/1413 |
| 40 | m | 0.73 | 1/958 (0.1%) | 0.92 | 1/1281 (0.1%) |
| 41 | n | 0.58 | 0/902 | 0.88 | 0/1209 |
| 42 | o | 0.64 | 0/929 | 0.83 | 0/1242 |
| 43 | p | 0.72 | 0/960 | 0.91 | 0/1278 |
| 44 | q | 0.60 | 0/829 | 0.82 | 1/1107 (0.1%) |
| 45 | r | 0.68 | 0/864 | 0.85 | 0/1156 |
| 46 | s | 0.58 | 0/744 | 0.81 | 0/994 |
| 47 | t | 0.56 | 0/787 | 0.86 | 0/1051 |
| 48 | u | 0.56 | 0/766 | 0.84 | 0/1025 |
| 49 | v | 0.67 | 0/576 | 0.82 | 0/762 |
| 50 | w | 0.67 | 0/635 | 0.86 | 0/848 |
| 51 | x | 0.51 | 0/502 | 0.97 | 0/667 |
| 52 | y | 0.58 | 0/448 | 0.89 | 1/598 (0.2%) |
| 53 | z | 0.72 | 0/450 | 0.91 | 0/599 |
| 54 | Z | 0.56 | 0/1813 | 0.83 | 1/2825 (0.0%) |
| 55 | 8 | 0.77 | 0/121 | 1.20 | 0/165 |
| All | All | 0.56 | 6/150949 (0.0%) | 0.88 | 56/225703 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 1 | a | 0 | 5 |
| 3 | 3 | 0 | 1 |
| 5 | K | 0 | 1 |
| 6 | L | 0 | 2 |
| 7 | d | 0 | 1 |
| 9 | 0 | 0 | 1 |
| 10 | 1 | 0 | 1 |
| 11 | 2 | 0 | 1 |
| 12 | B | 0 | 2 |
| 13 | C | 0 | 3 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 14 | D | 0 | 4 |
| 15 | E | 0 | 2 |
| 16 | F | 0 | 2 |
| 17 | G | 0 | 2 |
| 19 | I | 0 | 3 |
| 20 | J | 0 | 3 |
| 21 | M | 0 | 2 |
| 23 | O | 0 | 3 |
| 25 | Q | 0 | 3 |
| 26 | R | 0 | 1 |
| 28 | T | 0 | 3 |
| 29 | U | 0 | 2 |
| 32 | c | 0 | 4 |
| 33 | e | 0 | 3 |
| 34 | f | 0 | 2 |
| 35 | g | 0 | 1 |
| 37 | i | 0 | 3 |
| 38 | j | 0 | 1 |
| 39 | k | 0 | 1 |
| 41 | n | 0 | 1 |
| 42 | o | 0 | 2 |
| 43 | p | 0 | 2 |
| 44 | q | 0 | 1 |
| 48 | u | 0 | 1 |
| 49 | v | 0 | 1 |
| 50 | w | 0 | 2 |
| 51 | x | 0 | 2 |
| 53 | z | 0 | 1 |
| 55 | 8 | 0 | 2 |
| All | All | 0 | 78 |

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

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 5 | K | 120 | GLY | C-N | 17.33 | 1.56 | 1.33 |
| 8 | l | 79 | ALA | C-N | -6.83 | 1.23 | 1.33 |
| 40 | m | 3 | HIS | CG-CD2 | -6.34 | 1.28 | 1.35 |
| 8 | l | 83 | GLY | C-N | -5.66 | 1.25 | 1.33 |
| 1 | a | 2069 | G7M | O3'-P | 5.59 | 1.61 | 1.56 |

The worst 5 of 56 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | a | 2546 | U | O3'-P-O5' | -8.39 | 91.41 | 104.00 |
| 1 | a | 2601 | C | C4'-C3'-O3' | 7.89 | 124.83 | 113.00 |
| 1 | a | 204 | A | O3'-P-O5' | -7.44 | 92.85 | 104.00 |
| 1 | a | 781 | A | O3'-P-O5' | -6.98 | 93.53 | 104.00 |
| 1 | a | 1373 | A | O3'-P-O5' | -6.79 | 93.82 | 104.00 |

There are no chirality outliers.

5 of 78 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 1 | a | 249 | C | Sidechain |
| 1 | a | 395 | U | Sidechain |
| 1 | a | 463 | G | Sidechain |
| 1 | a | 512 | G | Sidechain |
| 1 | a | 980 | A | Sidechain |

## 5.2 Too-close contacts (i)

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 | a | 59130 | 0 | 29769 | 119 | 0 |
| 2 | A | 32612 | 0 | 16432 | 78 | 0 |
| 3 | 3 | 302 | 0 | 340 | 3 | 0 |
| 4 | 4 | 472 | 0 | 467 | 5 | 0 |
| 5 | K | 877 | 0 | 884 | 7 | 0 |
| 6 | L | 957 | 0 | 1017 | 7 | 0 |
| 7 | d | 1566 | 0 | 1618 | 15 | 0 |
| 8 | l | 1075 | 0 | 1146 | 15 | 0 |
| 9 | 0 | 405 | 0 | 437 | 4 | 0 |
| 10 | 1 | 367 | 0 | 405 | 1 | 0 |
| 11 | 2 | 504 | 0 | 572 | 5 | 0 |
| 12 | B | 1753 | 0 | 1780 | 12 | 0 |
| 13 | C | 1624 | 0 | 1696 | 6 | 0 |
| 14 | D | 1643 | 0 | 1707 | 19 | 0 |
| 15 | E | 1152 | 0 | 1196 | 10 | 0 |
| 16 | F | 839 | 0 | 833 | 7 | 0 |
| 17 | G | 1164 | 0 | 1213 | 5 | 0 |
| 18 | H | 979 | 0 | 1031 | 4 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 19 | I | 1022 | 0 | 1070 | 5 | 0 |
| 20 | J | 786 | 0 | 828 | 12 | 0 |
| 21 | M | 891 | 0 | 952 | 10 | 0 |
| 22 | N | 805 | 0 | 844 | 3 | 0 |
| 23 | O | 714 | 0 | 734 | 1 | 0 |
| 24 | P | 643 | 0 | 661 | 5 | 0 |
| 25 | Q | 624 | 0 | 658 | 7 | 0 |
| 26 | R | 455 | 0 | 478 | 5 | 0 |
| 27 | S | 668 | 0 | 693 | 5 | 0 |
| 28 | T | 670 | 0 | 719 | 3 | 0 |
| 29 | U | 589 | 0 | 629 | 1 | 0 |
| 30 | X | 131 | 0 | 66 | 1 | 0 |
| 31 | b | 2549 | 0 | 1291 | 6 | 0 |
| 32 | c | 2082 | 0 | 2154 | 10 | 0 |
| 33 | e | 1552 | 0 | 1619 | 8 | 0 |
| 34 | f | 1410 | 0 | 1444 | 4 | 0 |
| 35 | g | 1323 | 0 | 1371 | 17 | 0 |
| 36 | h | 303 | 0 | 327 | 2 | 0 |
| 37 | i | 1129 | 0 | 1162 | 11 | 0 |
| 38 | j | 946 | 0 | 1023 | 5 | 0 |
| 39 | k | 1053 | 0 | 1129 | 9 | 0 |
| 40 | m | 945 | 0 | 989 | 2 | 0 |
| 41 | n | 892 | 0 | 923 | 5 | 0 |
| 42 | o | 917 | 0 | 962 | 7 | 0 |
| 43 | p | 947 | 0 | 1019 | 3 | 0 |
| 44 | q | 816 | 0 | 839 | 6 | 0 |
| 45 | r | 857 | 0 | 922 | 3 | 0 |
| 46 | s | 738 | 0 | 807 | 0 | 0 |
| 47 | t | 779 | 0 | 831 | 9 | 0 |
| 48 | u | 753 | 0 | 780 | 9 | 0 |
| 49 | v | 569 | 0 | 581 | 3 | 0 |
| 50 | w | 625 | 0 | 652 | 1 | 0 |
| 51 | x | 501 | 0 | 531 | 2 | 0 |
| 52 | y | 444 | 0 | 483 | 2 | 0 |
| 53 | z | 444 | 0 | 458 | 4 | 0 |
| 54 | Z | 1623 | 0 | 825 | 1 | 0 |
| 55 | 8 | 115 | 0 | 113 | 0 | 0 |
| 56 | 3 | 1 | 0 | 0 | 0 | 0 |
| 56 | 4 | 1 | 0 | 0 | 0 | 0 |
| All | All | 139733 | 0 | 94110 | 440 | 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 2.

The worst 5 of 440 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) |
|---|---|---|---|
| 15:E:154:ALA:HA | 15:E:164:ILE:HD11 | 1.38 | 1.06 |
| 14:D:28:ILE:HG12 | 14:D:34:ILE:HD11 | 1.41 | 0.99 |
| 35:g:52:PHE:CZ | 35:g:72:LEU:HD12 | 2.04 | 0.92 |
| 13:C:77:ILE:HA | 13:C:84:VAL:HG23 | 1.57 | 0.85 |
| 37:i:18:VAL:HG21 | 37:i:142:ILE:HD12 | 1.59 | 0.85 |

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 | |
|---|---|---|---|---|---|---|---|
| 3 | 3 | 36/38 (95%) | 36 (100%) | 0 | 0 | 100 | 100 |
| 4 | 4 | 55/70 (79%) | 53 (96%) | 2 (4%) | 0 | 100 | 100 |
| 5 | K | 113/129 (88%) | 110 (97%) | 2 (2%) | 1 (1%) | 14 | 20 |
| 6 | L | 120/124 (97%) | 115 (96%) | 4 (3%) | 1 (1%) | 16 | 22 |
| 7 | d | 206/209 (99%) | 201 (98%) | 5 (2%) | 0 | 100 | 100 |
| 8 | l | 132/136 (97%) | 130 (98%) | 2 (2%) | 0 | 100 | 100 |
| 9 | 0 | 47/55 (86%) | 47 (100%) | 0 | 0 | 100 | 100 |
| 10 | 1 | 43/46 (94%) | 43 (100%) | 0 | 0 | 100 | 100 |
| 11 | 2 | 62/65 (95%) | 60 (97%) | 2 (3%) | 0 | 100 | 100 |
| 12 | B | 222/241 (92%) | 219 (99%) | 3 (1%) | 0 | 100 | 100 |
| 13 | C | 204/233 (88%) | 197 (97%) | 7 (3%) | 0 | 100 | 100 |
| 14 | D | 203/206 (98%) | 202 (100%) | 0 | 1 (0%) | 24 | 34 |
| 15 | E | 154/167 (92%) | 153 (99%) | 1 (1%) | 0 | 100 | 100 |
| 16 | F | 101/135 (75%) | 101 (100%) | 0 | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 17 | G | 143/179 (80%) | 137 (96%) | 6 (4%) | 0 | 100 | 100 |
| 18 | H | 127/130 (98%) | 122 (96%) | 5 (4%) | 0 | 100 | 100 |
| 19 | I | 125/130 (96%) | 123 (98%) | 2 (2%) | 0 | 100 | 100 |
| 20 | J | 96/103 (93%) | 93 (97%) | 2 (2%) | 1 (1%) | 12 | 17 |
| 21 | M | 113/118 (96%) | 111 (98%) | 2 (2%) | 0 | 100 | 100 |
| 22 | N | 98/101 (97%) | 98 (100%) | 0 | 0 | 100 | 100 |
| 23 | O | 86/89 (97%) | 85 (99%) | 1 (1%) | 0 | 100 | 100 |
| 24 | P | 79/82 (96%) | 76 (96%) | 3 (4%) | 0 | 100 | 100 |
| 25 | Q | 75/84 (89%) | 72 (96%) | 3 (4%) | 0 | 100 | 100 |
| 26 | R | 53/75 (71%) | 53 (100%) | 0 | 0 | 100 | 100 |
| 27 | S | 82/92 (89%) | 81 (99%) | 1 (1%) | 0 | 100 | 100 |
| 28 | T | 84/87 (97%) | 84 (100%) | 0 | 0 | 100 | 100 |
| 29 | U | 68/71 (96%) | 68 (100%) | 0 | 0 | 100 | 100 |
| 32 | c | 269/273 (98%) | 261 (97%) | 8 (3%) | 0 | 100 | 100 |
| 33 | e | 199/201 (99%) | 196 (98%) | 3 (2%) | 0 | 100 | 100 |
| 34 | f | 175/179 (98%) | 173 (99%) | 2 (1%) | 0 | 100 | 100 |
| 35 | g | 174/177 (98%) | 170 (98%) | 3 (2%) | 1 (1%) | 21 | 29 |
| 36 | h | 39/149 (26%) | 37 (95%) | 2 (5%) | 0 | 100 | 100 |
| 37 | i | 140/142 (99%) | 140 (100%) | 0 | 0 | 100 | 100 |
| 38 | j | 121/123 (98%) | 120 (99%) | 1 (1%) | 0 | 100 | 100 |
| 39 | k | 142/144 (99%) | 139 (98%) | 3 (2%) | 0 | 100 | 100 |
| 40 | m | 116/127 (91%) | 111 (96%) | 5 (4%) | 0 | 100 | 100 |
| 41 | n | 114/117 (97%) | 112 (98%) | 2 (2%) | 0 | 100 | 100 |
| 42 | o | 112/115 (97%) | 110 (98%) | 2 (2%) | 0 | 100 | 100 |
| 43 | p | 115/118 (98%) | 115 (100%) | 0 | 0 | 100 | 100 |
| 44 | q | 101/103 (98%) | 98 (97%) | 3 (3%) | 0 | 100 | 100 |
| 45 | r | 108/110 (98%) | 107 (99%) | 1 (1%) | 0 | 100 | 100 |
| 46 | s | 91/100 (91%) | 90 (99%) | 1 (1%) | 0 | 100 | 100 |
| 47 | t | 100/104 (96%) | 97 (97%) | 3 (3%) | 0 | 100 | 100 |
| 48 | u | 92/94 (98%) | 92 (100%) | 0 | 0 | 100 | 100 |
| 49 | v | 73/85 (86%) | 72 (99%) | 1 (1%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 50 | w | 75/78 (96%) | 75 (100%) | 0 | 0 | 100 | 100 |
| 51 | x | 60/63 (95%) | 60 (100%) | 0 | 0 | 100 | 100 |
| 52 | y | 55/59 (93%) | 54 (98%) | 1 (2%) | 0 | 100 | 100 |
| 53 | z | 54/57 (95%) | 53 (98%) | 1 (2%) | 0 | 100 | 100 |
| 55 | 8 | 11/19 (58%) | 10 (91%) | 1 (9%) | 0 | 100 | 100 |
| All | All | 5463/5932 (92%) | 5362 (98%) | 96 (2%) | 5 (0%) | 49 | 61 |

All (5) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 6 | L | 102 | LEU |
| 20 | J | 57 | VAL |
| 5 | K | 17 | SER |
| 14 | D | 46 | PRO |
| 35 | g | 61 | GLY |

### 5.3.2 Protein sidechains (i)

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 3 | 3 | 34/34 (100%) | 34 (100%) | 0 | 100 | 100 |
| 4 | 4 | 54/62 (87%) | 54 (100%) | 0 | 100 | 100 |
| 5 | K | 89/98 (91%) | 88 (99%) | 1 (1%) | 65 | 79 |
| 6 | L | 102/103 (99%) | 102 (100%) | 0 | 100 | 100 |
| 7 | d | 163/163 (100%) | 162 (99%) | 1 (1%) | 78 | 87 |
| 8 | l | 107/107 (100%) | 107 (100%) | 0 | 100 | 100 |
| 9 | 0 | 45/49 (92%) | 45 (100%) | 0 | 100 | 100 |
| 10 | 1 | 37/38 (97%) | 37 (100%) | 0 | 100 | 100 |
| 11 | 2 | 51/52 (98%) | 50 (98%) | 1 (2%) | 48 | 67 |
| 12 | B | 186/199 (94%) | 186 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 13 | C | 170/190 (90%) | 169 (99%) | 1 (1%) | 78 87 |
| 14 | D | 172/173 (99%) | 170 (99%) | 2 (1%) | 63 78 |
| 15 | E | 119/126 (94%) | 119 (100%) | 0 | 100 100 |
| 16 | F | 90/116 (78%) | 89 (99%) | 1 (1%) | 65 79 |
| 17 | G | 122/147 (83%) | 122 (100%) | 0 | 100 100 |
| 18 | H | 104/105 (99%) | 104 (100%) | 0 | 100 100 |
| 19 | I | 105/107 (98%) | 104 (99%) | 1 (1%) | 68 80 |
| 20 | J | 86/90 (96%) | 86 (100%) | 0 | 100 100 |
| 21 | M | 93/96 (97%) | 93 (100%) | 0 | 100 100 |
| 22 | N | 83/84 (99%) | 83 (100%) | 0 | 100 100 |
| 23 | O | 76/77 (99%) | 76 (100%) | 0 | 100 100 |
| 24 | P | 65/65 (100%) | 65 (100%) | 0 | 100 100 |
| 25 | Q | 71/78 (91%) | 71 (100%) | 0 | 100 100 |
| 26 | R | 48/65 (74%) | 48 (100%) | 0 | 100 100 |
| 27 | S | 72/79 (91%) | 72 (100%) | 0 | 100 100 |
| 28 | T | 65/66 (98%) | 65 (100%) | 0 | 100 100 |
| 29 | U | 60/61 (98%) | 60 (100%) | 0 | 100 100 |
| 32 | c | 216/218 (99%) | 216 (100%) | 0 | 100 100 |
| 33 | e | 165/165 (100%) | 165 (100%) | 0 | 100 100 |
| 34 | f | 148/150 (99%) | 146 (99%) | 2 (1%) | 59 75 |
| 35 | g | 137/138 (99%) | 136 (99%) | 1 (1%) | 76 85 |
| 36 | h | 32/114 (28%) | 32 (100%) | 0 | 100 100 |
| 37 | i | 116/116 (100%) | 116 (100%) | 0 | 100 100 |
| 38 | j | 104/104 (100%) | 104 (100%) | 0 | 100 100 |
| 39 | k | 103/103 (100%) | 103 (100%) | 0 | 100 100 |
| 40 | m | 98/103 (95%) | 98 (100%) | 0 | 100 100 |
| 41 | n | 86/87 (99%) | 85 (99%) | 1 (1%) | 63 78 |
| 42 | o | 99/100 (99%) | 99 (100%) | 0 | 100 100 |
| 43 | p | 89/90 (99%) | 89 (100%) | 0 | 100 100 |
| 44 | q | 84/84 (100%) | 84 (100%) | 0 | 100 100 |
| 45 | r | 93/93 (100%) | 92 (99%) | 1 (1%) | 65 79 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 46 | s | 80/84 (95%) | 79 (99%) | 1 (1%) | 61 76 |
| 47 | t | 83/85 (98%) | 81 (98%) | 2 (2%) | 43 61 |
| 48 | u | 78/78 (100%) | 78 (100%) | 0 | 100 100 |
| 49 | v | 56/63 (89%) | 56 (100%) | 0 | 100 100 |
| 50 | w | 67/68 (98%) | 67 (100%) | 0 | 100 100 |
| 51 | x | 54/55 (98%) | 54 (100%) | 0 | 100 100 |
| 52 | y | 48/49 (98%) | 48 (100%) | 0 | 100 100 |
| 53 | z | 47/48 (98%) | 47 (100%) | 0 | 100 100 |
| 55 | 8 | 13/18 (72%) | 13 (100%) | 0 | 100 100 |
| All | All | 4565/4843 (94%) | 4549 (100%) | 16 (0%) | 81 90 |

5 of 16 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 47 | t | 17 | LYS |
| 46 | s | 93 | LEU |
| 34 | f | 120 | LYS |
| 45 | r | 66 | ILE |
| 19 | I | 85 | ARG |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 79 such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 37 | i | 128 | ASN |
| 48 | u | 49 | ASN |
| 38 | j | 3 | GLN |
| 44 | q | 12 | HIS |
| 51 | x | 27 | ASN |

### 5.3.3 RNA (i)

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|---|---|---|---|---|
| 1 | a | 2749/2904 (94%) | 305 (11%) | 0 |
| 2 | A | 1516/1542 (98%) | 206 (13%) | 31 (2%) |
| 30 | X | 5/6 (83%) | 2 (40%) | 0 |
| 31 | b | 118/120 (98%) | 11 (9%) | 0 |
| 54 | Z | 75/77 (97%) | 22 (29%) | 2 (2%) |

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| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|---|---|---|---|---|
| All | All | 4463/4649 (95%) | 546 (12%) | 33 (0%) |

5 of 546 RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | a | 10 | A |
| 1 | a | 34 | U |
| 1 | a | 63 | A |
| 1 | a | 71 | A |
| 1 | a | 74 | A |

5 of 33 RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | A | 1397 | C |
| 2 | A | 1447 | A |
| 54 | Z | 46 | G |
| 2 | A | 776 | G |
| 2 | A | 641 | U |

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

40 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 | $\#\|Z\| > 2$ |
| 1 | OMC | a | 2498 | 1 | 19,22,23 | 0.52 | 0 | 26,31,34 | 0.55 | 0 |
| 1 | 3TD | a | 1915 | 1 | 18,22,23 | 0.85 | 1 (5%) | 22,32,35 | 0.62 | 0 |
| 2 | 2MG | A | 966 | 2 | 23,26,27 | 0.41 | 0 | 32,38,41 | 0.41 | 0 |
| 2 | 4OC | A | 1402 | 2 | 20,23,24 | 0.34 | 0 | 26,32,35 | 0.56 | 0 |
| 1 | G7M | a | 2069 | 1 | 23,26,27 | 0.80 | 0 | 35,39,42 | 0.71 | 0 |
| 8 | 4D4 | l | 81 | 8 | 9,11,12 | 1.87 | 2 (22%) | 8,13,15 | 1.29 | 0 |
| 6 | D2T | L | 89 | 6 | 7,9,10 | 1.01 | 0 | 6,11,13 | 1.77 | 3 (50%) |
| 1 | PSU | a | 2457 | 1 | 18,21,22 | 0.93 | 1 (5%) | 22,30,33 | 0.63 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 1 | 2MA | a | 2503 | 1 | 22,25,26 | 0.55 | 0 | 33,37,40 | 0.76 | 1 (3%) |
| 1 | PSU | a | 955 | 1 | 18,21,22 | 0.93 | 1 (5%) | 22,30,33 | 0.69 | 0 |
| 1 | 1MG | a | 745 | 1 | 22,26,27 | 0.88 | 2 (9%) | 33,39,42 | 0.44 | 0 |
| 1 | PSU | a | 2504 | 1 | 18,21,22 | 0.90 | 1 (5%) | 22,30,33 | 0.71 | 1 (4%) |
| 7 | MEQ | d | 150 | 7 | 8,9,10 | 0.59 | 0 | 5,10,12 | 0.89 | 0 |
| 1 | 5MC | a | 1962 | 1 | 18,22,23 | 0.40 | 0 | 26,32,35 | 0.65 | 0 |
| 1 | OMG | a | 2251 | 54,1 | 23,26,27 | 0.46 | 0 | 33,38,41 | 0.45 | 0 |
| 1 | PSU | a | 2605 | 1 | 18,21,22 | 0.96 | 1 (5%) | 22,30,33 | 0.92 | 1 (4%) |
| 1 | PSU | a | 2580 | 1 | 18,21,22 | 1.03 | 1 (5%) | 22,30,33 | 0.79 | 1 (4%) |
| 2 | 5MC | A | 1407 | 2 | 18,22,23 | 0.32 | 0 | 26,32,35 | 0.68 | 0 |
| 2 | 2MG | A | 1207 | 2 | 23,26,27 | 0.38 | 0 | 32,38,41 | 0.43 | 0 |
| 2 | 2MG | A | 1516 | 2 | 23,26,27 | 0.43 | 0 | 32,38,41 | 0.53 | 0 |
| 1 | PSU | a | 746 | 1 | 18,21,22 | 0.98 | 1 (5%) | 22,30,33 | 0.71 | 0 |
| 1 | 6MZ | a | 1618 | 1 | 22,25,26 | 0.40 | 0 | 30,36,39 | 0.62 | 0 |
| 2 | MA6 | A | 1518 | 2 | 23,26,27 | 0.35 | 0 | 34,38,41 | 0.74 | 1 (2%) |
| 1 | PSU | a | 1917 | 1 | 18,21,22 | 0.87 | 1 (5%) | 22,30,33 | 0.63 | 0 |
| 2 | PSU | A | 516 | 2 | 18,21,22 | 0.90 | 1 (5%) | 22,30,33 | 0.68 | 0 |
| 1 | 2MG | a | 1835 | 1 | 23,26,27 | 0.38 | 0 | 32,38,41 | 0.44 | 0 |
| 2 | G7M | A | 527 | 2 | 23,26,27 | 0.78 | 1 (4%) | 35,39,42 | 0.64 | 1 (2%) |
| 1 | 5MU | a | 1939 | 1 | 19,22,23 | 0.50 | 0 | 28,32,35 | 0.36 | 0 |
| 2 | 5MC | A | 967 | 2 | 18,22,23 | 0.36 | 0 | 26,32,35 | 0.56 | 0 |
| 1 | 2MG | a | 2445 | 1 | 23,26,27 | 0.54 | 0 | 32,38,41 | 0.40 | 0 |
| 1 | 6MZ | a | 2030 | 1 | 22,25,26 | 0.81 | 0 | 30,36,39 | 0.69 | 0 |
| 1 | H2U | a | 2449 | 1 | 18,21,22 | 0.70 | 0 | 21,30,33 | 0.98 | 2 (9%) |
| 1 | PSU | a | 2604 | 1 | 18,21,22 | 1.01 | 2 (11%) | 22,30,33 | 0.83 | 1 (4%) |
| 1 | 5MU | a | 747 | 1 | 19,22,23 | 0.43 | 0 | 28,32,35 | 0.49 | 0 |
| 8 | MS6 | l | 82 | 8 | 5,7,8 | 0.23 | 0 | 2,7,9 | 0.27 | 0 |
| 5 | IAS | K | 119 | 5 | 6,7,8 | 1.36 | 1 (16%) | 6,8,10 | 0.88 | 0 |
| 1 | PSU | a | 1911 | 1 | 18,21,22 | 0.86 | 1 (5%) | 22,30,33 | 0.60 | 0 |
| 1 | OMU | a | 2552 | 1 | 19,22,23 | 0.50 | 0 | 26,31,34 | 0.48 | 0 |
| 2 | MA6 | A | 1519 | 2 | 23,26,27 | 0.42 | 0 | 34,38,41 | 0.80 | 1 (2%) |
| 2 | UR3 | A | 1498 | 2 | 19,22,23 | 0.42 | 0 | 26,32,35 | 0.69 | 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 |
|---|---|---|---|---|---|---|---|
| 1 | OMC | a | 2498 | 1 | - | 0/9/27/28 | 0/2/2/2 |
| 1 | 3TD | a | 1915 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 2 | 2MG | A | 966 | 2 | - | 0/9/27/28 | 0/3/3/3 |
| 2 | 4OC | A | 1402 | 2 | - | 0/9/29/30 | 0/2/2/2 |
| 1 | G7M | a | 2069 | 1 | - | 2/7/25/26 | 0/3/3/3 |
| 8 | 4D4 | l | 81 | 8 | - | 1/11/12/14 | - |
| 6 | D2T | L | 89 | 6 | - | 5/7/12/14 | - |
| 1 | PSU | a | 2457 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | 2MA | a | 2503 | 1 | - | 2/7/25/26 | 0/3/3/3 |
| 1 | PSU | a | 955 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | 1MG | a | 745 | 1 | - | 0/7/25/26 | 0/3/3/3 |
| 1 | PSU | a | 2504 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 7 | MEQ | d | 150 | 7 | - | 2/8/9/11 | - |
| 1 | 5MC | a | 1962 | 1 | - | 1/7/25/26 | 0/2/2/2 |
| 1 | OMG | a | 2251 | 54,1 | - | 0/9/27/28 | 0/3/3/3 |
| 1 | PSU | a | 2605 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | PSU | a | 2580 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 2 | 5MC | A | 1407 | 2 | - | 0/7/25/26 | 0/2/2/2 |
| 2 | 2MG | A | 1207 | 2 | - | 0/9/27/28 | 0/3/3/3 |
| 2 | 2MG | A | 1516 | 2 | - | 0/9/27/28 | 0/3/3/3 |
| 1 | PSU | a | 746 | 1 | - | 1/7/25/26 | 0/2/2/2 |
| 1 | 6MZ | a | 1618 | 1 | - | 0/9/27/28 | 0/3/3/3 |
| 2 | MA6 | A | 1518 | 2 | - | 0/11/29/30 | 0/3/3/3 |
| 1 | PSU | a | 1917 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 2 | PSU | A | 516 | 2 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | 2MG | a | 1835 | 1 | - | 0/9/27/28 | 0/3/3/3 |
| 2 | G7M | A | 527 | 2 | - | 1/7/25/26 | 0/3/3/3 |
| 1 | 5MU | a | 1939 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 2 | 5MC | A | 967 | 2 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | 2MG | a | 2445 | 1 | - | 0/9/27/28 | 0/3/3/3 |
| 1 | 6MZ | a | 2030 | 1 | - | 2/9/27/28 | 0/3/3/3 |
| 1 | H2U | a | 2449 | 1 | - | 0/7/38/39 | 0/2/2/2 |
| 1 | PSU | a | 2604 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | 5MU | a | 747 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 8 | MS6 | l | 82 | 8 | - | 1/4/6/8 | - |
| 5 | IAS | K | 119 | 5 | - | 0/7/7/8 | - |
| 1 | PSU | a | 1911 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | OMU | a | 2552 | 1 | - | 0/9/27/28 | 0/2/2/2 |
| 2 | MA6 | A | 1519 | 2 | - | 2/11/29/30 | 0/3/3/3 |
| 2 | UR3 | A | 1498 | 2 | - | 0/7/25/26 | 0/2/2/2 |

The worst 5 of 18 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 8 | l | 81 | 4D4 | CZ-NE | 4.01 | 1.41 | 1.33 |
| 2 | A | 516 | PSU | C6-C5 | 3.46 | 1.39 | 1.35 |
| 1 | a | 1915 | 3TD | C6-C5 | 3.40 | 1.39 | 1.35 |
| 1 | a | 2504 | PSU | C6-C5 | 3.32 | 1.39 | 1.35 |
| 1 | a | 1911 | PSU | C6-C5 | 3.25 | 1.39 | 1.35 |

The worst 5 of 13 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | A | 1518 | MA6 | C2-N1-C6 | 3.11 | 119.11 | 111.75 |
| 2 | A | 1519 | MA6 | C2-N1-C6 | 3.05 | 118.96 | 111.75 |
| 1 | a | 2449 | H2U | N3-C2-N1 | 2.61 | 119.42 | 116.65 |
| 6 | L | 89 | D2T | OD1-CG-CB | -2.56 | 117.07 | 122.44 |
| 1 | a | 2503 | 2MA | C5-C4-N3 | -2.40 | 124.49 | 127.19 |

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 6 | L | 89 | D2T | O-C-CA-CB |
| 6 | L | 89 | D2T | CA-CB-CG-OD1 |
| 6 | L | 89 | D2T | CA-CB-CG-OD2 |
| 6 | L | 89 | D2T | SB-CB-CG-OD2 |
| 1 | a | 2030 | 6MZ | O4'-C4'-C5'-O5' |

There are no ring outliers.

6 monomers are involved in 7 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 1 | a | 1915 | 3TD | 2 | 0 |
| 1 | a | 1939 | 5MU | 1 | 0 |
| 1 | a | 2030 | 6MZ | 2 | 0 |
| 1 | a | 2604 | PSU | 1 | 0 |
| 5 | K | 119 | IAS | 1 | 0 |
| 1 | a | 2552 | OMU | 1 | 0 |

## 5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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.

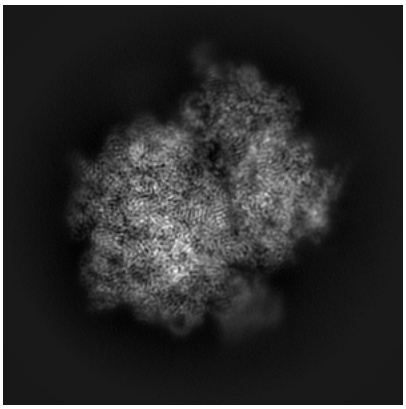
# 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-55845. These allow visual inspection of the internal detail of the map and identification of artifacts.

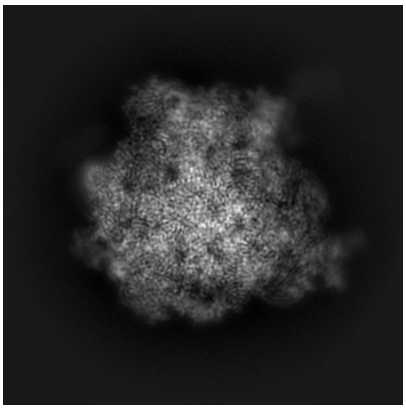
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

## 6.1 Orthogonal projections

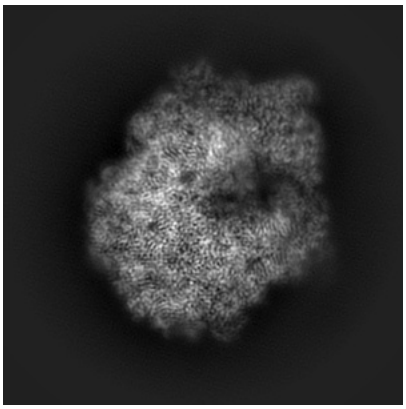
### 6.1.1 Primary map



X

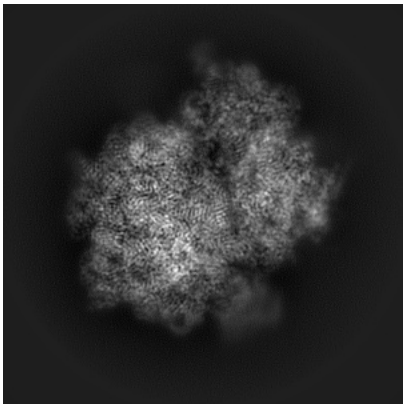


Y

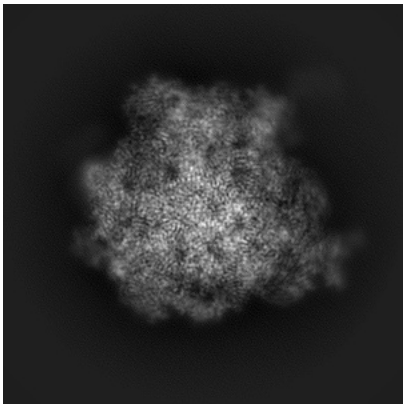


Z

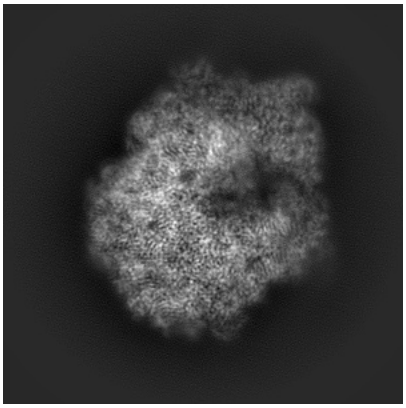
### 6.1.2 Raw map



X



Y

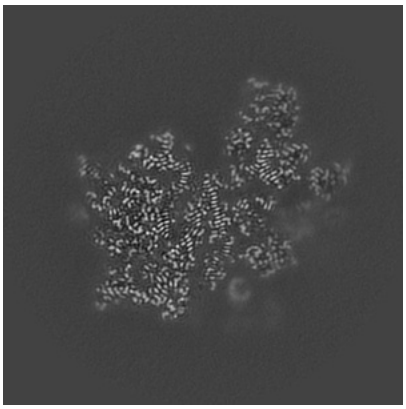


Z

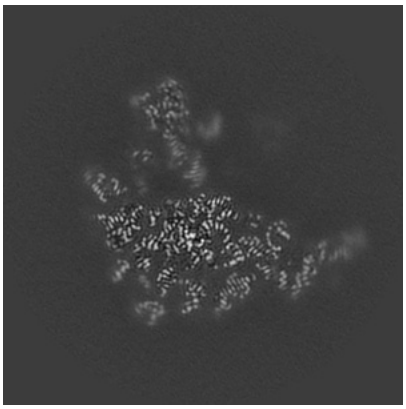
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices (i)

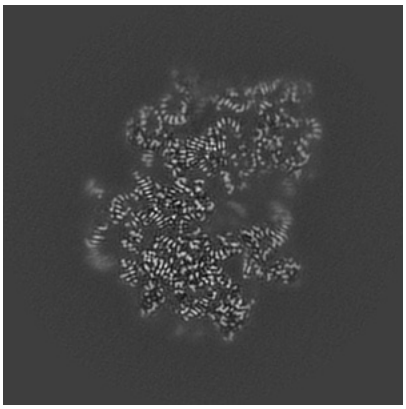
### 6.2.1 Primary map



X Index: 208

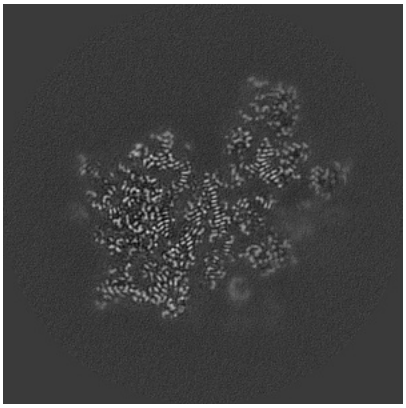


Y Index: 208

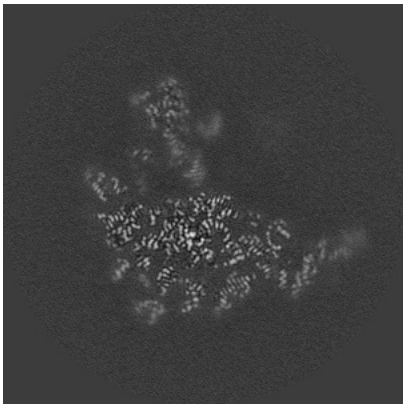


Z Index: 208

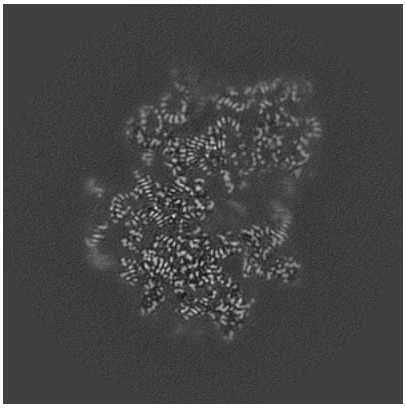
### 6.2.2 Raw map



X Index: 208



Y Index: 208

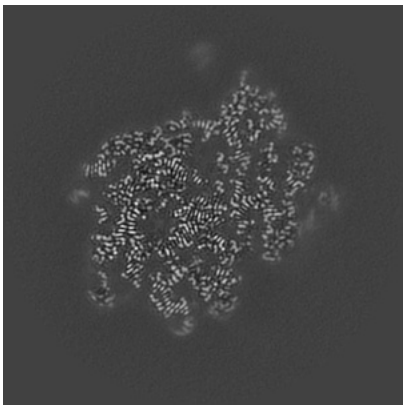


Z Index: 208

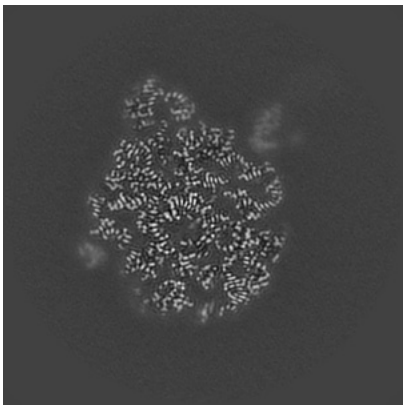
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices (i)

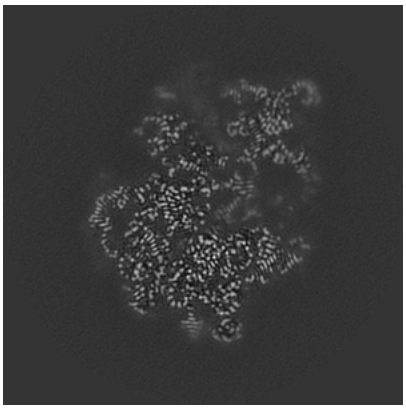
### 6.3.1 Primary map



X Index: 178

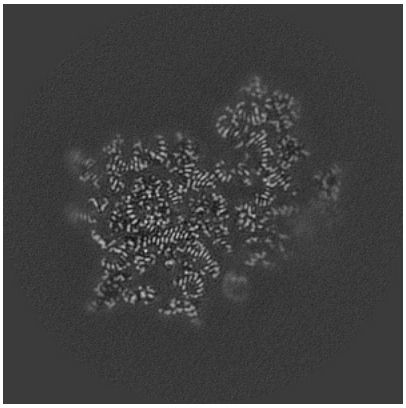


Y Index: 169

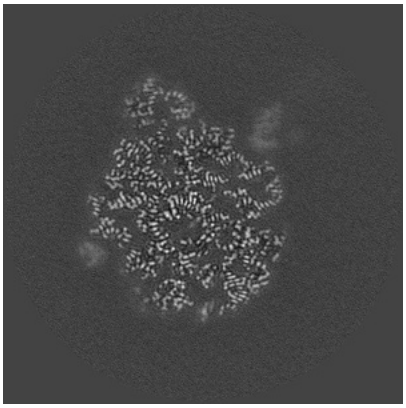


Z Index: 194

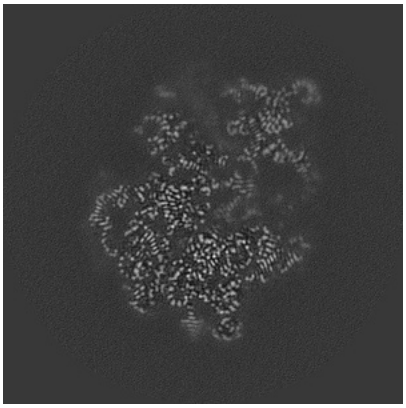
### 6.3.2 Raw map



X Index: 199



Y Index: 169

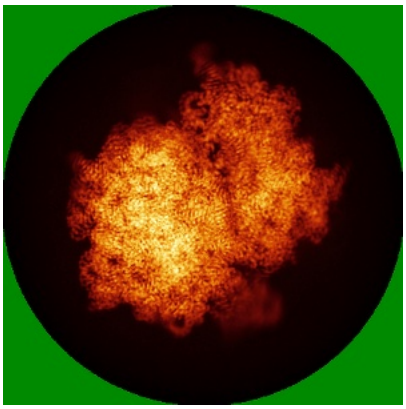


Z Index: 194

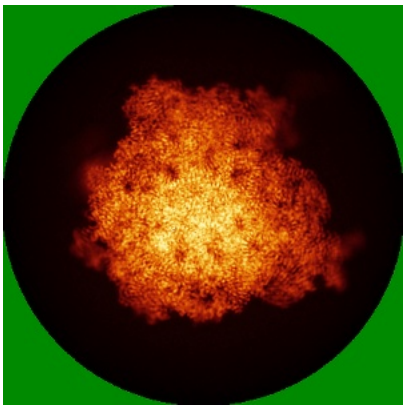
The images above show the largest variance slices of the map in three orthogonal directions.

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

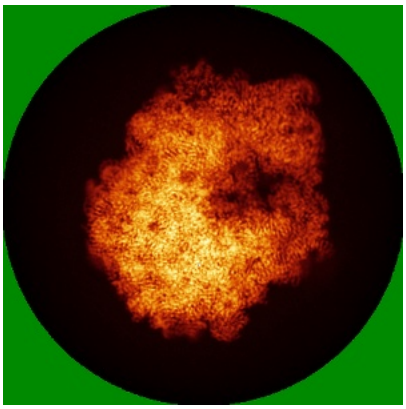
### 6.4.1 Primary map



X

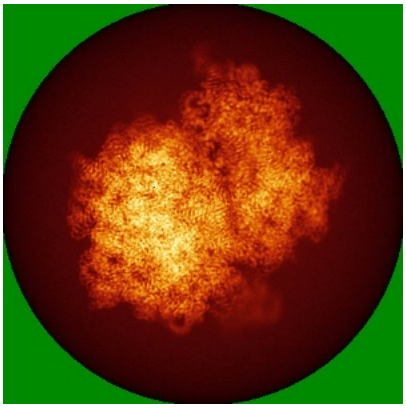


Y

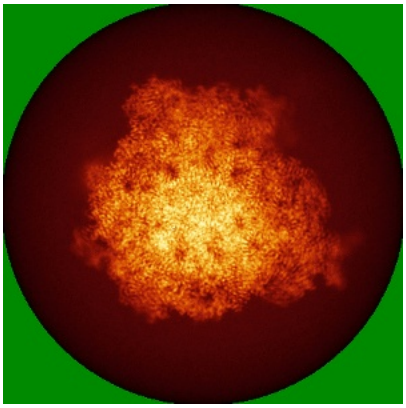


Z

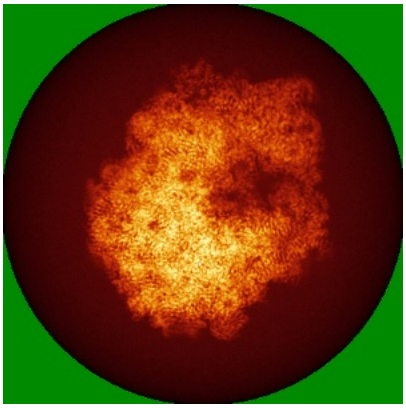
### 6.4.2 Raw map



X



Y

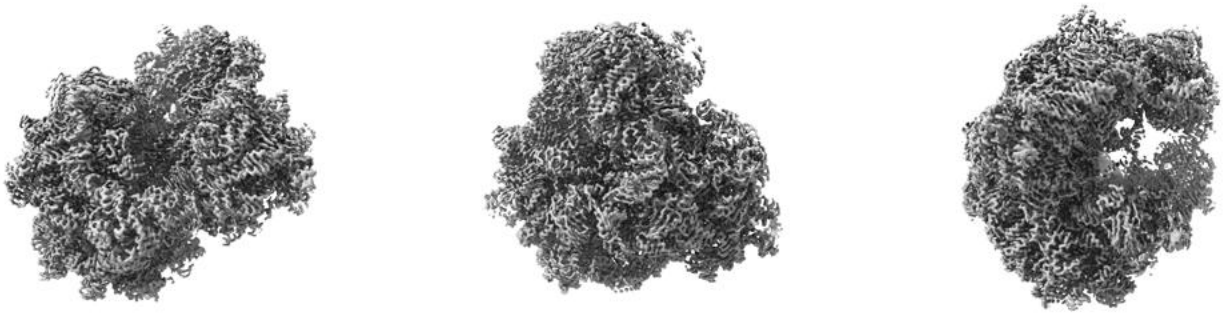


Z

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)

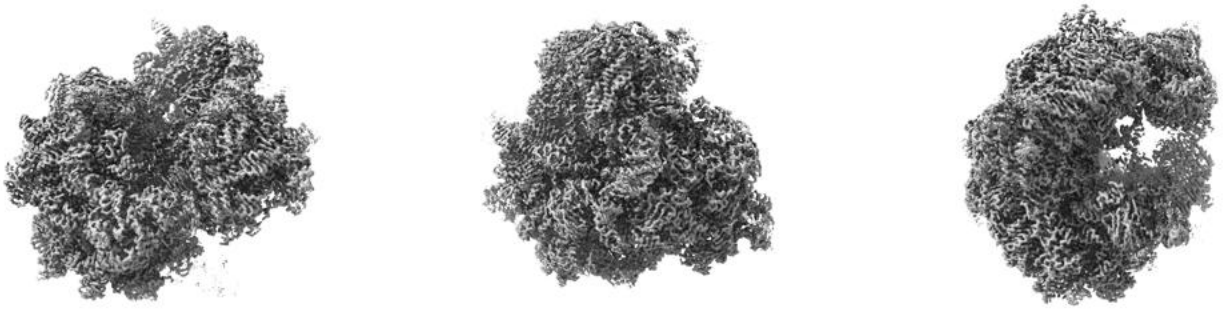
### 6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.01. 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.

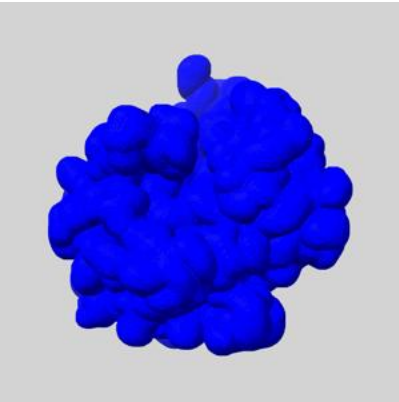
## 6.6 Mask visualisation (i)

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

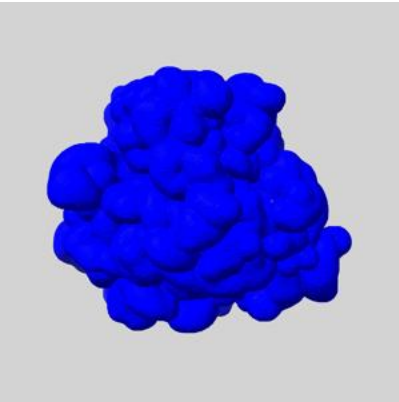
A mask typically either:

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

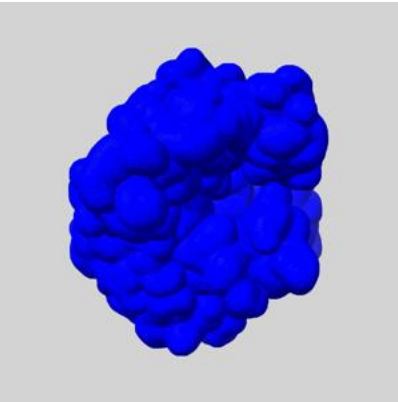
### 6.6.1 emd_55845_msk_1.map (i)



X



Y

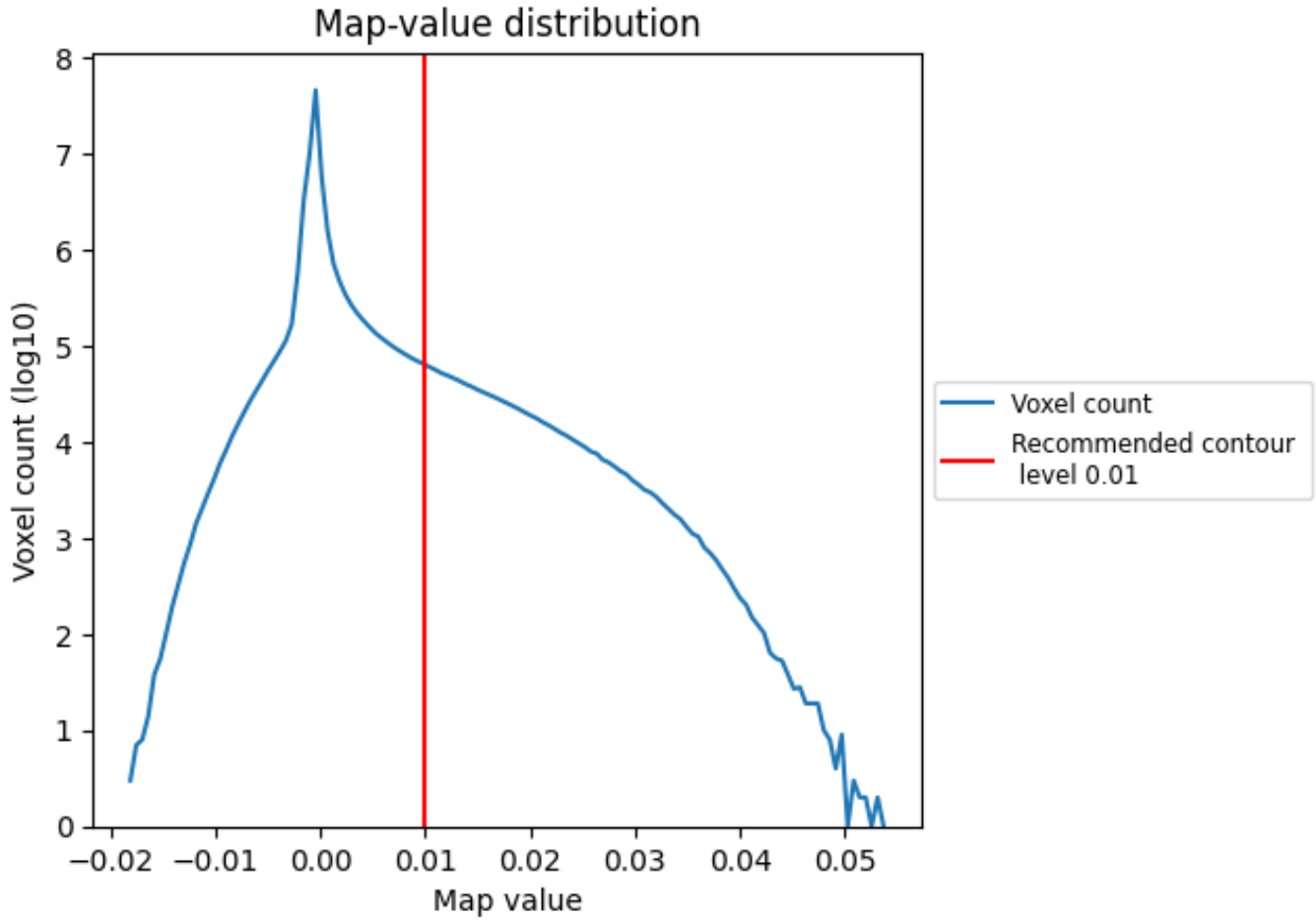


Z

# 7 Map analysis

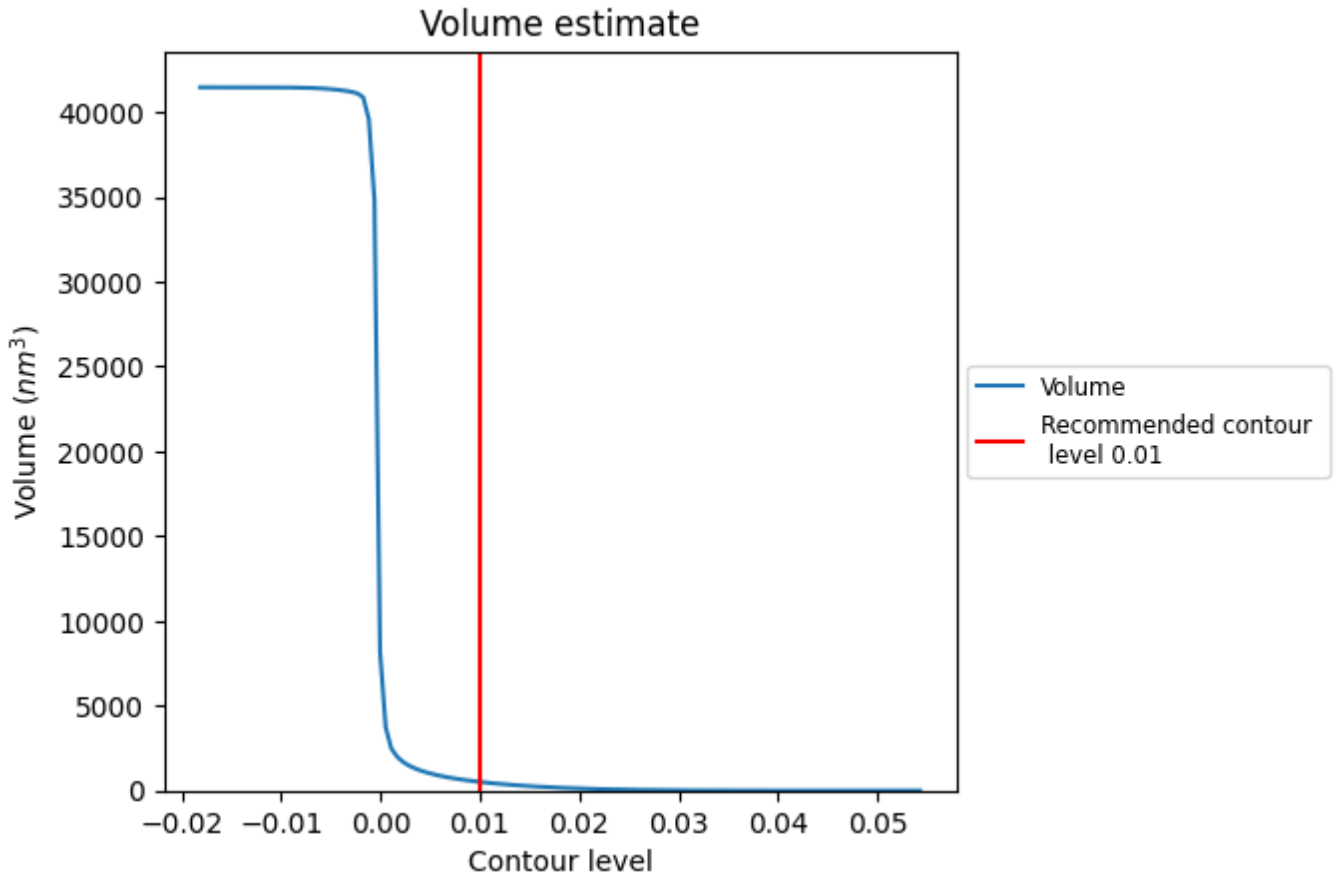
This section contains the results of statistical analysis of the map.

## 7.1 Map-value distribution




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.

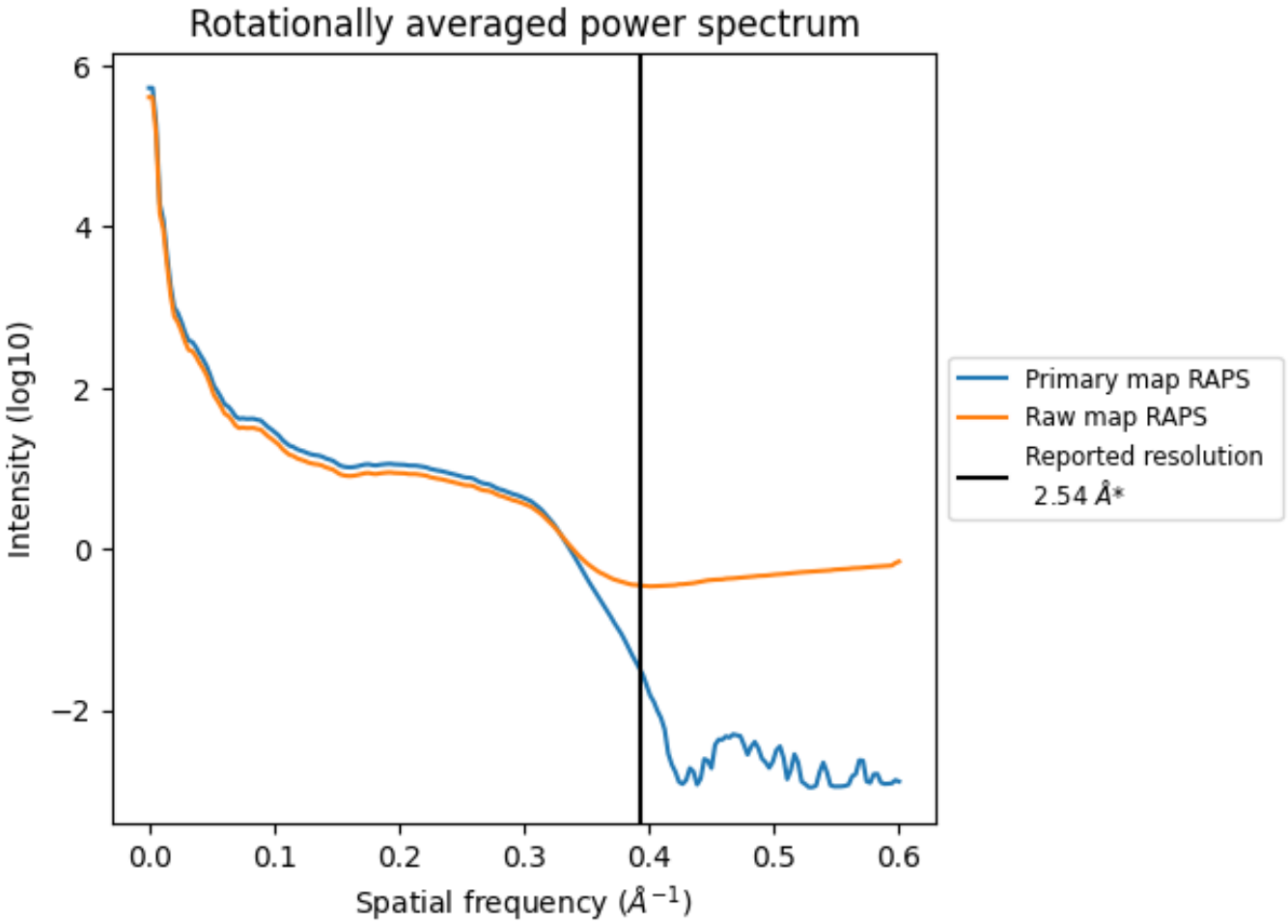
## 7.2 Volume estimate (i)




The volume at the recommended contour level is 511 $nm^3$; this corresponds to an approximate mass of 461 kDa.

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

## 7.3 Rotationally averaged power spectrum (i)

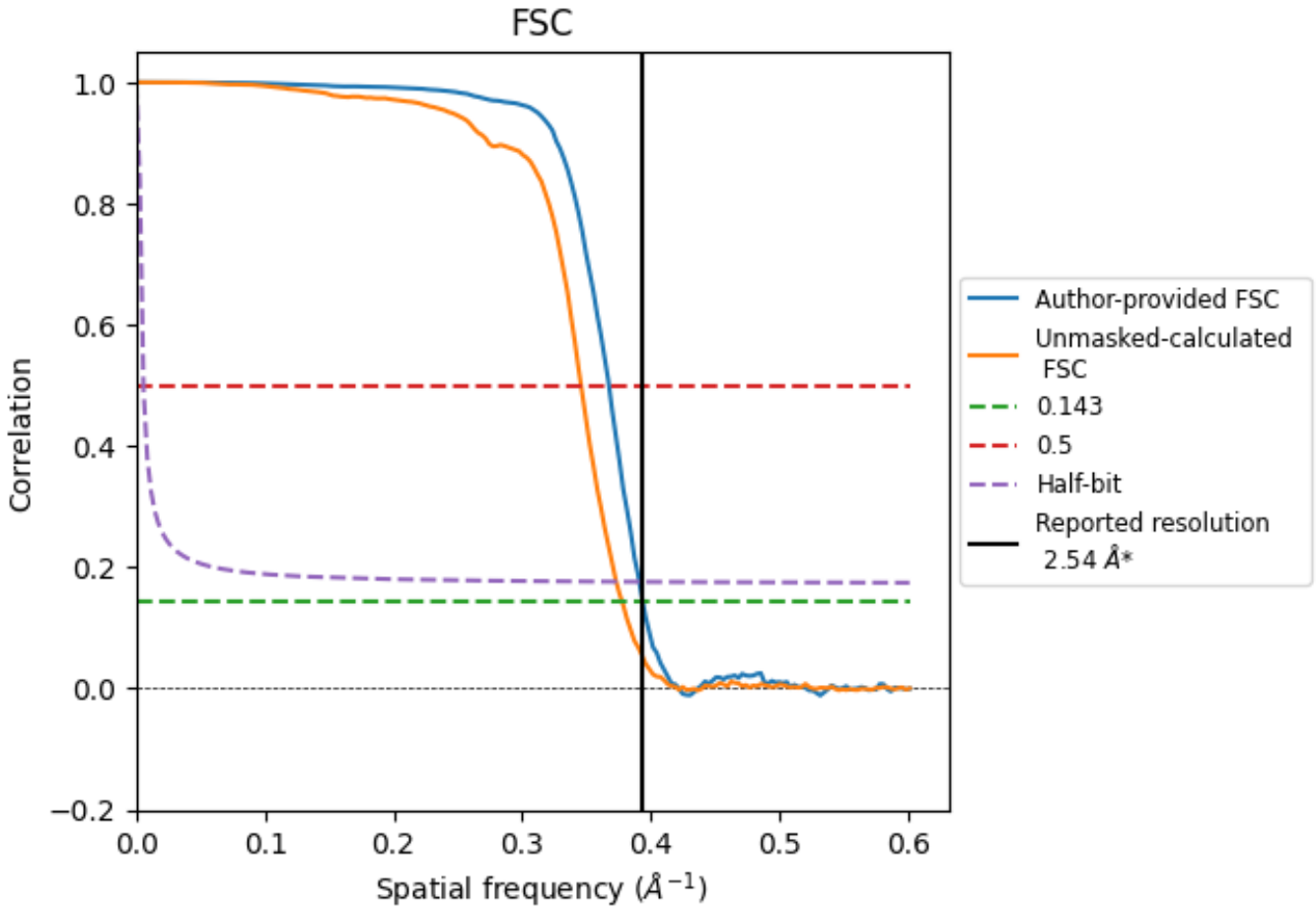



*Reported resolution corresponds to spatial frequency of 0.394 Å$^{-1}$

# 8 Fourier-Shell correlation

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




*Reported resolution corresponds to spatial frequency of 0.394 Å$^{-1}$

## 8.2 Resolution estimates (i)

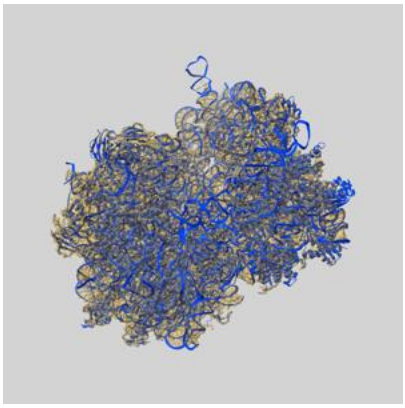
| Resolution estimate (Å) | Estimation criterion (FSC cut-off) | | |
|---|---|---|---|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | 2.54 | - | - |
| Author-provided FSC curve | 2.54 | 2.72 | 2.56 |
| Unmasked-calculated* | 2.65 | 2.89 | 2.68 |

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

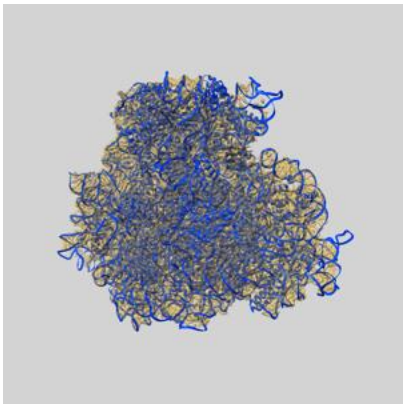
# 9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-55845 and PDB model 9TEX. Per-residue inclusion information can be found in section 3 on page 15.

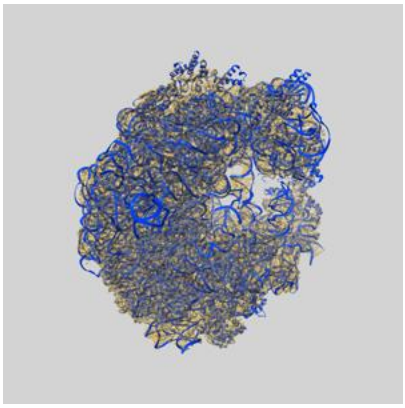
## 9.1 Map-model overlay



X



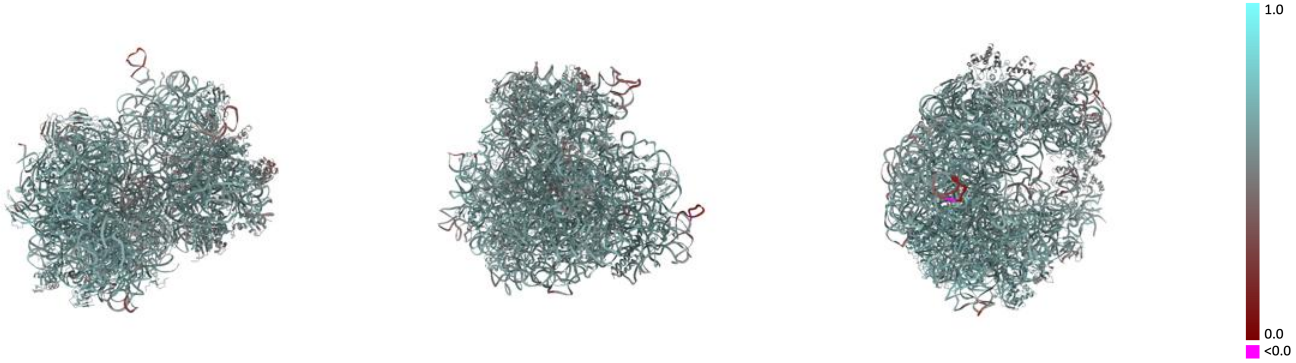
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.01 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.

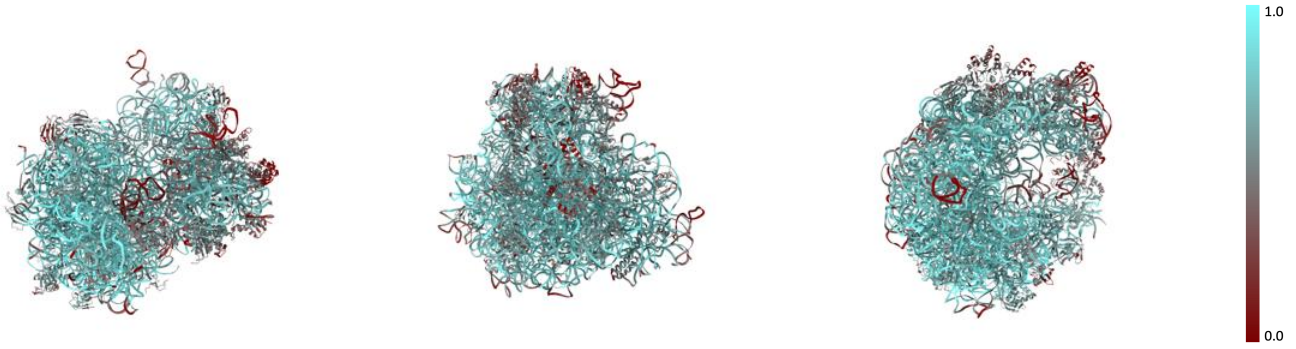
## 9.2 Q-score mapped to coordinate model (i)




X Y Z

The images above show the model with each residue coloured according 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.

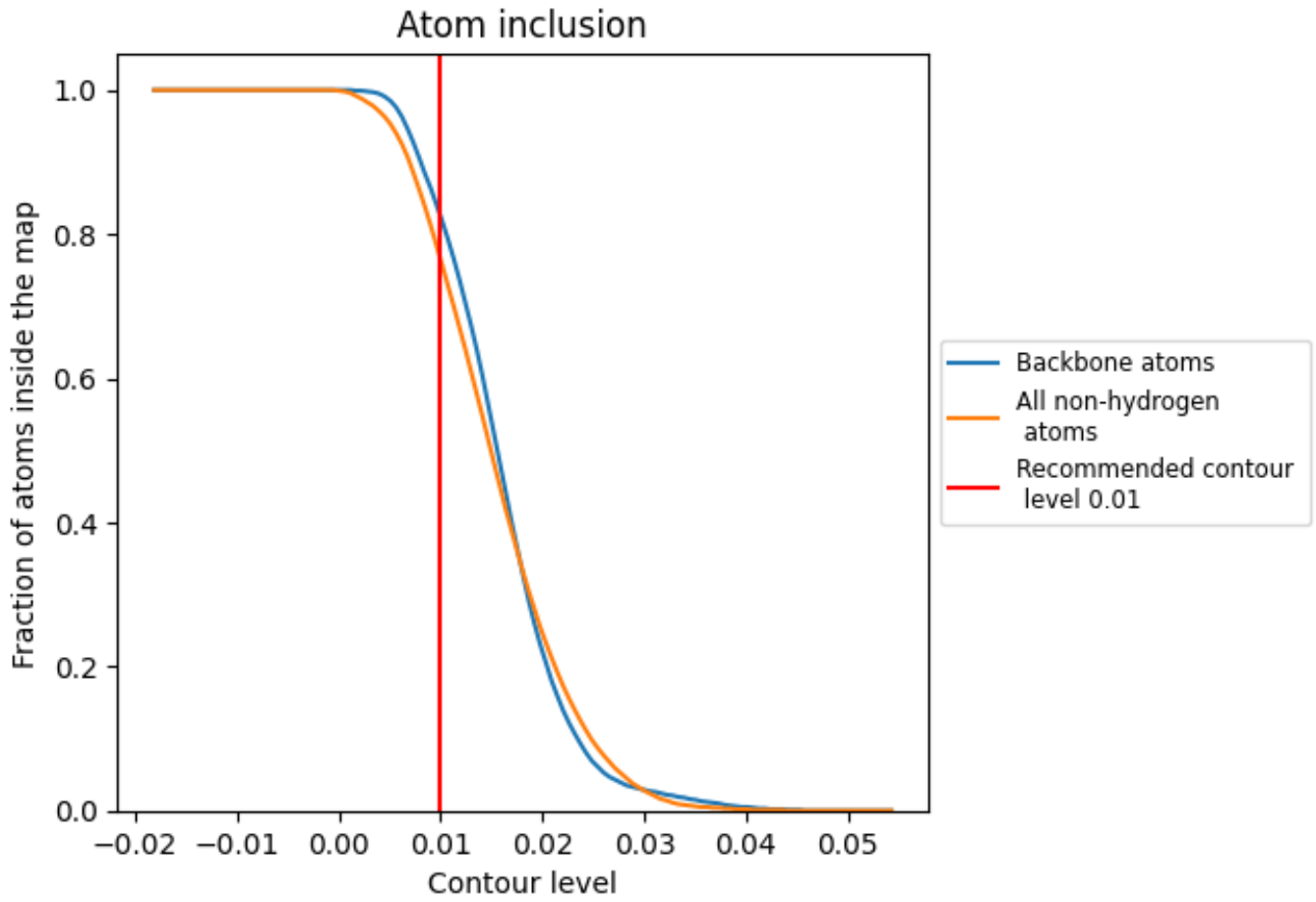
## 9.3 Atom inclusion mapped to coordinate model (i)




X Y Z

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 (0.01).

## 9.4 Atom inclusion (i)




At the recommended contour level, 82% of all backbone atoms, 76% 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 (0.01) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|---|---|---|
| All | 0.7650 | 0.6110 |
| 0 | 0.6420 | 0.6070 |
| 1 | 0.8320 | 0.6610 |
| 2 | 0.8150 | 0.6580 |
| 3 | 0.6890 | 0.6210 |
| 4 | 0.2740 | 0.5110 |
| 8 | 0.6360 | 0.6310 |
| A | 0.7830 | 0.6000 |
| B | 0.3690 | 0.5250 |
| C | 0.5120 | 0.5750 |
| D | 0.5110 | 0.5710 |
| E | 0.6150 | 0.6040 |
| F | 0.4990 | 0.5540 |
| G | 0.4330 | 0.5360 |
| H | 0.5910 | 0.5930 |
| I | 0.4830 | 0.5600 |
| J | 0.3360 | 0.5260 |
| K | 0.5790 | 0.5850 |
| L | 0.5800 | 0.6000 |
| M | 0.4480 | 0.5580 |
| N | 0.5320 | 0.5770 |
| O | 0.5840 | 0.5890 |
| P | 0.5880 | 0.5910 |
| Q | 0.5110 | 0.5760 |
| R | 0.5780 | 0.5780 |
| S | 0.4080 | 0.5500 |
| T | 0.5360 | 0.5750 |
| U | 0.3420 | 0.5200 |
| X | 0.4960 | 0.5600 |
| Z | 0.4390 | 0.5590 |
| a | 0.8860 | 0.6330 |
| b | 0.7980 | 0.6050 |
| c | 0.7690 | 0.6450 |
| d | 0.7610 | 0.6400 |
| e | 0.6490 | 0.6090 |

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| Chain | Atom inclusion | Q-score |
|---|---|---|
| f | 0.4060 | 0.5480 |
| g | 0.4230 | 0.5380 |
| h | 0.5130 | 0.5600 |
| i | 0.7610 | 0.6360 |
| j | 0.7080 | 0.6320 |
| k | 0.7140 | 0.6290 |
| l | 0.7050 | 0.6290 |
| m | 0.8150 | 0.6510 |
| n | 0.6030 | 0.5800 |
| o | 0.7040 | 0.6260 |
| p | 0.7910 | 0.6470 |
| q | 0.7000 | 0.6210 |
| r | 0.7190 | 0.6330 |
| s | 0.6070 | 0.6020 |
| t | 0.5610 | 0.5830 |
| u | 0.6040 | 0.5920 |
| v | 0.7620 | 0.6330 |
| w | 0.7270 | 0.6350 |
| x | 0.5460 | 0.5700 |
| y | 0.6920 | 0.6240 |
| z | 0.7290 | 0.6310 |