# wwPDB EM Validation Summary Report

Sep 17, 2026 – 12:24 AM EDT

| | | |
|---|---|---|
| PDB ID | : | 6OUO / pdb_00006ouo |
| EMDB ID | : | EMD-20204 |
| Title | : | RF2 accommodated state bound 70S complex at long incubation time |
| Authors | : | Fu, Z.; Indrisiunaite, G.; Kaledhonkar, S.; Shah, B.; Sun, M.; Chen, B.; Grassucci, R.A.; Ehrenberg, M.; Frank, J. |
| Deposited on | : | 2019-05-05 |
| Resolution | : | 3.70 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 ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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The following versions of software and data (see references ⓘ) were used in the production of this report:

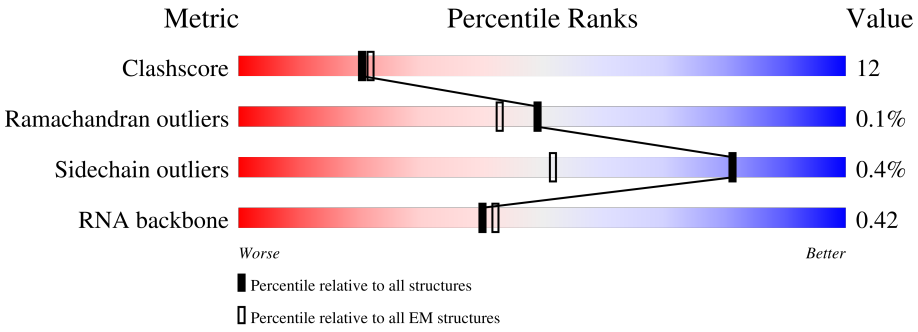
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev133 |
| Mogul | : | 2022.3.0, CSD as543be (2022) |
| MolProbity | : | 4-5-2 with Phenix2.0 |
| Percentile statistics | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| EM percentile statistics | : | 202505.v01 (Using 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 |

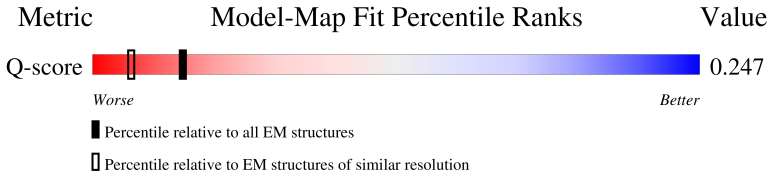
# 1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.70 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 | 11569 ( 3.20 - 4.20 ) |

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 | 1 | 2903 | 54% 36% 10% |
| 2 | 2 | 1534 | 50% 41% 9% |
| 3 | 3 | 120 | 61% 32% 8% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 4 | 4 | 9 | 78% 11% 11% |
| 5 | B | 271 | 75% 25% |
| 6 | C | 209 | 76% 23% |
| 7 | D | 201 | 79% 21% |
| 8 | E | 177 | 75% 25% |
| 9 | F | 175 | 79% 21% |
| 10 | G | 149 | 56% 72% 28% |
| 11 | J | 142 | 88% 12% |
| 12 | K | 123 | 77% 23% |
| 13 | L | 144 | 83% 17% |
| 14 | M | 136 | 82% 18% |
| 15 | N | 119 | 67% 32% |
| 16 | O | 116 | 78% 22% |
| 17 | P | 114 | 76% 24% |
| 18 | Q | 117 | 76% 24% |
| 19 | R | 103 | 68% 30% |
| 20 | S | 110 | 79% 21% |
| 21 | T | 94 | 79% 21% |
| 22 | U | 103 | 74% 26% |
| 23 | V | 94 | 72% 28% |
| 24 | W | 76 | 72% 28% |
| 25 | X | 77 | 77% 23% |
| 26 | Y | 62 | 74% 26% |
| 27 | Z | 58 | 66% 34% |
| 28 | a | 66 | 8% 71% 29% |

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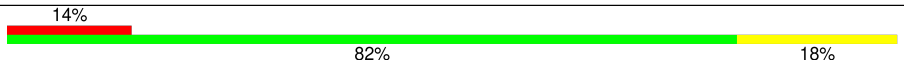
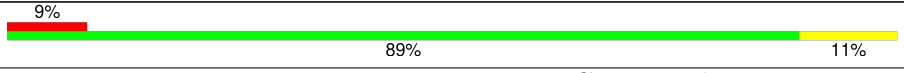
| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 29 | b | 56 | |
| 30 | c | 52 | |
| 31 | d | 46 | |
| 32 | e | 64 | |
| 33 | f | 38 | |
| 34 | g | 225 |   |
| 35 | h | 208 | |
| 36 | i | 205 | |
| 37 | j | 156 | |
| 38 | k | 104 | |
| 39 | l | 151 | |
| 40 | m | 129 | |
| 41 | n | 127 | |
| 42 | o | 99 | |
| 43 | p | 117 | |
| 44 | q | 87 | |
| 45 | r | 116 | |
| 46 | s | 100 | |
| 47 | t | 88 | |
| 48 | u | 82 | |
| 49 | v | 80 | |
| 50 | w | 66 | |
| 51 | x | 83 | |
| 52 | y | 86 | |
| 53 | z | 70 |   |

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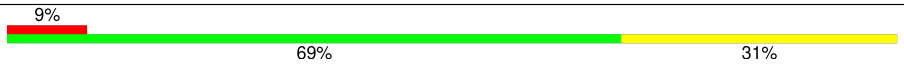
| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 54 | 5 | 76 | |
| 55 | A | 357 |   |

# 2 Entry composition (i)

There are 57 unique types of molecules in this entry. The entry contains 146867 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 ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 1 | 1 | 2903 | 62336 | 27816 | 11470 | 20147 | 2903 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 2 | 2 | 1534 | 32929 | 14693 | 6041 | 10661 | 1534 | 0 | 0 |

- Molecule 3 is a RNA chain called 5S ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 3 | 3 | 120 | 2569 | 1144 | 468 | 837 | 120 | 0 | 0 |

- Molecule 4 is a RNA chain called mRNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 4 | 4 | 9 | 184 | 83 | 26 | 66 | 9 | 0 | 0 |

- Molecule 5 is a protein called 50S ribosomal protein L2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 5 | B | 271 | 2082 | 1288 | 423 | 364 | 7 | 0 | 0 |

- Molecule 6 is a protein called 50S ribosomal protein L3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 6 | C | 209 | 1565 | 979 | 288 | 294 | 4 | 0 | 0 |

- Molecule 7 is a protein called 50S ribosomal protein L4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 7 | D | 201 | Total | C | N | O | S | 0 | 0 |
| | | | 1552 | 974 | 283 | 290 | 5 | | |

- Molecule 8 is a protein called 50S ribosomal protein L5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 8 | E | 177 | Total | C | N | O | S | 0 | 0 |
| | | | 1410 | 899 | 249 | 256 | 6 | | |

- Molecule 9 is a protein called 50S ribosomal protein L6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 9 | F | 175 | Total | C | N | O | S | 0 | 0 |
| | | | 1313 | 826 | 241 | 244 | 2 | | |

- Molecule 10 is a protein called 50S ribosomal protein L9.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 10 | G | 149 | Total | C | N | O | S | 0 | 0 |
| | | | 1111 | 699 | 197 | 214 | 1 | | |

- Molecule 11 is a protein called 50S ribosomal protein L13.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 11 | J | 142 | Total | C | N | O | S | 0 | 0 |
| | | | 1129 | 714 | 212 | 199 | 4 | | |

- Molecule 12 is a protein called 50S ribosomal protein L14.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 12 | K | 123 | Total | C | N | O | S | 0 | 0 |
| | | | 946 | 593 | 181 | 166 | 6 | | |

- Molecule 13 is a protein called 50S ribosomal protein L15.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 13 | L | 144 | Total | C | N | O | S | 0 | 0 |
| | | | 1053 | 654 | 207 | 190 | 2 | | |

- Molecule 14 is a protein called 50S ribosomal protein L16.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 14 | M | 136 | Total | C | N | O | S | 0 | 0 |
| | | | 1074 | 686 | 205 | 177 | 6 | | |

- Molecule 15 is a protein called 50S ribosomal protein L17.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 15 | N | 119 | Total | C | N | O | S | 0 | 0 |
| | | | 951 | 588 | 195 | 163 | 5 | | |

- Molecule 16 is a protein called 50S ribosomal protein L18.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 16 | O | 116 | Total | C | N | O | 0 | 0 |
| | | | 892 | 552 | 178 | 162 | | |

- Molecule 17 is a protein called 50S ribosomal protein L19.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 17 | P | 114 | Total | C | N | O | S | 0 | 0 |
| | | | 917 | 574 | 179 | 163 | 1 | | |

- Molecule 18 is a protein called 50S ribosomal protein L20.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 18 | Q | 117 | Total | C | N | O | 0 | 0 |
| | | | 947 | 604 | 192 | 151 | | |

- Molecule 19 is a protein called 50S ribosomal protein L21.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 19 | R | 103 | Total | C | N | O | S | 0 | 0 |
| | | | 816 | 516 | 153 | 145 | 2 | | |

- Molecule 20 is a protein called 50S ribosomal protein L22.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 20 | S | 110 | Total | C | N | O | S | 0 | 0 |
| | | | 857 | 532 | 166 | 156 | 3 | | |

- Molecule 21 is a protein called 50S ribosomal protein L23.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 21 | T | 94 | Total | C | N | O | S | 0 | 0 |
| | | | 746 | 470 | 140 | 134 | 2 | | |

- Molecule 22 is a protein called 50S ribosomal protein L24.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 22 | U | 103 | Total | C | N | O | 0 | 0 |
| | | | 788 | 498 | 148 | 142 | | |

- Molecule 23 is a protein called 50S ribosomal protein L25.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 23 | V | 94 | Total | C | N | O | S | 0 | 0 |
| | | | 753 | 479 | 137 | 134 | 3 | | |

- Molecule 24 is a protein called 50S ribosomal protein L27.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 24 | W | 76 | Total | C | N | O | S | 0 | 0 |
| | | | 582 | 360 | 117 | 104 | 1 | | |

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

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

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

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

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 27 | Z | 58 | Total | C | N | O | S | 0 | 0 |
| | | | 448 | 281 | 87 | 78 | 2 | | |

- Molecule 28 is a protein called 50S ribosomal protein L31.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 28 | a | 66 | Total | C | N | O | S | 0 | 0 |
| | | | 522 | 323 | 99 | 94 | 6 | | |

- Molecule 29 is a protein called 50S ribosomal protein L32.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 29 | b | 56 | Total | C | N | O | S | 0 | 0 |
| | | | 444 | 269 | 94 | 80 | 1 | | |

- Molecule 30 is a protein called 50S ribosomal protein L33.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 30 | c | 52 | Total | C | N | O | 0 | 0 |
| | | | 426 | 275 | 78 | 73 | | |

- Molecule 31 is a protein called 50S ribosomal protein L34.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 31 | d | 46 | Total | C | N | O | S | 0 | 0 |
| | | | 377 | 228 | 90 | 57 | 2 | | |

- Molecule 32 is a protein called 50S ribosomal protein L35.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 32 | e | 64 | Total | C | N | O | S | 0 | 0 |
| | | | 504 | 323 | 105 | 74 | 2 | | |

- Molecule 33 is a protein called 50S ribosomal protein L36.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 33 | f | 38 | Total | C | N | O | S | 0 | 0 |
| | | | 302 | 185 | 65 | 48 | 4 | | |

- Molecule 34 is a protein called 30S ribosomal protein S2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 34 | g | 225 | Total | C | N | O | S | 0 | 0 |
| | | | 1760 | 1113 | 316 | 323 | 8 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 35 | h | 208 | Total | C | N | O | S | 0 | 0 |
| | | | 1636 | 1036 | 307 | 290 | 3 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 36 | i | 205 | Total | C | N | O | S | 0 | 0 |
| | | | 1643 | 1026 | 315 | 298 | 4 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 37 | j | 156 | Total | C | N | O | S | 0 | 0 |
| | | | 1152 | 717 | 217 | 212 | 6 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 38 | k | 104 | Total | C | N | O | S | 0 | 0 |
| | | | 848 | 536 | 153 | 152 | 7 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 39 | l | 151 | Total | C | N | O | S | 0 | 0 |
| | | | 1181 | 735 | 227 | 215 | 4 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 40 | m | 129 | Total | C | N | O | S | 0 | 0 |
| | | | 979 | 616 | 173 | 184 | 6 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 41 | n | 127 | Total | C | N | O | S | 0 | 0 |
| | | | 1022 | 634 | 206 | 179 | 3 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 42 | o | 99 | Total<br>790 | C<br>495 | N<br>151 | O<br>143 | S<br>1 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 43 | p | 117 | Total<br>877 | C<br>540 | N<br>174 | O<br>160 | S<br>3 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 44 | q | 87 | Total<br>673 | C<br>417 | N<br>137 | O<br>116 | S<br>3 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 45 | r | 116 | Total<br>900 | C<br>558 | N<br>181 | O<br>158 | S<br>3 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 46 | s | 100 | Total<br>805 | C<br>499 | N<br>164 | O<br>139 | S<br>3 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 47 | t | 88 | Total<br>714 | C<br>439 | N<br>144 | O<br>130 | S<br>1 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 48 | u | 82 | Total<br>649 | C<br>406 | N<br>128 | O<br>114 | S<br>1 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 49 | v | 80 | Total<br>648 | C<br>411 | N<br>121 | O<br>113 | S<br>3 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 50 | w | 66 | Total<br>544 | C<br>344 | N<br>102 | O<br>97 | S<br>1 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 51 | x | 83 | Total<br>663 | C<br>424 | N<br>126 | O<br>111 | S<br>2 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 52 | y | 86 | Total<br>669 | C<br>414 | N<br>138 | O<br>114 | S<br>3 | 0 | 0 |

- Molecule 53 is a protein called 30S ribosomal protein S21.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 53 | z | 70 | Total<br>589 | C<br>366 | N<br>125 | O<br>97 | S<br>1 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 54 | 5 | 76 | Total<br>1627 | C<br>727 | N<br>296 | O<br>527 | P<br>76 | S<br>1 | 0 | 0 |

- Molecule 55 is a protein called Peptide chain release factor 2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 55 | A | 357 | Total<br>2833 | C<br>1742 | N<br>498 | O<br>583 | S<br>10 | 0 | 0 |

- Molecule 56 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 56 | 1 | 2 | Total Mg<br>2 2 | 0 |
| 56 | 2 | 1 | Total Mg<br>1 1 | 0 |
| 56 | 3 | 8 | Total Mg<br>8 8 | 0 |
| 56 | i | 1 | Total Mg<br>1 1 | 0 |

- Molecule 57 is ZINC ION (CCD ID: ZN) (formula: Zn).

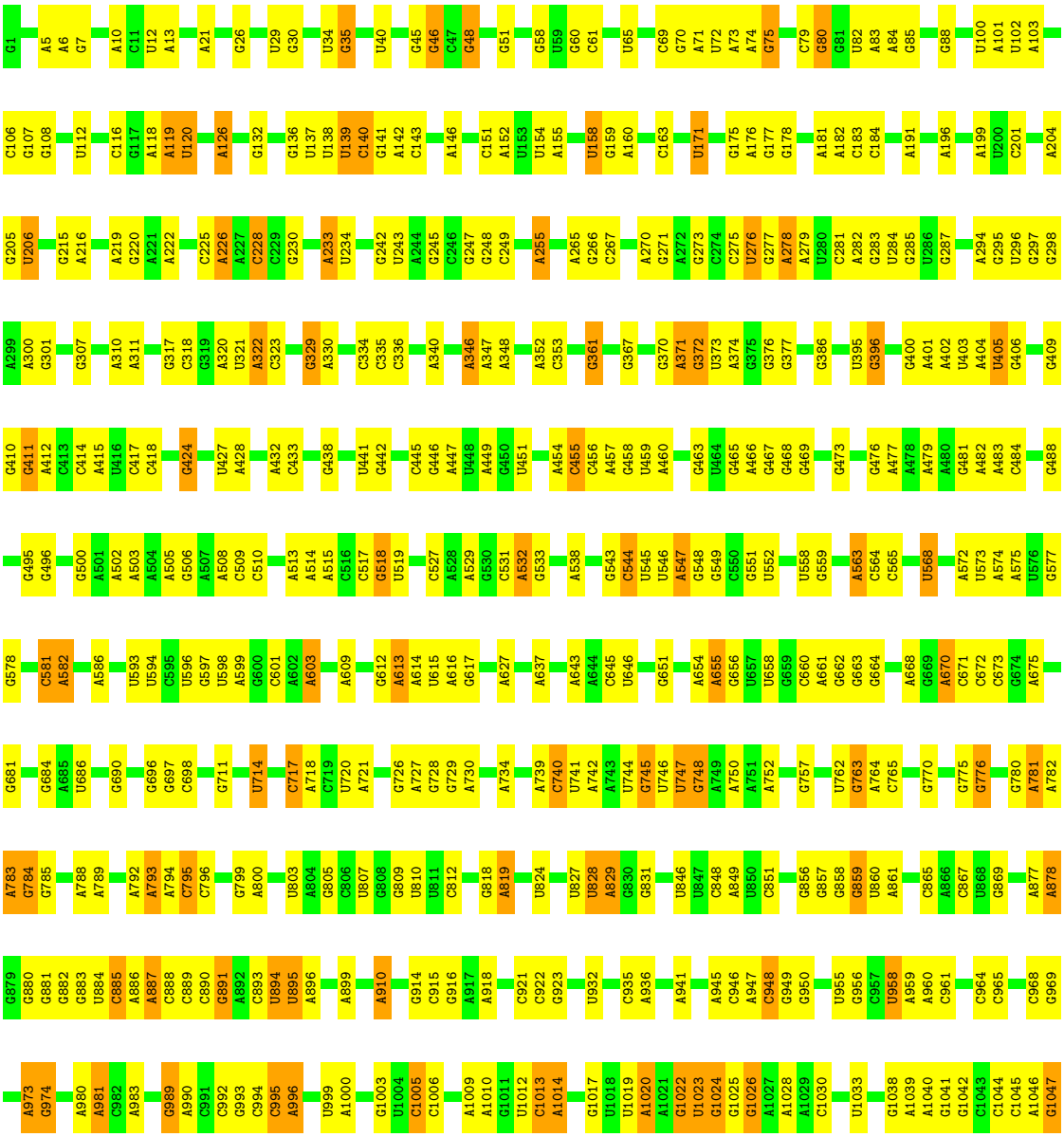
| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 57 | a | 1 | Total Zn<br>1 1 | 0 |
| 57 | f | 1 | Total Zn<br>1 1 | 0 |

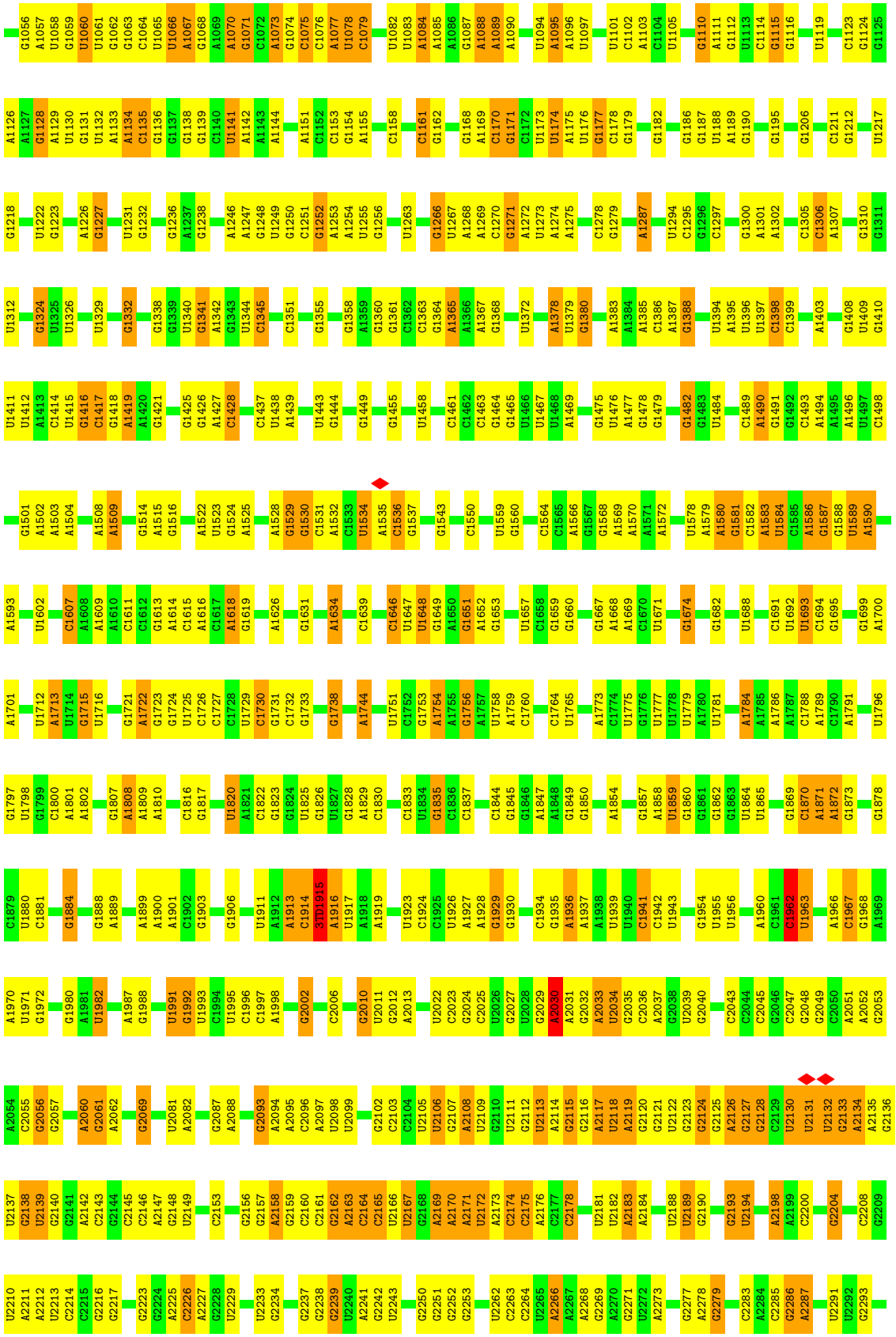
# 3 Residue-property plots (i)

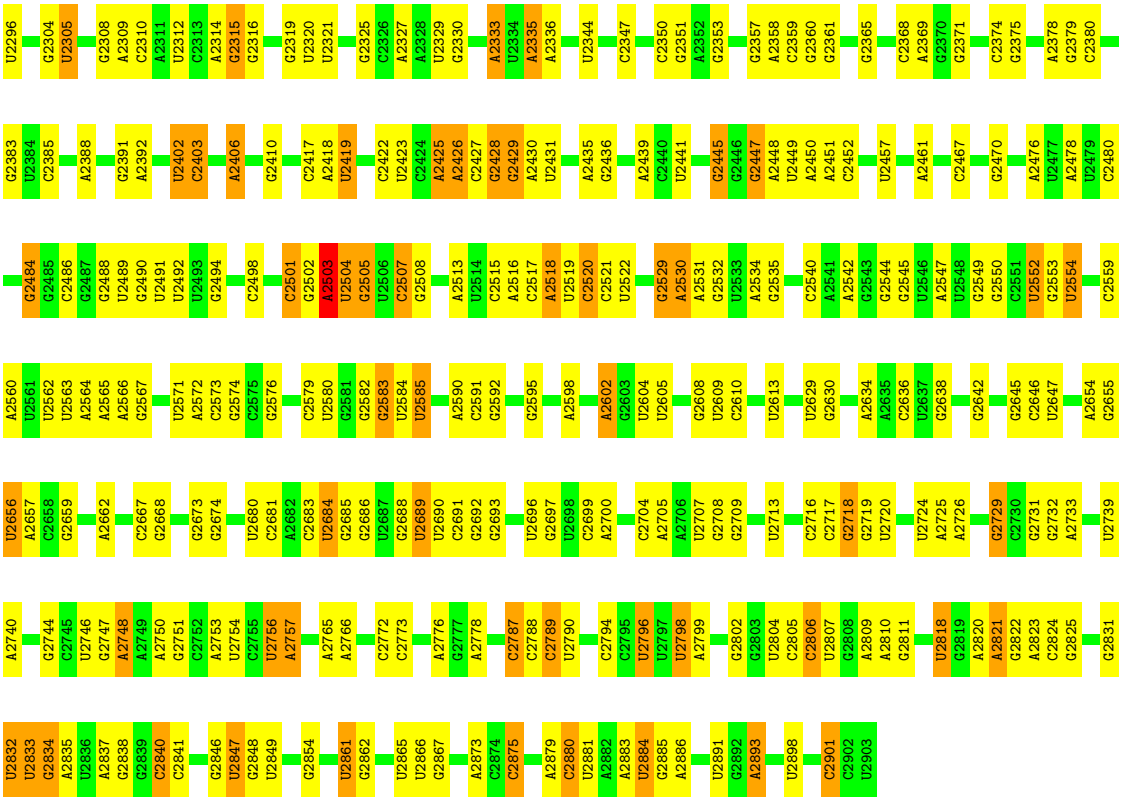
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: 23S ribosomal RNA

Chain 1:

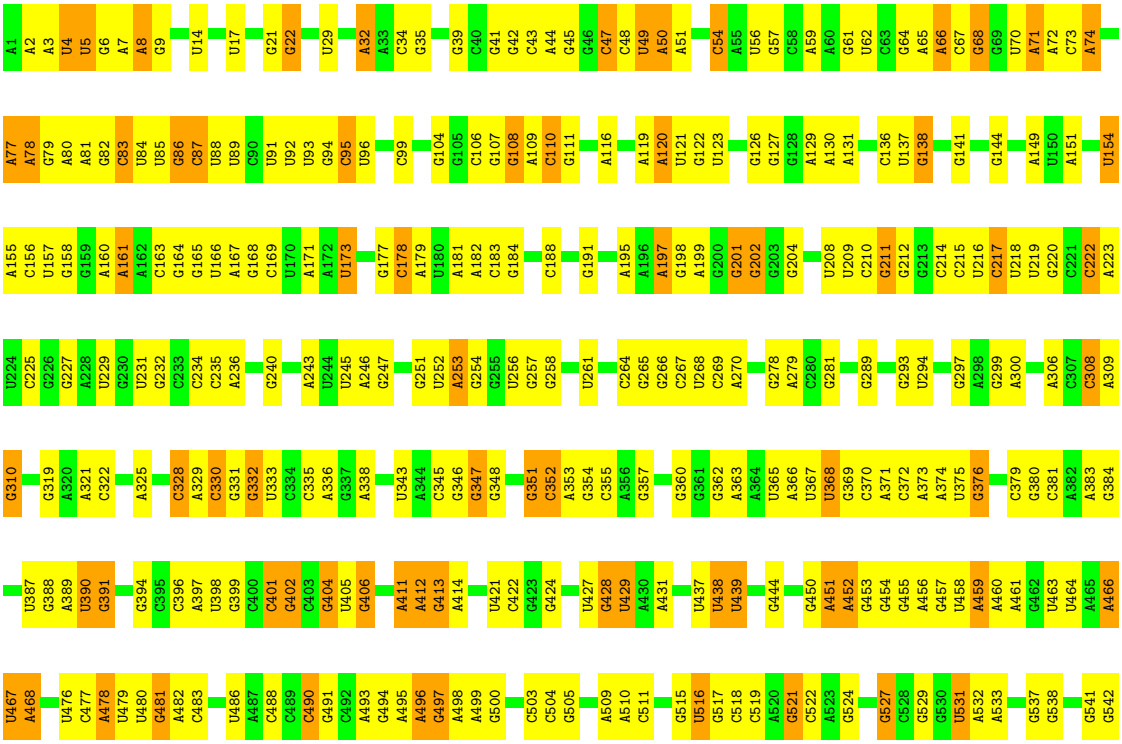


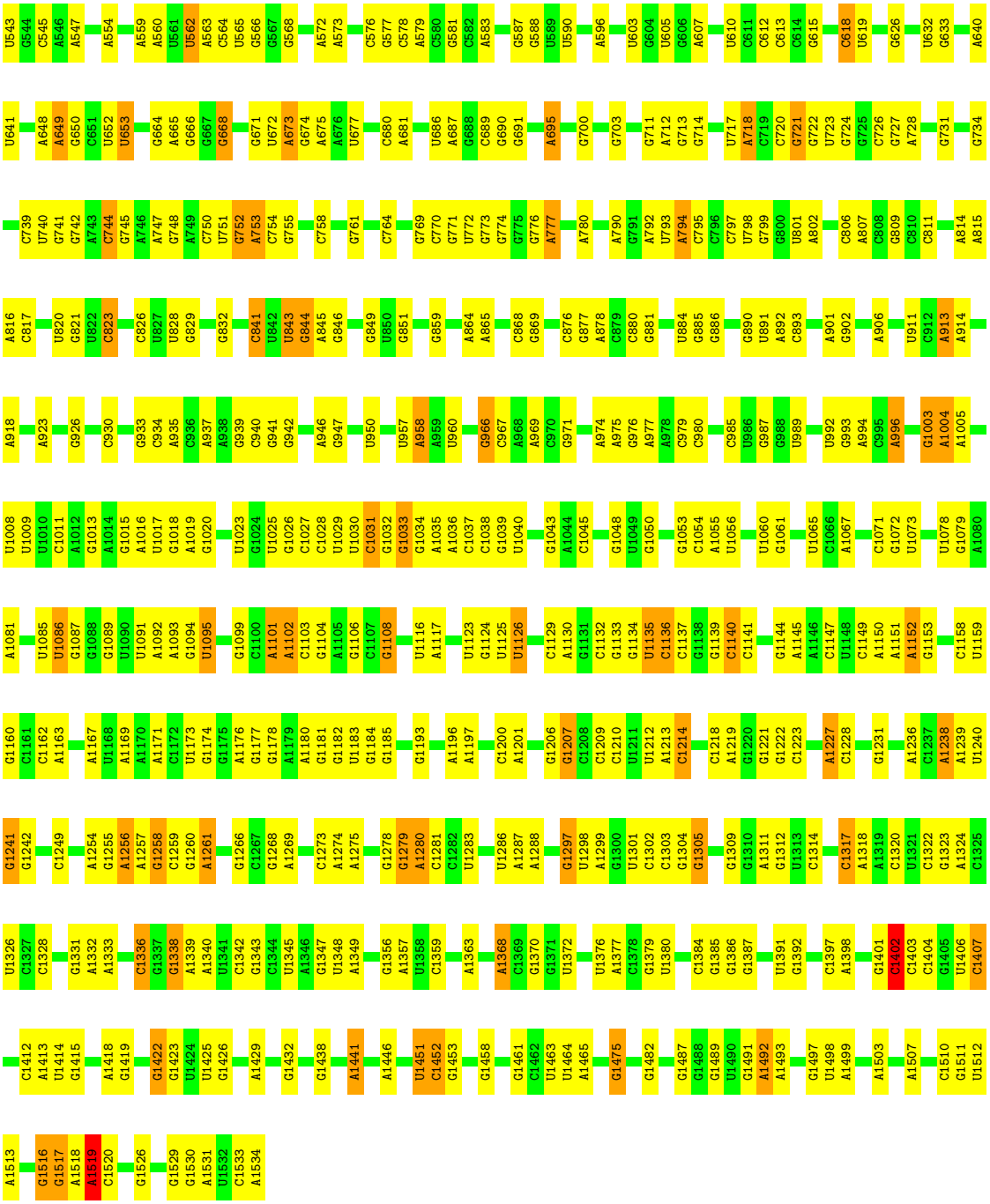




• Molecule 2: 16S ribosomal RNA

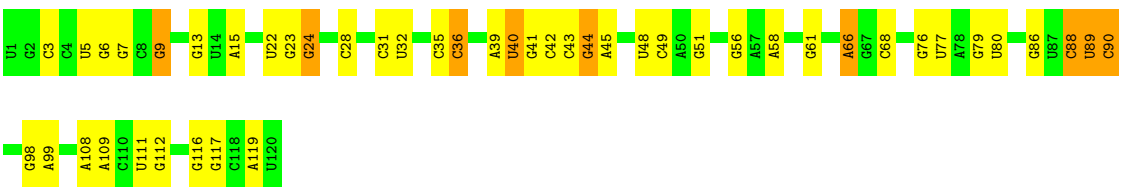
Chain 2:





• Molecule 3: 5S ribosomal RNA

Chain 3:

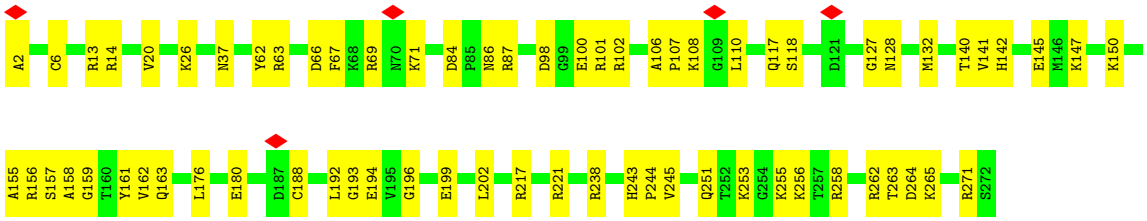


• Molecule 4: mRNA

Chain 4:

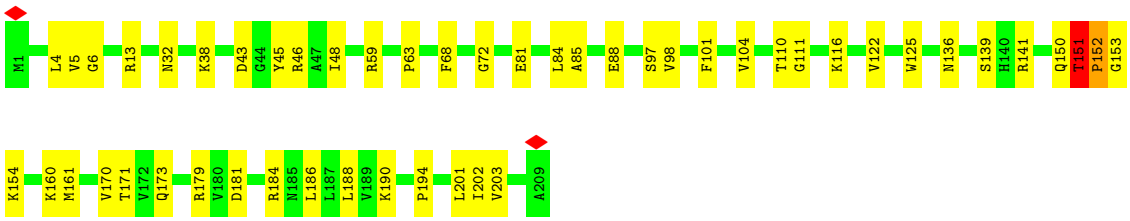
• Molecule 5: 50S ribosomal protein L2

Chain B:



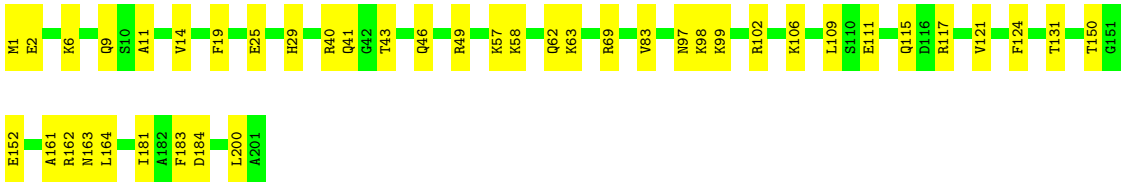

• Molecule 6: 50S ribosomal protein L3

Chain C:



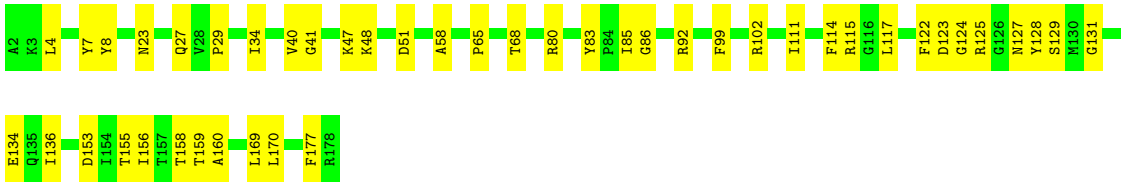

• Molecule 7: 50S ribosomal protein L4

Chain D:



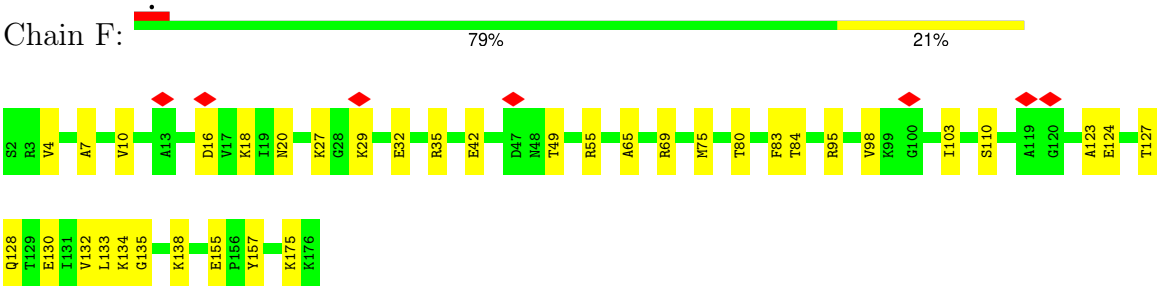

• Molecule 8: 50S ribosomal protein L5

Chain E:



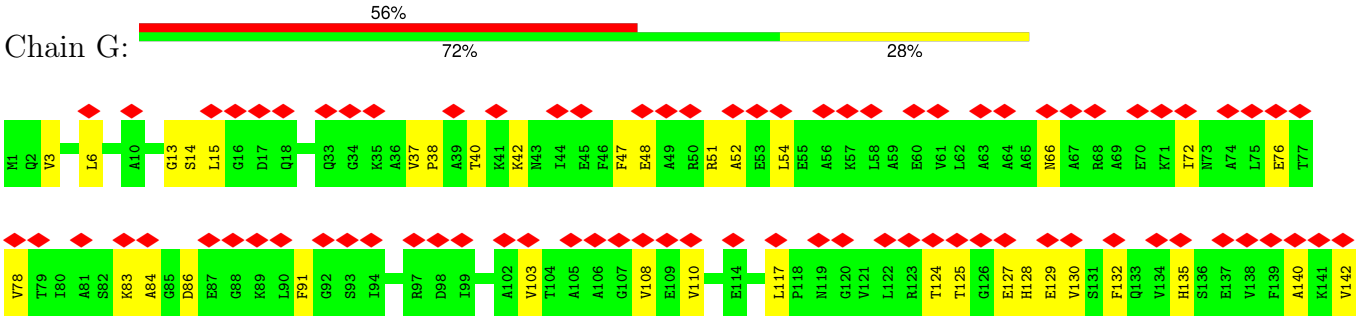

• Molecule 9: 50S ribosomal protein L6

Chain F:



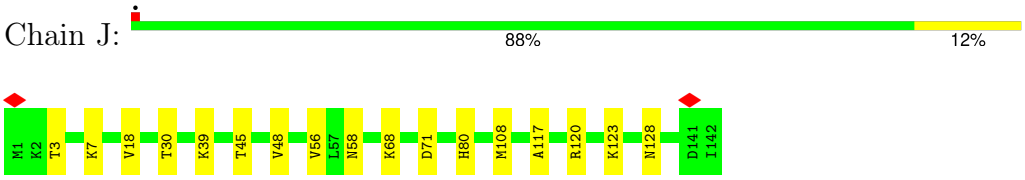

• Molecule 10: 50S ribosomal protein L9

Chain G:



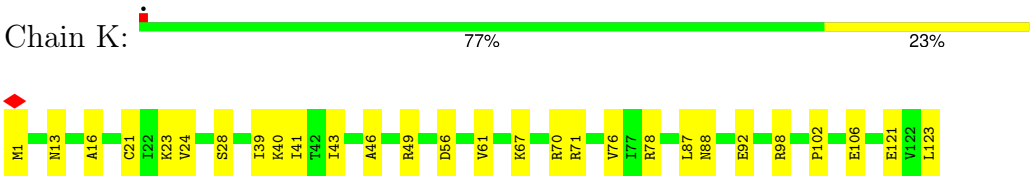

• Molecule 11: 50S ribosomal protein L13

Chain J:



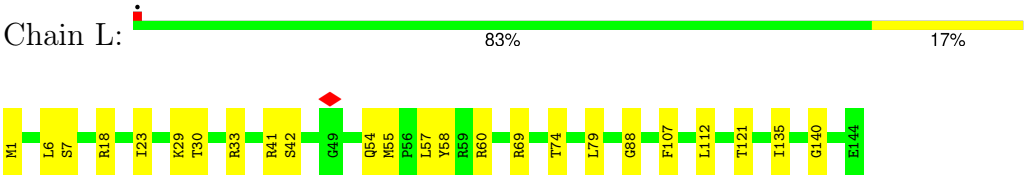

• Molecule 12: 50S ribosomal protein L14

Chain K:



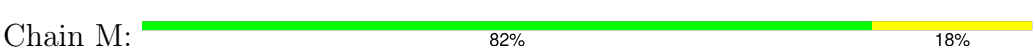

• Molecule 13: 50S ribosomal protein L15

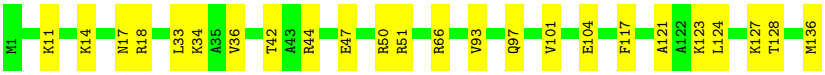
Chain L:




• Molecule 14: 50S ribosomal protein L16

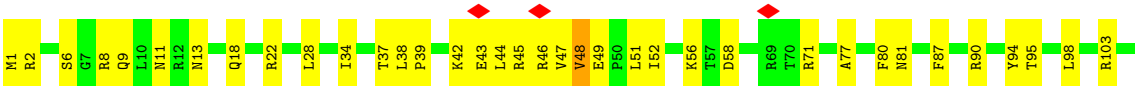
Chain M:





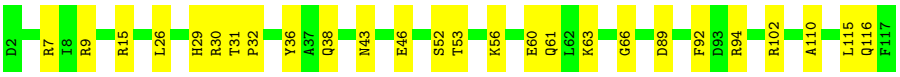

• Molecule 15: 50S ribosomal protein L17

Chain N:



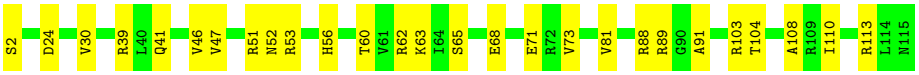
• Molecule 16: 50S ribosomal protein L18

Chain O:




• Molecule 17: 50S ribosomal protein L19

Chain P:

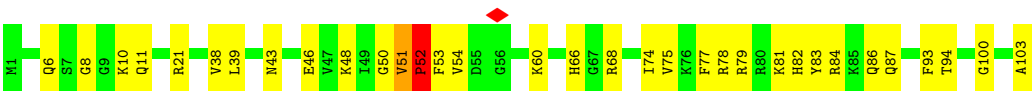



• Molecule 18: 50S ribosomal protein L20

Chain Q:

• Molecule 19: 50S ribosomal protein L21

Chain R:

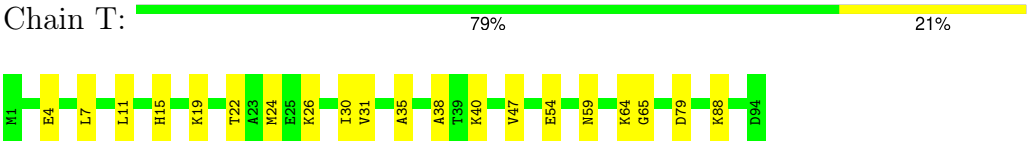



• Molecule 20: 50S ribosomal protein L22

Chain S:

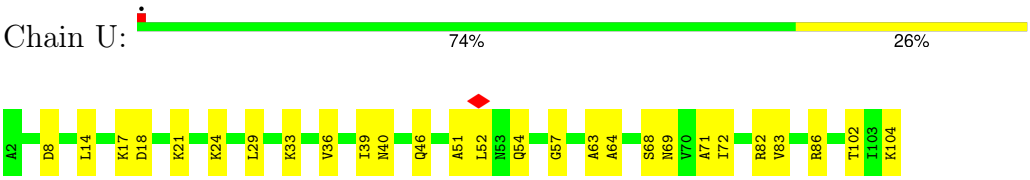
• Molecule 21: 50S ribosomal protein L23

Chain T:



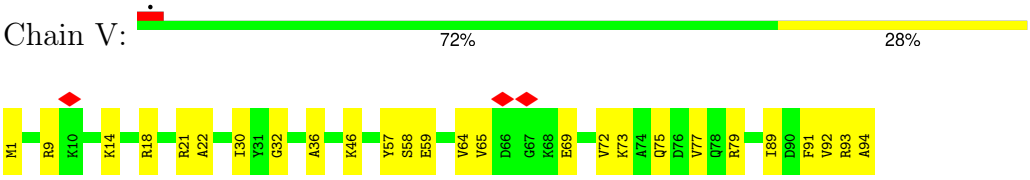

• Molecule 22: 50S ribosomal protein L24

Chain U:



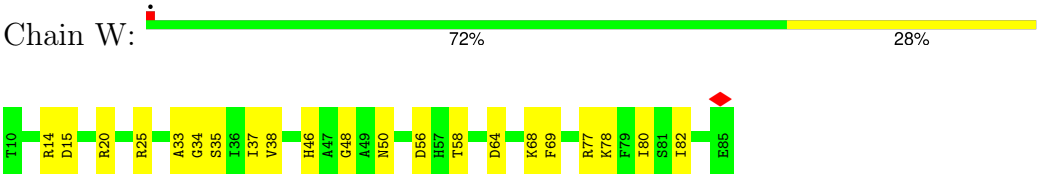

• Molecule 23: 50S ribosomal protein L25

Chain V:



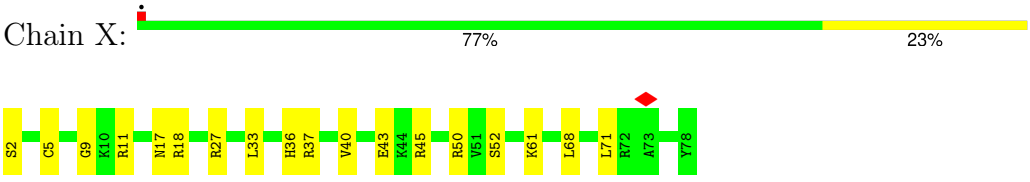

• Molecule 24: 50S ribosomal protein L27

Chain W:



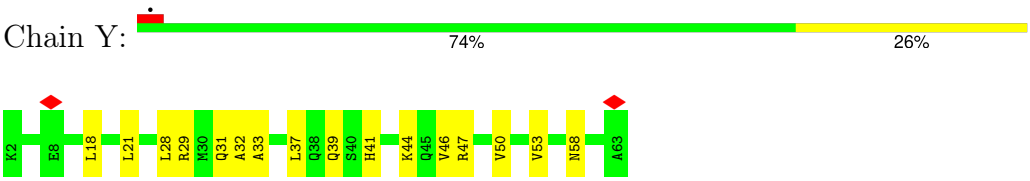

• Molecule 25: 50S ribosomal protein L28

Chain X:




• Molecule 26: 50S ribosomal protein L29

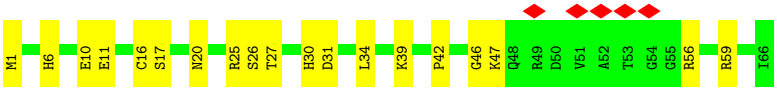
Chain Y:



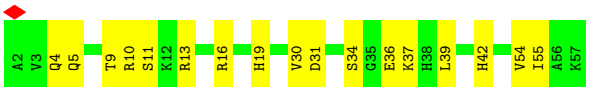

• Molecule 27: 50S ribosomal protein L30

Chain Z:

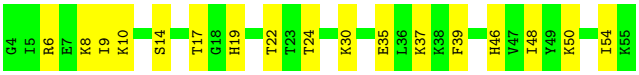
• Molecule 28: 50S ribosomal protein L31



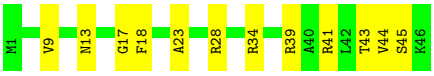

• Molecule 29: 50S ribosomal protein L32



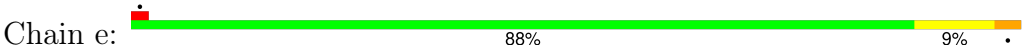

• Molecule 30: 50S ribosomal protein L33

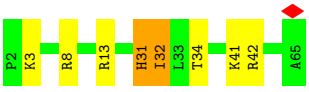



• Molecule 31: 50S ribosomal protein L34

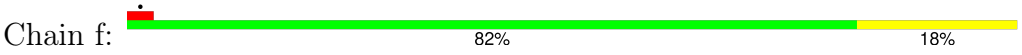


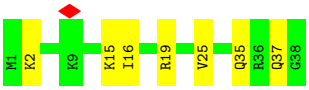

• Molecule 32: 50S ribosomal protein L35



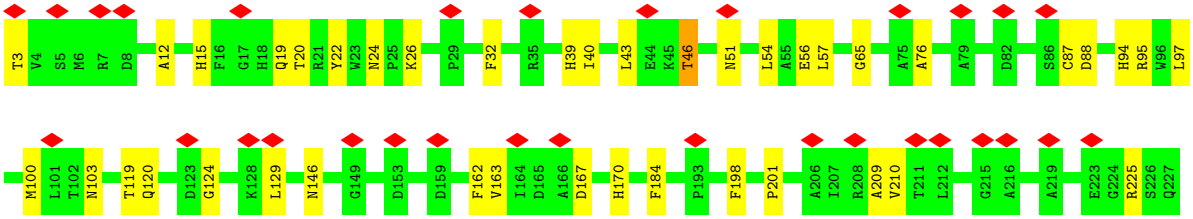

• Molecule 33: 50S ribosomal protein L36



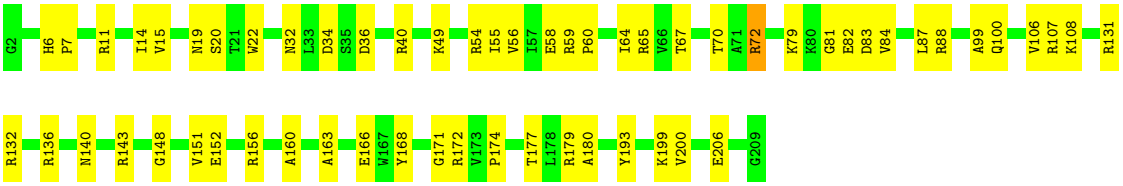

• Molecule 34: 30S ribosomal protein S2

Chain g:



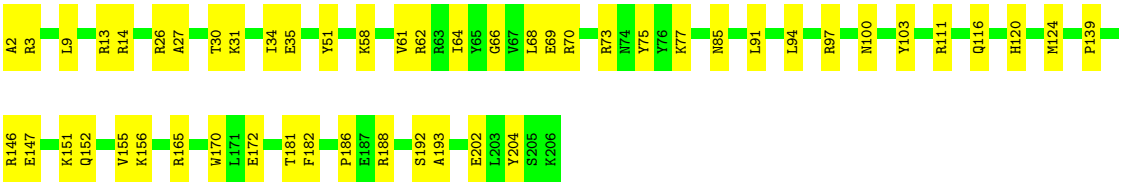

• Molecule 35: 30S ribosomal protein S3

Chain h:



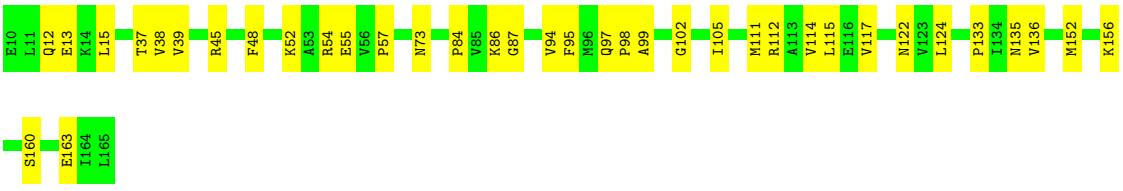

• Molecule 36: 30S ribosomal protein S4

Chain i:



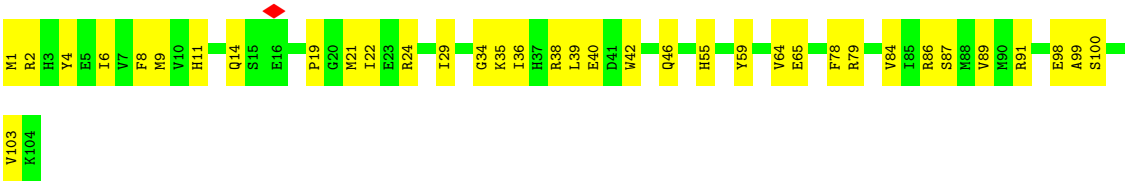

• Molecule 37: 30S ribosomal protein S5

Chain j:



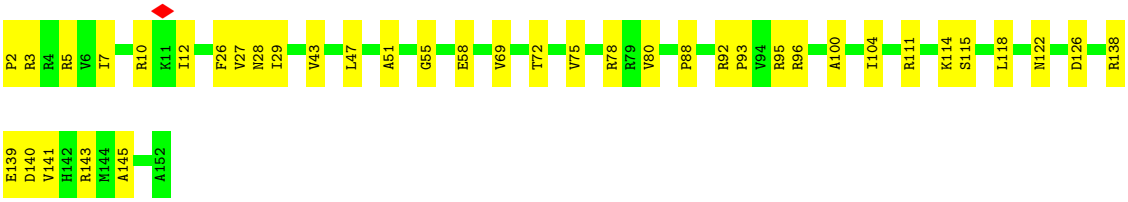

• Molecule 38: 30S ribosomal protein S6

Chain k:



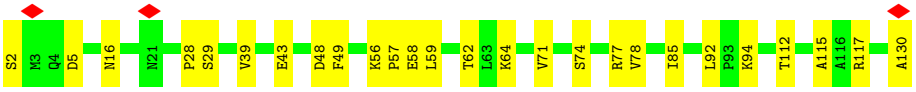
• Molecule 39: 30S ribosomal protein S7

Chain l:




• Molecule 40: 30S ribosomal protein S8

Chain m:

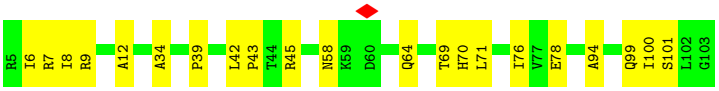



• Molecule 41: 30S ribosomal protein S9

Chain n:

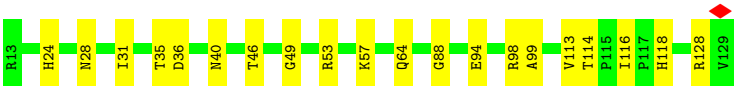
• Molecule 42: 30S ribosomal protein S10

Chain o:



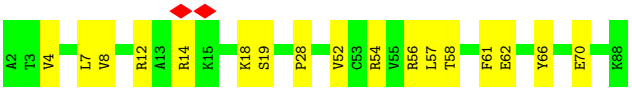

• Molecule 43: 30S ribosomal protein S11

Chain p:



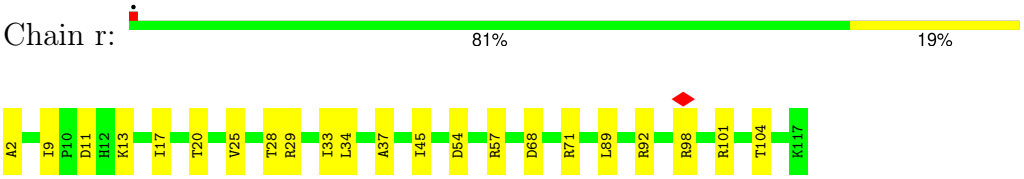

• Molecule 44: 30S ribosomal protein S12

Chain q:



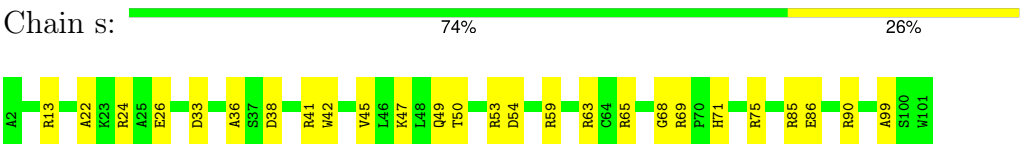

• Molecule 45: 30S ribosomal protein S13

Chain r:



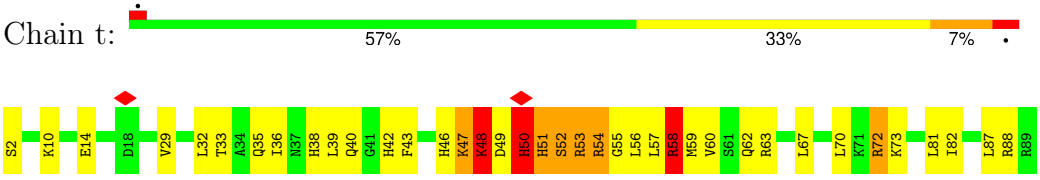

• Molecule 46: 30S ribosomal protein S14

Chain s:



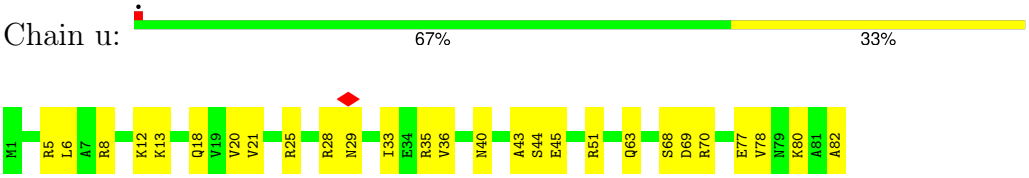

• Molecule 47: 30S ribosomal protein S15

Chain t:



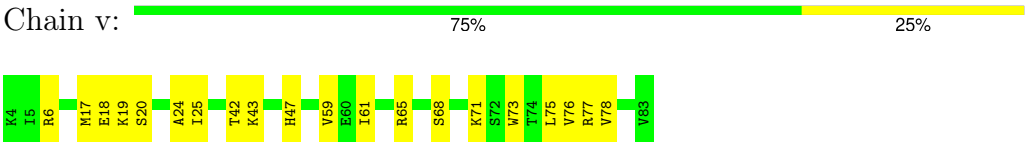

• Molecule 48: 30S ribosomal protein S16

Chain u:



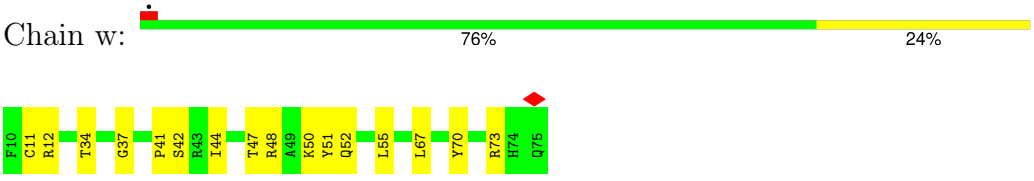

• Molecule 49: 30S ribosomal protein S17

Chain v:



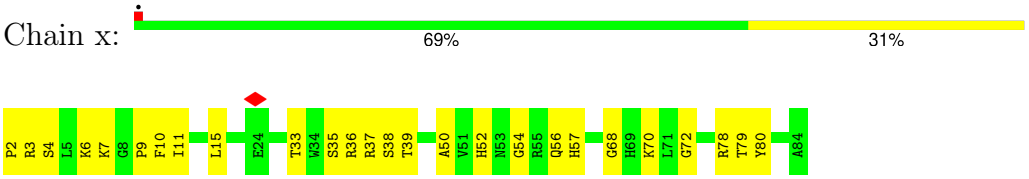

• Molecule 50: 30S ribosomal protein S18

Chain w:



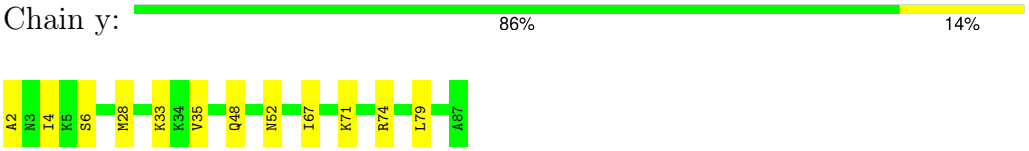

• Molecule 51: 30S ribosomal protein S19

Chain x:



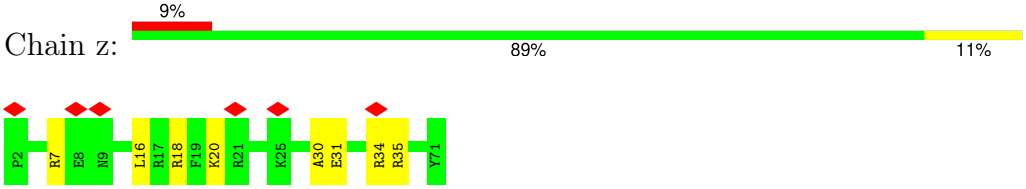
• Molecule 52: 30S ribosomal protein S20

Chain y:



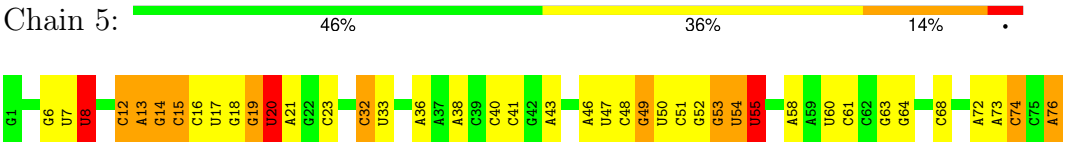

• Molecule 53: 30S ribosomal protein S21

Chain z:



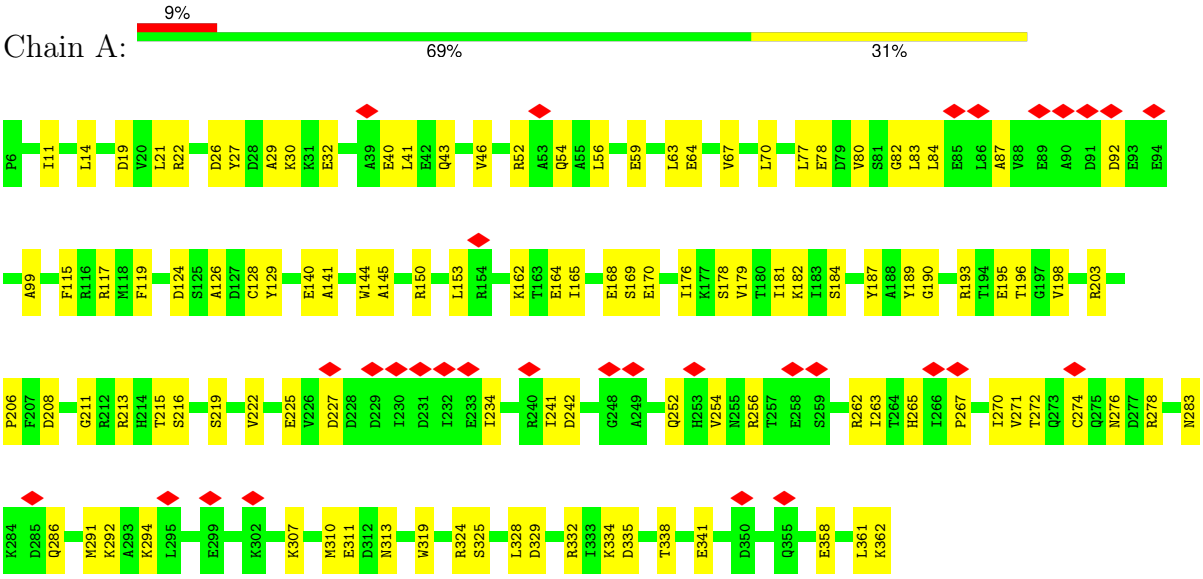

• Molecule 54: P-tRNA

Chain 5:




• Molecule 55: Peptide chain release factor 2

Chain A:



# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 94709 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope | FEI POLARA 300 | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/Å^2$) | 41.6 | Depositor |
| Minimum defocus (nm) | Not provided | |
| Maximum defocus (nm) | Not provided | |
| Magnification | Not provided | |
| Image detector | GATAN K2 SUMMIT (4k x 4k) | Depositor |
| Maximum map value | 0.089 | Depositor |
| Minimum map value | -0.029 | Depositor |
| Average map value | -0.000 | Depositor |
| Map value standard deviation | 0.004 | Depositor |
| Recommended contour level | 0.01 | Depositor |
| Map size (Å) | 526.4, 526.4, 526.4 | wwPDB |
| Map dimensions | 320, 320, 320 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 1.6450001, 1.6450001, 1.6450001 | Depositor |

# 5 Model quality (i)

## 5.1 Standard geometry (i)

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

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 | 1 | 0.37 | 0/69286 | 0.37 | 2/108087 (0.0%) |
| 2 | 2 | 0.35 | 0/36590 | 0.37 | 0/57074 |
| 3 | 3 | 0.33 | 0/2872 | 0.34 | 0/4478 |
| 4 | 4 | 0.29 | 0/203 | 0.36 | 0/312 |
| 5 | B | 0.36 | 0/2121 | 0.60 | 0/2852 |
| 6 | C | 0.38 | 0/1586 | 0.65 | 1/2134 (0.0%) |
| 7 | D | 0.34 | 0/1571 | 0.56 | 0/2113 |
| 8 | E | 0.33 | 0/1434 | 0.57 | 0/1926 |
| 9 | F | 0.31 | 0/1333 | 0.52 | 0/1805 |
| 10 | G | 0.28 | 0/1122 | 0.62 | 1/1515 (0.1%) |
| 11 | J | 0.35 | 0/1152 | 0.57 | 0/1551 |
| 12 | K | 0.34 | 0/955 | 0.61 | 0/1279 |
| 13 | L | 0.33 | 0/1062 | 0.59 | 0/1413 |
| 14 | M | 0.34 | 0/1093 | 0.57 | 0/1460 |
| 15 | N | 0.38 | 0/964 | 0.79 | 0/1289 |
| 16 | O | 0.30 | 0/902 | 0.56 | 0/1209 |
| 17 | P | 0.38 | 0/929 | 0.66 | 0/1242 |
| 18 | Q | 0.35 | 0/960 | 0.57 | 0/1278 |
| 19 | R | 0.43 | 1/829 (0.1%) | 0.65 | 1/1107 (0.1%) |
| 20 | S | 0.35 | 0/864 | 0.58 | 0/1156 |
| 21 | T | 0.33 | 0/752 | 0.57 | 0/1005 |
| 22 | U | 0.36 | 0/796 | 0.63 | 0/1062 |
| 23 | V | 0.32 | 0/766 | 0.51 | 0/1025 |
| 24 | W | 0.33 | 0/589 | 0.51 | 0/779 |
| 25 | X | 0.39 | 0/635 | 0.56 | 0/848 |
| 26 | Y | 0.32 | 0/502 | 0.57 | 0/667 |
| 27 | Z | 0.30 | 0/452 | 0.55 | 0/605 |
| 28 | a | 0.31 | 0/531 | 0.57 | 0/709 |
| 29 | b | 0.34 | 0/450 | 0.57 | 0/599 |
| 30 | c | 0.30 | 0/433 | 0.56 | 0/576 |
| 31 | d | 0.38 | 0/380 | 0.62 | 0/498 |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 32 | e | 0.41 | 0/513 | 0.67 | 1/676 (0.1%) |
| 33 | f | 0.30 | 0/303 | 0.60 | 0/397 |
| 34 | g | 0.32 | 0/1791 | 0.66 | 2/2413 (0.1%) |
| 35 | h | 0.33 | 0/1663 | 0.59 | 0/2241 |
| 36 | i | 0.30 | 0/1665 | 0.55 | 0/2227 |
| 37 | j | 0.35 | 0/1165 | 0.61 | 0/1568 |
| 38 | k | 0.33 | 0/867 | 0.63 | 0/1171 |
| 39 | l | 0.29 | 0/1195 | 0.56 | 0/1602 |
| 40 | m | 0.32 | 0/989 | 0.55 | 0/1326 |
| 41 | n | 0.30 | 0/1034 | 0.61 | 0/1375 |
| 42 | o | 0.29 | 0/800 | 0.59 | 0/1082 |
| 43 | p | 0.31 | 0/893 | 0.52 | 0/1205 |
| 44 | q | 0.33 | 0/682 | 0.57 | 0/918 |
| 45 | r | 0.31 | 0/909 | 0.63 | 0/1215 |
| 46 | s | 0.30 | 0/817 | 0.53 | 0/1088 |
| 47 | t | 0.48 | 0/722 | 0.84 | 1/964 (0.1%) |
| 48 | u | 0.33 | 0/659 | 0.66 | 0/884 |
| 49 | v | 0.32 | 0/657 | 0.64 | 0/881 |
| 50 | w | 0.30 | 0/553 | 0.54 | 0/743 |
| 51 | x | 0.30 | 0/680 | 0.55 | 0/915 |
| 52 | y | 0.34 | 0/675 | 0.54 | 0/895 |
| 53 | z | 0.29 | 0/597 | 0.56 | 0/792 |
| 54 | 5 | 0.33 | 0/1704 | 0.37 | 0/2654 |
| 55 | A | 0.32 | 0/2873 | 0.64 | 4/3870 (0.1%) |
| All | All | 0.35 | 1/158520 (0.0%) | 0.45 | 13/236755 (0.0%) |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 19 | R | 52 | PRO | N-CA | -6.14 | 1.39 | 1.47 |

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

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | 1 | 784 | G | C4'-C3'-O3' | 6.65 | 122.97 | 113.00 |
| 32 | e | 31 | HIS | O-C-N | 6.46 | 130.62 | 123.25 |
| 34 | g | 46 | THR | CA-C-N | 5.84 | 126.04 | 120.43 |
| 34 | g | 46 | THR | C-N-CA | 5.84 | 126.04 | 120.43 |
| 55 | A | 338 | THR | CA-C-N | 5.50 | 131.60 | 121.70 |

There are no chirality outliers.

There are no planarity outliers.

## 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 | 1 | 62336 | 0 | 31370 | 662 | 0 |
| 2 | 2 | 32929 | 0 | 16587 | 410 | 0 |
| 3 | 3 | 2569 | 0 | 1301 | 34 | 0 |
| 4 | 4 | 184 | 0 | 95 | 1 | 0 |
| 5 | B | 2082 | 0 | 2154 | 50 | 0 |
| 6 | C | 1565 | 0 | 1616 | 48 | 0 |
| 7 | D | 1552 | 0 | 1619 | 31 | 0 |
| 8 | E | 1410 | 0 | 1444 | 32 | 0 |
| 9 | F | 1313 | 0 | 1358 | 22 | 0 |
| 10 | G | 1111 | 0 | 1148 | 28 | 0 |
| 11 | J | 1129 | 0 | 1162 | 13 | 0 |
| 12 | K | 946 | 0 | 1023 | 20 | 0 |
| 13 | L | 1053 | 0 | 1129 | 20 | 0 |
| 14 | M | 1074 | 0 | 1157 | 16 | 0 |
| 15 | N | 951 | 0 | 994 | 34 | 0 |
| 16 | O | 892 | 0 | 923 | 20 | 0 |
| 17 | P | 917 | 0 | 962 | 24 | 0 |
| 18 | Q | 947 | 0 | 1019 | 22 | 0 |
| 19 | R | 816 | 0 | 839 | 36 | 0 |
| 20 | S | 857 | 0 | 922 | 19 | 0 |
| 21 | T | 746 | 0 | 811 | 13 | 0 |
| 22 | U | 788 | 0 | 844 | 20 | 0 |
| 23 | V | 753 | 0 | 780 | 17 | 0 |
| 24 | W | 582 | 0 | 599 | 13 | 0 |
| 25 | X | 625 | 0 | 652 | 17 | 0 |
| 26 | Y | 501 | 0 | 531 | 10 | 0 |
| 27 | Z | 448 | 0 | 488 | 11 | 0 |
| 28 | a | 522 | 0 | 520 | 14 | 0 |
| 29 | b | 444 | 0 | 458 | 14 | 0 |
| 30 | c | 426 | 0 | 464 | 13 | 0 |
| 31 | d | 377 | 0 | 418 | 8 | 0 |
| 32 | e | 504 | 0 | 572 | 11 | 0 |
| 33 | f | 302 | 0 | 340 | 6 | 0 |
| 34 | g | 1760 | 0 | 1787 | 24 | 0 |
| 35 | h | 1636 | 0 | 1710 | 35 | 0 |
| 36 | i | 1643 | 0 | 1707 | 38 | 0 |
| 37 | j | 1152 | 0 | 1196 | 28 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 38 | k | 848 | 0 | 846 | 25 | 0 |
| 39 | l | 1181 | 0 | 1238 | 27 | 0 |
| 40 | m | 979 | 0 | 1031 | 17 | 0 |
| 41 | n | 1022 | 0 | 1070 | 22 | 0 |
| 42 | o | 790 | 0 | 831 | 16 | 0 |
| 43 | p | 877 | 0 | 887 | 13 | 0 |
| 44 | q | 673 | 0 | 720 | 14 | 0 |
| 45 | r | 900 | 0 | 965 | 17 | 0 |
| 46 | s | 805 | 0 | 844 | 21 | 0 |
| 47 | t | 714 | 0 | 734 | 90 | 0 |
| 48 | u | 649 | 0 | 666 | 22 | 0 |
| 49 | v | 648 | 0 | 691 | 14 | 0 |
| 50 | w | 544 | 0 | 560 | 10 | 0 |
| 51 | x | 663 | 0 | 688 | 23 | 0 |
| 52 | y | 669 | 0 | 719 | 8 | 0 |
| 53 | z | 589 | 0 | 629 | 5 | 0 |
| 54 | 5 | 1627 | 0 | 832 | 25 | 0 |
| 55 | A | 2833 | 0 | 2729 | 79 | 0 |
| 56 | 1 | 2 | 0 | 0 | 0 | 0 |
| 56 | 2 | 1 | 0 | 0 | 0 | 0 |
| 56 | 3 | 8 | 0 | 0 | 0 | 0 |
| 56 | i | 1 | 0 | 0 | 0 | 0 |
| 57 | a | 1 | 0 | 0 | 0 | 0 |
| 57 | f | 1 | 0 | 0 | 0 | 0 |
| All | All | 146867 | 0 | 99379 | 1926 | 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 12.

The worst 5 of 1926 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) |
|---|---|---|---|
| 19:R:51:VAL:HG13 | 19:R:52:PRO:CD | 1.51 | 1.38 |
| 19:R:51:VAL:CG1 | 19:R:52:PRO:HD3 | 1.55 | 1.35 |
| 2:2:764:C:C5' | 47:t:53:ARG:HH11 | 1.40 | 1.35 |
| 2:2:764:C:H5' | 47:t:53:ARG:NH1 | 1.51 | 1.23 |
| 6:C:151:THR:OG1 | 6:C:152:PRO:HD3 | 1.34 | 1.22 |

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 | |
|---|---|---|---|---|---|---|---|
| 5 | B | 269/271 (99%) | 254 (94%) | 15 (6%) | 0 | 100 | 100 |
| 6 | C | 207/209 (99%) | 198 (96%) | 7 (3%) | 2 (1%) | 12 | 43 |
| 7 | D | 199/201 (99%) | 191 (96%) | 8 (4%) | 0 | 100 | 100 |
| 8 | E | 175/177 (99%) | 160 (91%) | 14 (8%) | 1 (1%) | 21 | 52 |
| 9 | F | 173/175 (99%) | 164 (95%) | 9 (5%) | 0 | 100 | 100 |
| 10 | G | 147/149 (99%) | 135 (92%) | 12 (8%) | 0 | 100 | 100 |
| 11 | J | 140/142 (99%) | 134 (96%) | 6 (4%) | 0 | 100 | 100 |
| 12 | K | 121/123 (98%) | 117 (97%) | 4 (3%) | 0 | 100 | 100 |
| 13 | L | 142/144 (99%) | 139 (98%) | 3 (2%) | 0 | 100 | 100 |
| 14 | M | 134/136 (98%) | 129 (96%) | 5 (4%) | 0 | 100 | 100 |
| 15 | N | 117/119 (98%) | 106 (91%) | 11 (9%) | 0 | 100 | 100 |
| 16 | O | 114/116 (98%) | 110 (96%) | 4 (4%) | 0 | 100 | 100 |
| 17 | P | 112/114 (98%) | 107 (96%) | 5 (4%) | 0 | 100 | 100 |
| 18 | Q | 115/117 (98%) | 114 (99%) | 1 (1%) | 0 | 100 | 100 |
| 19 | R | 101/103 (98%) | 90 (89%) | 10 (10%) | 1 (1%) | 12 | 43 |
| 20 | S | 108/110 (98%) | 105 (97%) | 3 (3%) | 0 | 100 | 100 |
| 21 | T | 92/94 (98%) | 87 (95%) | 5 (5%) | 0 | 100 | 100 |
| 22 | U | 101/103 (98%) | 92 (91%) | 9 (9%) | 0 | 100 | 100 |
| 23 | V | 92/94 (98%) | 88 (96%) | 4 (4%) | 0 | 100 | 100 |
| 24 | W | 74/76 (97%) | 68 (92%) | 6 (8%) | 0 | 100 | 100 |
| 25 | X | 75/77 (97%) | 74 (99%) | 1 (1%) | 0 | 100 | 100 |
| 26 | Y | 60/62 (97%) | 59 (98%) | 1 (2%) | 0 | 100 | 100 |
| 27 | Z | 56/58 (97%) | 53 (95%) | 3 (5%) | 0 | 100 | 100 |
| 28 | a | 64/66 (97%) | 56 (88%) | 8 (12%) | 0 | 100 | 100 |
| 29 | b | 54/56 (96%) | 51 (94%) | 3 (6%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 30 | c | 50/52 (96%) | 49 (98%) | 1 (2%) | 0 | 100 | 100 |
| 31 | d | 44/46 (96%) | 44 (100%) | 0 | 0 | 100 | 100 |
| 32 | e | 62/64 (97%) | 57 (92%) | 4 (6%) | 1 (2%) | 7 | 35 |
| 33 | f | 36/38 (95%) | 36 (100%) | 0 | 0 | 100 | 100 |
| 34 | g | 223/225 (99%) | 214 (96%) | 9 (4%) | 0 | 100 | 100 |
| 35 | h | 206/208 (99%) | 189 (92%) | 17 (8%) | 0 | 100 | 100 |
| 36 | i | 203/205 (99%) | 197 (97%) | 6 (3%) | 0 | 100 | 100 |
| 37 | j | 154/156 (99%) | 142 (92%) | 12 (8%) | 0 | 100 | 100 |
| 38 | k | 102/104 (98%) | 99 (97%) | 3 (3%) | 0 | 100 | 100 |
| 39 | l | 149/151 (99%) | 147 (99%) | 2 (1%) | 0 | 100 | 100 |
| 40 | m | 127/129 (98%) | 124 (98%) | 3 (2%) | 0 | 100 | 100 |
| 41 | n | 125/127 (98%) | 114 (91%) | 11 (9%) | 0 | 100 | 100 |
| 42 | o | 97/99 (98%) | 90 (93%) | 7 (7%) | 0 | 100 | 100 |
| 43 | p | 115/117 (98%) | 108 (94%) | 7 (6%) | 0 | 100 | 100 |
| 44 | q | 85/87 (98%) | 80 (94%) | 5 (6%) | 0 | 100 | 100 |
| 45 | r | 114/116 (98%) | 110 (96%) | 4 (4%) | 0 | 100 | 100 |
| 46 | s | 98/100 (98%) | 97 (99%) | 1 (1%) | 0 | 100 | 100 |
| 47 | t | 86/88 (98%) | 73 (85%) | 11 (13%) | 2 (2%) | 5 | 30 |
| 48 | u | 80/82 (98%) | 74 (92%) | 6 (8%) | 0 | 100 | 100 |
| 49 | v | 78/80 (98%) | 73 (94%) | 5 (6%) | 0 | 100 | 100 |
| 50 | w | 64/66 (97%) | 63 (98%) | 1 (2%) | 0 | 100 | 100 |
| 51 | x | 81/83 (98%) | 77 (95%) | 4 (5%) | 0 | 100 | 100 |
| 52 | y | 84/86 (98%) | 84 (100%) | 0 | 0 | 100 | 100 |
| 53 | z | 68/70 (97%) | 66 (97%) | 2 (3%) | 0 | 100 | 100 |
| 55 | A | 355/357 (99%) | 331 (93%) | 24 (7%) | 0 | 100 | 100 |
| All | All | 5928/6028 (98%) | 5619 (95%) | 302 (5%) | 7 (0%) | 49 | 78 |

5 of 7 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 6 | C | 151 | THR |
| 47 | t | 48 | LYS |
| 19 | R | 52 | PRO |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 47 | t | 50 | HIS |
| 32 | e | 32 | ILE |

### 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 | |
|---|---|---|---|---|---|---|
| 5 | B | 216/216 (100%) | 216 (100%) | 0 | 100 | 100 |
| 6 | C | 164/164 (100%) | 163 (99%) | 1 (1%) | 78 | 79 |
| 7 | D | 165/165 (100%) | 165 (100%) | 0 | 100 | 100 |
| 8 | E | 148/148 (100%) | 147 (99%) | 1 (1%) | 76 | 77 |
| 9 | F | 136/136 (100%) | 136 (100%) | 0 | 100 | 100 |
| 10 | G | 114/114 (100%) | 114 (100%) | 0 | 100 | 100 |
| 11 | J | 116/116 (100%) | 116 (100%) | 0 | 100 | 100 |
| 12 | K | 104/104 (100%) | 104 (100%) | 0 | 100 | 100 |
| 13 | L | 103/103 (100%) | 103 (100%) | 0 | 100 | 100 |
| 14 | M | 109/109 (100%) | 109 (100%) | 0 | 100 | 100 |
| 15 | N | 99/99 (100%) | 97 (98%) | 2 (2%) | 48 | 64 |
| 16 | O | 86/86 (100%) | 86 (100%) | 0 | 100 | 100 |
| 17 | P | 99/99 (100%) | 99 (100%) | 0 | 100 | 100 |
| 18 | Q | 89/89 (100%) | 89 (100%) | 0 | 100 | 100 |
| 19 | R | 84/84 (100%) | 83 (99%) | 1 (1%) | 63 | 72 |
| 20 | S | 93/93 (100%) | 93 (100%) | 0 | 100 | 100 |
| 21 | T | 81/81 (100%) | 81 (100%) | 0 | 100 | 100 |
| 22 | U | 84/84 (100%) | 84 (100%) | 0 | 100 | 100 |
| 23 | V | 78/78 (100%) | 77 (99%) | 1 (1%) | 61 | 71 |
| 24 | W | 58/58 (100%) | 58 (100%) | 0 | 100 | 100 |
| 25 | X | 67/67 (100%) | 67 (100%) | 0 | 100 | 100 |
| 26 | Y | 54/54 (100%) | 54 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 27 | Z | 48/48 (100%) | 48 (100%) | 0 | 100 | 100 |
| 28 | a | 59/59 (100%) | 59 (100%) | 0 | 100 | 100 |
| 29 | b | 47/47 (100%) | 47 (100%) | 0 | 100 | 100 |
| 30 | c | 47/47 (100%) | 47 (100%) | 0 | 100 | 100 |
| 31 | d | 38/38 (100%) | 38 (100%) | 0 | 100 | 100 |
| 32 | e | 51/51 (100%) | 51 (100%) | 0 | 100 | 100 |
| 33 | f | 34/34 (100%) | 34 (100%) | 0 | 100 | 100 |
| 34 | g | 187/187 (100%) | 186 (100%) | 1 (0%) | 81 | 80 |
| 35 | h | 171/171 (100%) | 169 (99%) | 2 (1%) | 63 | 72 |
| 36 | i | 172/172 (100%) | 172 (100%) | 0 | 100 | 100 |
| 37 | j | 119/119 (100%) | 119 (100%) | 0 | 100 | 100 |
| 38 | k | 91/91 (100%) | 91 (100%) | 0 | 100 | 100 |
| 39 | l | 124/124 (100%) | 124 (100%) | 0 | 100 | 100 |
| 40 | m | 104/104 (100%) | 104 (100%) | 0 | 100 | 100 |
| 41 | n | 105/105 (100%) | 105 (100%) | 0 | 100 | 100 |
| 42 | o | 86/86 (100%) | 86 (100%) | 0 | 100 | 100 |
| 43 | p | 90/90 (100%) | 90 (100%) | 0 | 100 | 100 |
| 44 | q | 74/74 (100%) | 74 (100%) | 0 | 100 | 100 |
| 45 | r | 94/94 (100%) | 94 (100%) | 0 | 100 | 100 |
| 46 | s | 83/83 (100%) | 83 (100%) | 0 | 100 | 100 |
| 47 | t | 76/76 (100%) | 67 (88%) | 9 (12%) | 5 | 23 |
| 48 | u | 65/65 (100%) | 65 (100%) | 0 | 100 | 100 |
| 49 | v | 74/74 (100%) | 74 (100%) | 0 | 100 | 100 |
| 50 | w | 57/57 (100%) | 57 (100%) | 0 | 100 | 100 |
| 51 | x | 72/72 (100%) | 72 (100%) | 0 | 100 | 100 |
| 52 | y | 65/65 (100%) | 65 (100%) | 0 | 100 | 100 |
| 53 | z | 60/60 (100%) | 60 (100%) | 0 | 100 | 100 |
| 55 | A | 304/305 (100%) | 304 (100%) | 0 | 100 | 100 |
| All | All | 4944/4945 (100%) | 4926 (100%) | 18 (0%) | 81 | 81 |

5 of 18 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 47 | t | 53 | ARG |
| 47 | t | 72 | ARG |
| 47 | t | 58 | ARG |
| 35 | h | 179 | ARG |
| 47 | t | 52 | SER |

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

| Mol | Chain | Res | Type |
|---|---|---|---|
| 38 | k | 46 | GLN |
| 50 | w | 52 | GLN |
| 38 | k | 68 | GLN |
| 44 | q | 5 | ASN |
| 55 | A | 255 | ASN |

### 5.3.3 RNA (i)

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|---|---|---|---|---|
| 1 | 1 | 2902/2903 (99%) | 758 (26%) | 15 (0%) |
| 2 | 2 | 1531/1534 (99%) | 415 (27%) | 4 (0%) |
| 3 | 3 | 119/120 (99%) | 23 (19%) | 0 |
| 4 | 4 | 8/9 (88%) | 2 (25%) | 0 |
| 54 | 5 | 75/76 (98%) | 22 (29%) | 1 (1%) |
| All | All | 4635/4642 (99%) | 1220 (26%) | 20 (0%) |

5 of 1220 RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 1 | 10 | A |
| 1 | 1 | 34 | U |
| 1 | 1 | 35 | G |
| 1 | 1 | 40 | U |
| 1 | 1 | 46 | G |

5 of 20 RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 1 | 2756 | U |
| 2 | 2 | 496 | A |
| 54 | 5 | 15 | C |
| 2 | 2 | 516 | PSU |

*Continued on next page...*

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 1 | 1252 | G |

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

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

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 2 | 4OC | 2 | 1402 | 2 | 20,23,24 | 3.00 | 8 (40%) | 25,32,35 | 1.26 | 4 (16%) |
| 1 | PSU | 1 | 2504 | 1 | 18,21,22 | 1.21 | 2 (11%) | 21,30,33 | 1.93 | 4 (19%) |
| 2 | 5MC | 2 | 1407 | 2 | 19,22,23 | 3.81 | 8 (42%) | 26,32,35 | 1.12 | 2 (7%) |
| 1 | 6MZ | 1 | 2030 | 1 | 22,25,26 | 2.90 | 6 (27%) | 29,36,39 | 4.48 | 13 (44%) |
| 1 | 5MU | 1 | 1939 | 1 | 19,22,23 | 4.77 | 7 (36%) | 27,32,35 | 3.83 | 10 (37%) |
| 1 | 5MC | 1 | 1962 | 1 | 19,22,23 | 3.79 | 8 (42%) | 26,32,35 | 1.02 | 2 (7%) |
| 1 | PSU | 1 | 955 | 1 | 18,21,22 | 1.04 | 1 (5%) | 21,30,33 | 1.80 | 3 (14%) |
| 1 | 6MZ | 1 | 1618 | 1 | 22,25,26 | 2.85 | 6 (27%) | 29,36,39 | 4.44 | 14 (48%) |
| 1 | OMC | 1 | 2498 | 1 | 19,22,23 | 2.90 | 7 (36%) | 25,31,34 | 0.91 | 1 (4%) |
| 1 | 2MG | 1 | 2445 | 1 | 23,26,27 | 2.94 | 6 (26%) | 33,38,41 | 2.27 | 7 (21%) |
| 2 | MA6 | 2 | 1519 | 2 | 23,26,27 | 1.53 | 4 (17%) | 33,38,41 | 2.76 | 13 (39%) |
| 1 | 2MG | 1 | 1835 | 1 | 23,26,27 | 2.89 | 7 (30%) | 33,38,41 | 2.20 | 10 (30%) |
| 1 | OMG | 1 | 2251 | 54,1 | 23,26,27 | 2.40 | 8 (34%) | 32,38,41 | 1.96 | 8 (25%) |
| 2 | MA6 | 2 | 1518 | 2 | 23,26,27 | 1.56 | 5 (21%) | 33,38,41 | 2.71 | 12 (36%) |
| 1 | 3TD | 1 | 1915 | 1 | 19,22,23 | 4.26 | 5 (26%) | 23,32,35 | 2.01 | 4 (17%) |
| 2 | PSU | 2 | 516 | 2 | 18,21,22 | 1.02 | 1 (5%) | 21,30,33 | 1.94 | 5 (23%) |
| 1 | 2MA | 1 | 2503 | 1 | 22,25,26 | 3.71 | 8 (36%) | 32,37,40 | 2.44 | 7 (21%) |
| 2 | 5MC | 2 | 967 | 2 | 19,22,23 | 3.84 | 8 (42%) | 26,32,35 | 0.99 | 1 (3%) |
| 1 | PSU | 1 | 2580 | 1 | 18,21,22 | 1.10 | 2 (11%) | 21,30,33 | 2.08 | 6 (28%) |
| 1 | G7M | 1 | 2069 | 1 | 23,26,27 | 2.58 | 8 (34%) | 34,39,42 | 2.51 | 11 (32%) |
| 54 | PSU | 5 | 55 | 54 | 18,21,22 | 1.11 | 1 (5%) | 21,30,33 | 1.88 | 4 (19%) |
| 2 | 2MG | 2 | 966 | 2 | 23,26,27 | 3.00 | 7 (30%) | 33,38,41 | 2.30 | 7 (21%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 1 | PSU | 1 | 746 | 1 | 18,21,22 | 1.09 | 2 (11%) | 21,30,33 | 1.80 | 3 (14%) |
| 54 | H2U | 5 | 20 | 54 | 18,21,22 | 3.37 | 5 (27%) | 19,30,33 | 1.54 | 4 (21%) |
| 2 | G7M | 2 | 527 | 2 | 23,26,27 | 3.59 | 12 (52%) | 34,39,42 | 1.58 | 7 (20%) |
| 54 | 5MU | 5 | 54 | 54 | 19,22,23 | 4.81 | 7 (36%) | 27,32,35 | 3.53 | 8 (29%) |
| 1 | PSU | 1 | 2457 | 1 | 18,21,22 | 1.17 | 3 (16%) | 21,30,33 | 2.03 | 6 (28%) |
| 54 | 4SU | 5 | 8 | 54 | 18,21,22 | 3.70 | 7 (38%) | 25,30,33 | 2.22 | 5 (20%) |
| 1 | PSU | 1 | 2605 | 1 | 18,21,22 | 1.13 | 2 (11%) | 21,30,33 | 2.08 | 5 (23%) |
| 2 | 2MG | 2 | 1516 | 2 | 23,26,27 | 2.95 | 8 (34%) | 33,38,41 | 2.14 | 10 (30%) |
| 1 | PSU | 1 | 1911 | 1 | 18,21,22 | 1.13 | 2 (11%) | 21,30,33 | 2.16 | 5 (23%) |
| 2 | UR3 | 2 | 1498 | 2 | 19,22,23 | 2.53 | 7 (36%) | 26,32,35 | 1.56 | 3 (11%) |
| 2 | 2MG | 2 | 1207 | 2 | 23,26,27 | 2.89 | 7 (30%) | 33,38,41 | 2.33 | 9 (27%) |
| 1 | PSU | 1 | 1917 | 1 | 18,21,22 | 1.11 | 1 (5%) | 21,30,33 | 1.88 | 4 (19%) |
| 1 | 1MG | 1 | 745 | 1 | 23,26,27 | 2.83 | 7 (30%) | 33,39,42 | 2.07 | 9 (27%) |
| 54 | 4OC | 5 | 32 | 54 | 20,23,24 | 3.00 | 8 (40%) | 25,32,35 | 1.02 | 2 (8%) |
| 1 | OMU | 1 | 2552 | 1 | 19,22,23 | 2.88 | 8 (42%) | 25,31,34 | 1.92 | 5 (20%) |
| 1 | 5MU | 1 | 747 | 1 | 19,22,23 | 4.81 | 7 (36%) | 27,32,35 | 3.93 | 9 (33%) |

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 |
|---|---|---|---|---|---|---|---|
| 2 | 4OC | 2 | 1402 | 2 | - | 2/9/29/30 | 0/2/2/2 |
| 1 | PSU | 1 | 2504 | 1 | - | 2/7/25/26 | 0/2/2/2 |
| 2 | 5MC | 2 | 1407 | 2 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | 6MZ | 1 | 2030 | 1 | - | 3/9/27/28 | 0/3/3/3 |
| 1 | 5MU | 1 | 1939 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | 5MC | 1 | 1962 | 1 | - | 2/7/25/26 | 0/2/2/2 |
| 1 | PSU | 1 | 955 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | 6MZ | 1 | 1618 | 1 | - | 4/9/27/28 | 0/3/3/3 |
| 1 | OMC | 1 | 2498 | 1 | - | 0/9/27/28 | 0/2/2/2 |
| 1 | 2MG | 1 | 2445 | 1 | - | 2/9/27/28 | 0/3/3/3 |
| 2 | MA6 | 2 | 1519 | 2 | - | 3/11/29/30 | 0/3/3/3 |
| 1 | 2MG | 1 | 1835 | 1 | - | 2/9/27/28 | 0/3/3/3 |
| 1 | OMG | 1 | 2251 | 54,1 | - | 0/9/27/28 | 0/3/3/3 |
| 2 | MA6 | 2 | 1518 | 2 | - | 0/11/29/30 | 0/3/3/3 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 1 | 3TD | 1 | 1915 | 1 | - | 4/7/25/26 | 0/2/2/2 |
| 2 | PSU | 2 | 516 | 2 | - | 2/7/25/26 | 0/2/2/2 |
| 1 | 2MA | 1 | 2503 | 1 | - | 5/7/25/26 | 0/3/3/3 |
| 2 | 5MC | 2 | 967 | 2 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | PSU | 1 | 2580 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | G7M | 1 | 2069 | 1 | - | 1/7/25/26 | 0/3/3/3 |
| 54 | PSU | 5 | 55 | 54 | - | 1/7/25/26 | 0/2/2/2 |
| 2 | 2MG | 2 | 966 | 2 | - | 0/9/27/28 | 0/3/3/3 |
| 1 | PSU | 1 | 746 | 1 | - | 2/7/25/26 | 0/2/2/2 |
| 54 | H2U | 5 | 20 | 54 | - | 4/7/38/39 | 0/2/2/2 |
| 2 | G7M | 2 | 527 | 2 | - | 2/7/25/26 | 0/3/3/3 |
| 54 | 5MU | 5 | 54 | 54 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | PSU | 1 | 2457 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 54 | 4SU | 5 | 8 | 54 | - | 3/7/25/26 | 0/2/2/2 |
| 1 | PSU | 1 | 2605 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 2 | 2MG | 2 | 1516 | 2 | - | 0/9/27/28 | 0/3/3/3 |
| 1 | PSU | 1 | 1911 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 2 | UR3 | 2 | 1498 | 2 | - | 0/7/25/26 | 0/2/2/2 |
| 2 | 2MG | 2 | 1207 | 2 | - | 2/9/27/28 | 0/3/3/3 |
| 1 | PSU | 1 | 1917 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | 1MG | 1 | 745 | 1 | - | 0/7/25/26 | 0/3/3/3 |
| 54 | 4OC | 5 | 32 | 54 | - | 0/9/29/30 | 0/2/2/2 |
| 1 | OMU | 1 | 2552 | 1 | - | 1/9/27/28 | 0/2/2/2 |
| 1 | 5MU | 1 | 747 | 1 | - | 1/7/25/26 | 0/2/2/2 |

The worst 5 of 216 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | 1 | 1915 | 3TD | C6-C5 | 13.15 | 1.49 | 1.35 |
| 1 | 1 | 2503 | 2MA | C4-N3 | 11.40 | 1.49 | 1.34 |
| 1 | 1 | 2030 | 6MZ | C6-N6 | 11.37 | 1.47 | 1.34 |
| 1 | 1 | 747 | 5MU | C2-N1 | 11.29 | 1.56 | 1.38 |
| 54 | 5 | 20 | H2U | C2-N1 | 11.12 | 1.51 | 1.35 |

The worst 5 of 242 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | 1 | 1618 | 6MZ | C4-N9-C8 | 14.18 | 120.63 | 105.74 |
| 1 | 1 | 2030 | 6MZ | C4-N9-C8 | 13.95 | 120.39 | 105.74 |
| 1 | 1 | 747 | 5MU | C5-C4-N3 | 12.91 | 126.55 | 115.32 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | 1 | 1939 | 5MU | C5-C4-N3 | 12.57 | 126.25 | 115.32 |
| 54 | 5 | 54 | 5MU | C5-C4-N3 | 12.04 | 125.79 | 115.32 |

There are no chirality outliers.

5 of 48 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 1 | 1 | 1618 | 6MZ | C5-C6-N6-C9 |
| 1 | 1 | 1618 | 6MZ | N1-C6-N6-C9 |
| 1 | 1 | 1915 | 3TD | O4'-C1'-C5-C4 |
| 1 | 1 | 1915 | 3TD | O4'-C1'-C5-C6 |
| 1 | 1 | 2504 | PSU | O4'-C4'-C5'-O5' |

There are no ring outliers.

15 monomers are involved in 22 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 2 | 2 | 1402 | 4OC | 1 | 0 |
| 2 | 2 | 1407 | 5MC | 2 | 0 |
| 1 | 1 | 2030 | 6MZ | 1 | 0 |
| 1 | 1 | 1962 | 5MC | 1 | 0 |
| 2 | 2 | 1519 | MA6 | 1 | 0 |
| 1 | 1 | 1915 | 3TD | 4 | 0 |
| 1 | 1 | 2503 | 2MA | 4 | 0 |
| 54 | 5 | 55 | PSU | 1 | 0 |
| 54 | 5 | 20 | H2U | 1 | 0 |
| 54 | 5 | 54 | 5MU | 1 | 0 |
| 54 | 5 | 8 | 4SU | 1 | 0 |
| 2 | 2 | 1516 | 2MG | 1 | 0 |
| 1 | 1 | 745 | 1MG | 1 | 0 |
| 54 | 5 | 32 | 4OC | 1 | 0 |
| 1 | 1 | 2552 | OMU | 2 | 0 |

## 5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry (i)

Of 14 ligands modelled in this entry, 14 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.

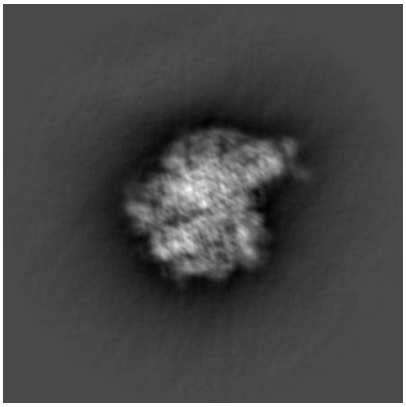
# 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-20204. These allow visual inspection of the internal detail of the map and identification of artifacts.

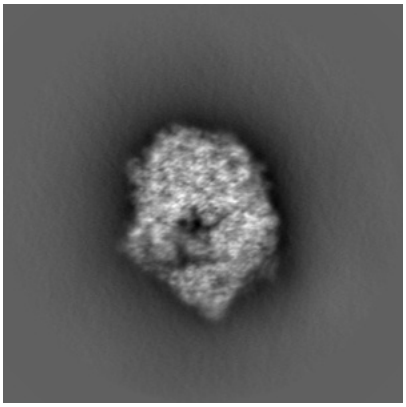
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

## 6.1 Orthogonal projections

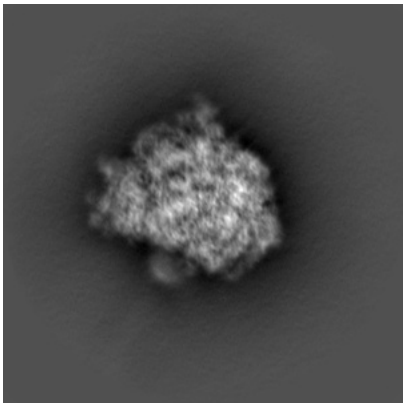
### 6.1.1 Primary map



X



Y

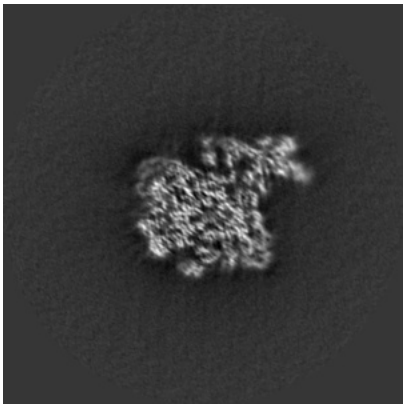


Z

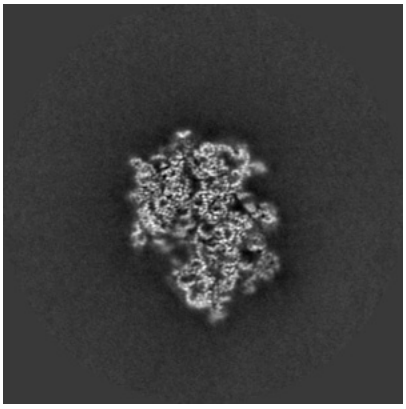
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices

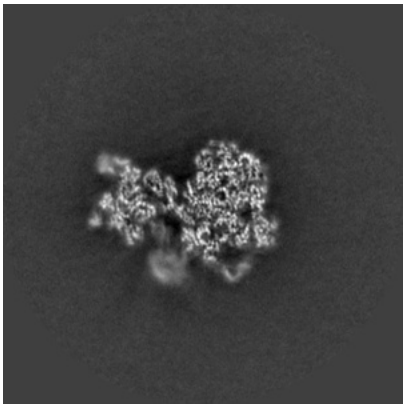
### 6.2.1 Primary map



X Index: 160



Y Index: 160

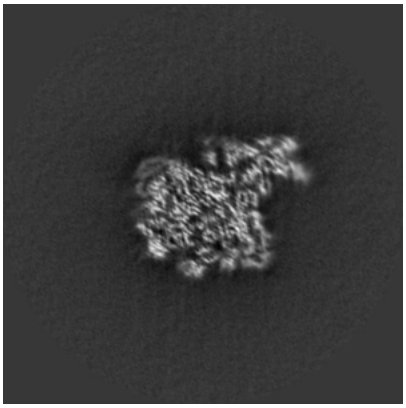


Z Index: 160

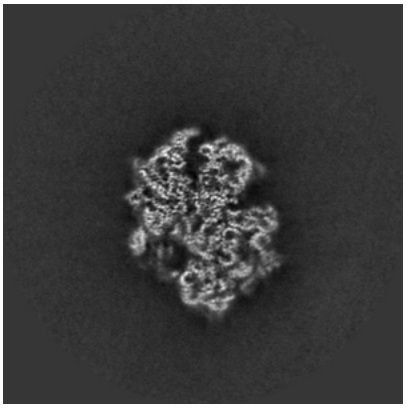
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices (i)

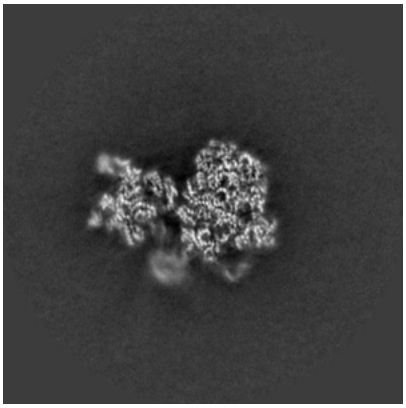
### 6.3.1 Primary map



X Index: 161



Y Index: 156

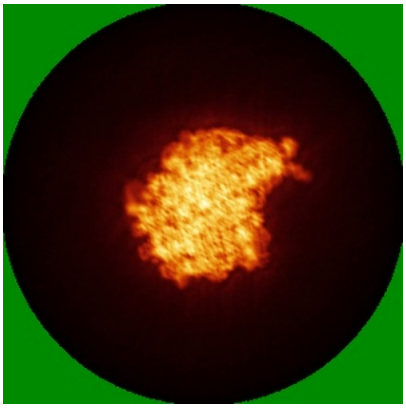


Z Index: 161

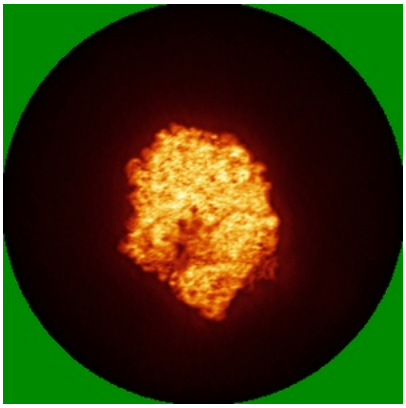
The images above show the largest variance slices of the map in three orthogonal directions.

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

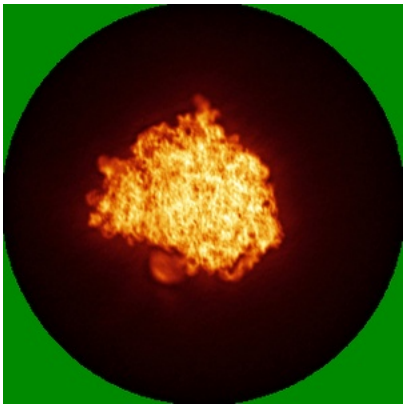
### 6.4.1 Primary map



X



Y

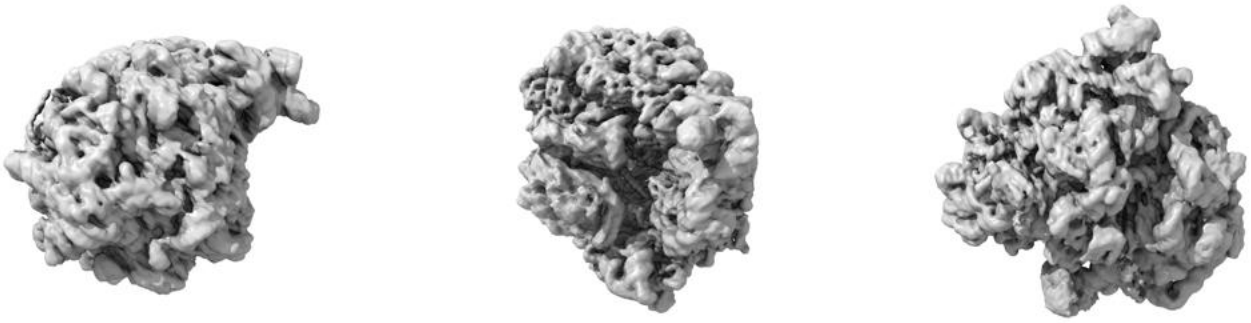


Z

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

## 6.5 Orthogonal surface views (i)

### 6.5.1 Primary map



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.

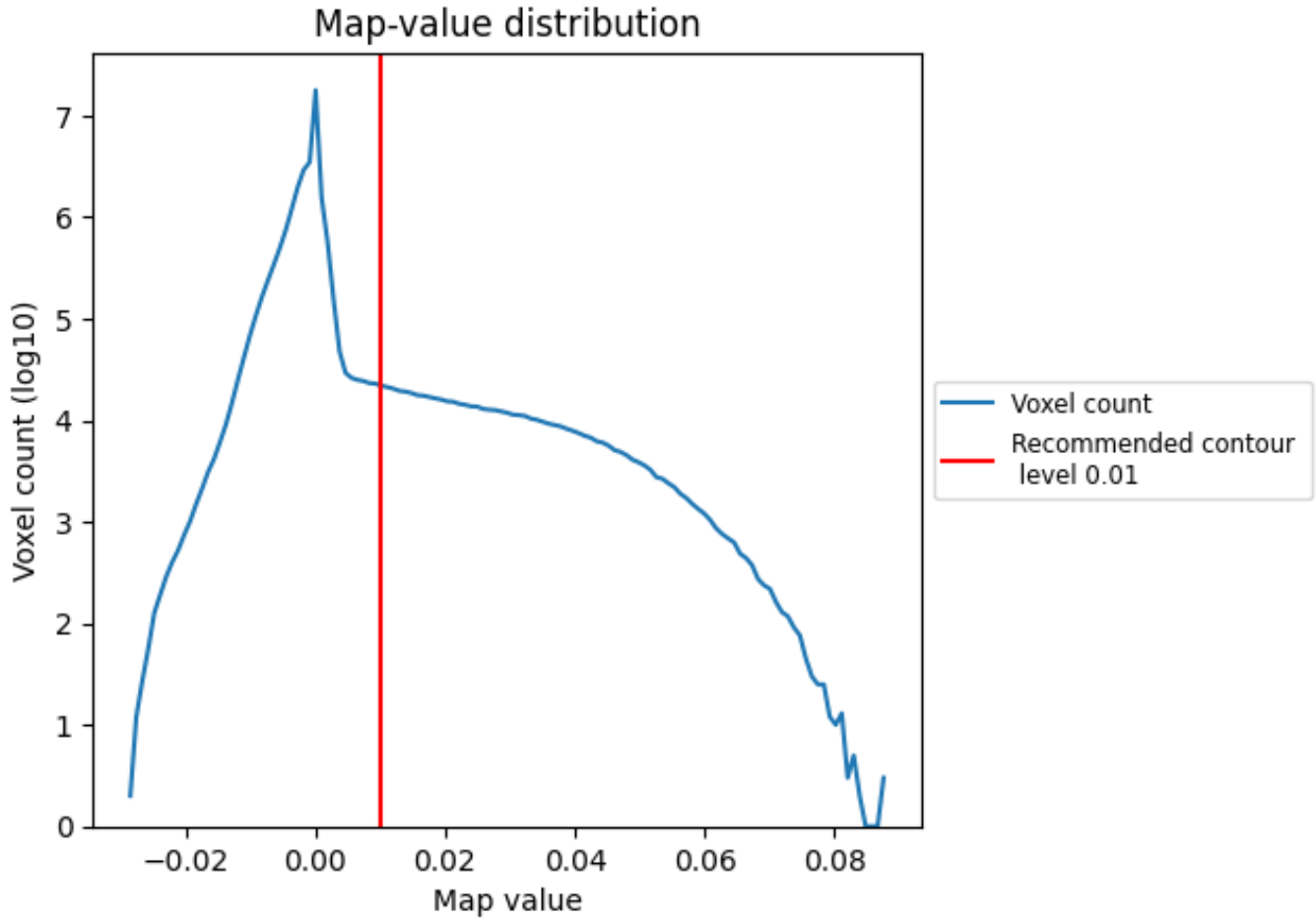
## 6.6 Mask visualisation (i)

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

# 7 Map analysis

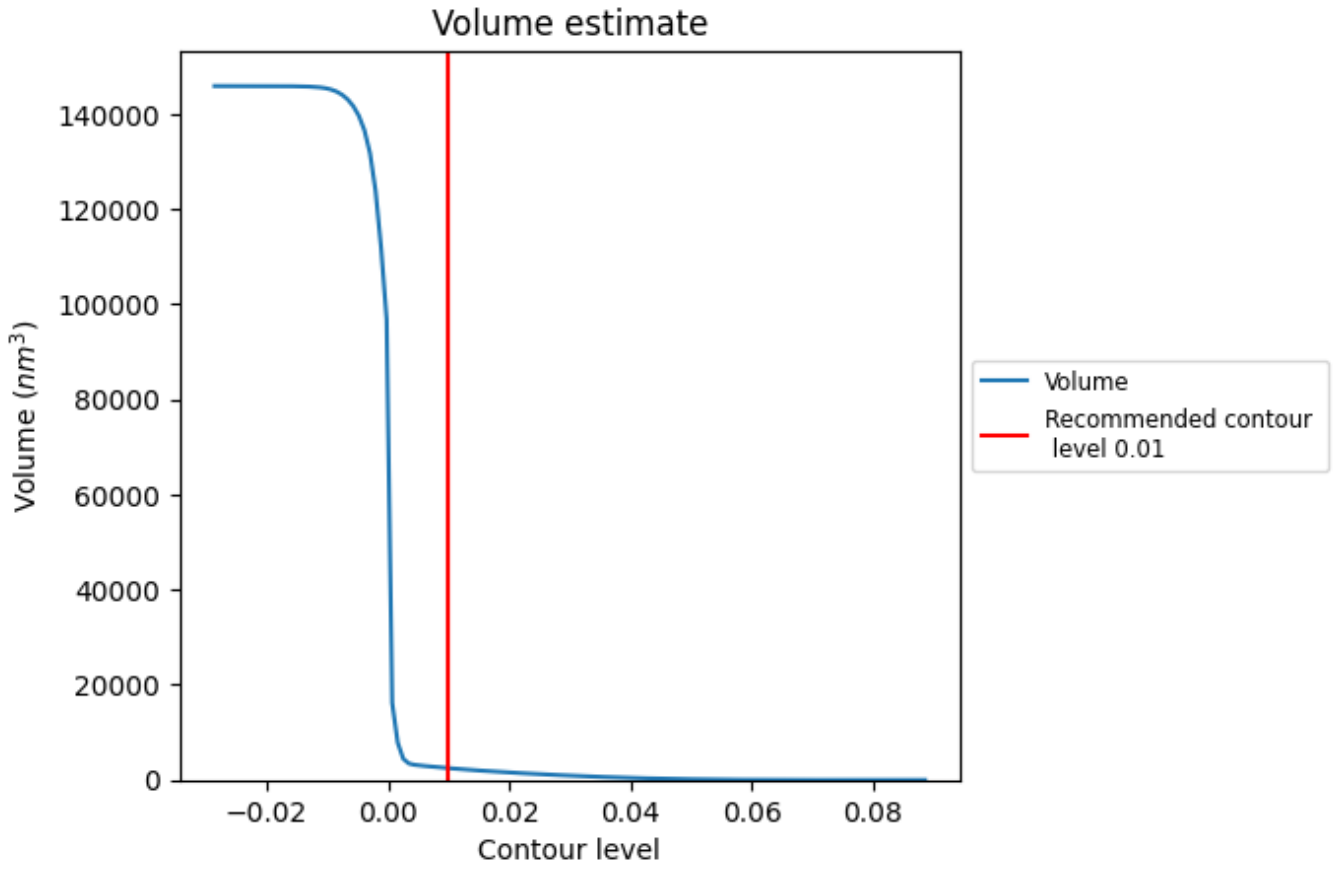
This section contains the results of statistical analysis of the map.

## 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.

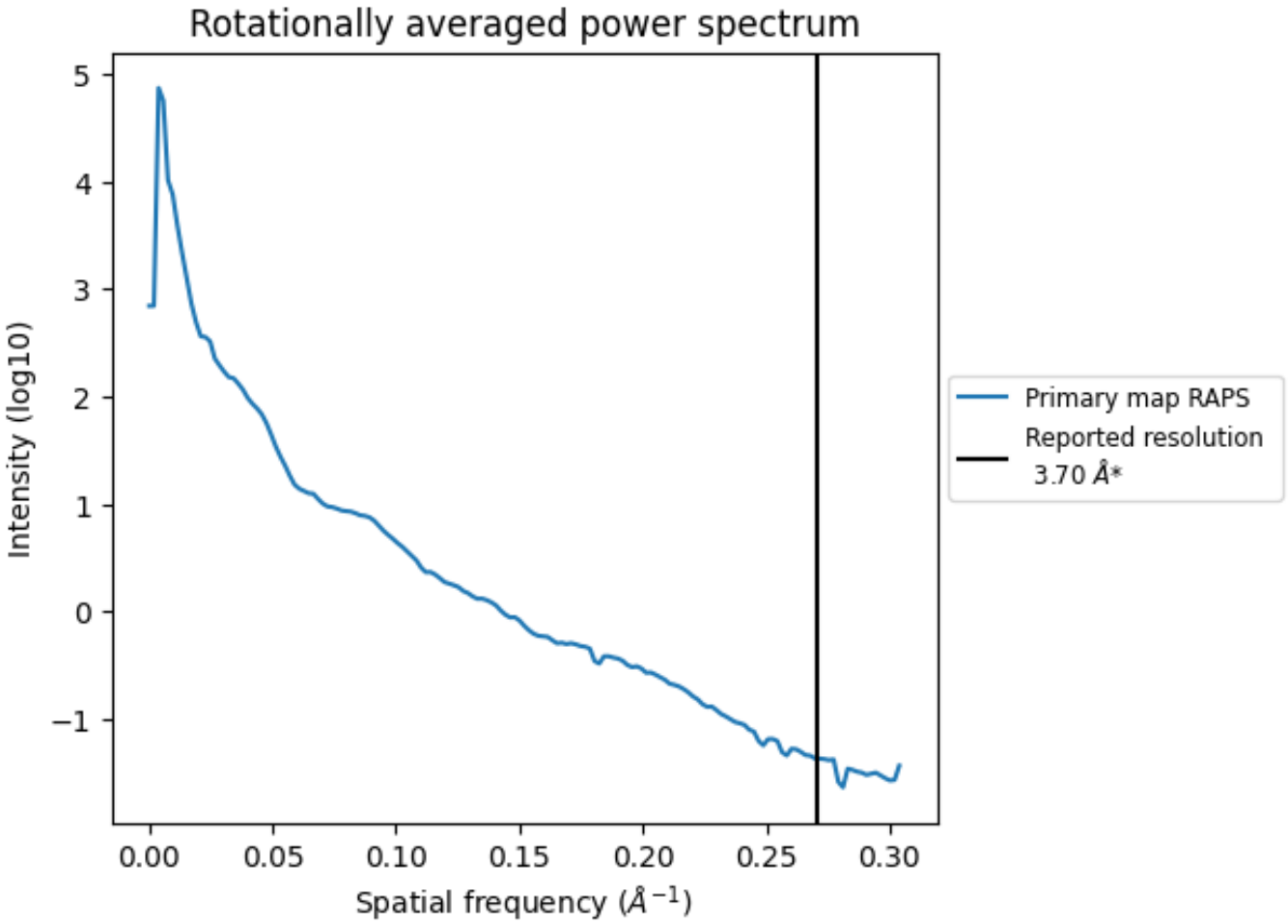
## 7.2 Volume estimate (i)




The volume at the recommended contour level is 2485 $nm^3$; this corresponds to an approximate mass of 2245 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 0.270 Å$^{-1}$

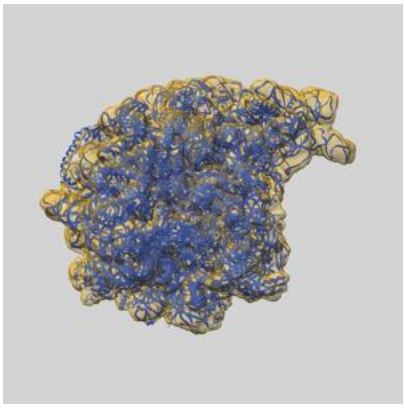
# 8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

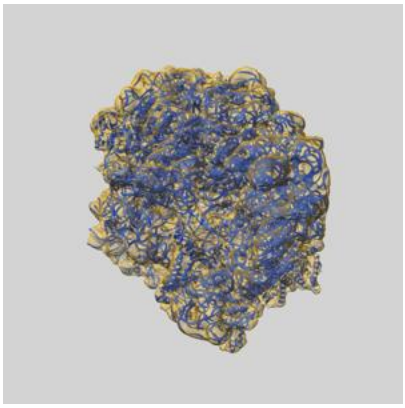
# 9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-20204 and PDB model 6OUO. Per-residue inclusion information can be found in section 3 on page 15.

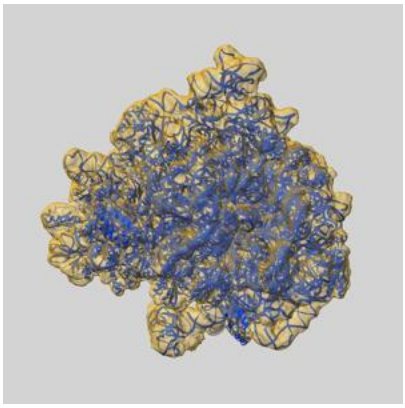
## 9.1 Map-model overlay



X



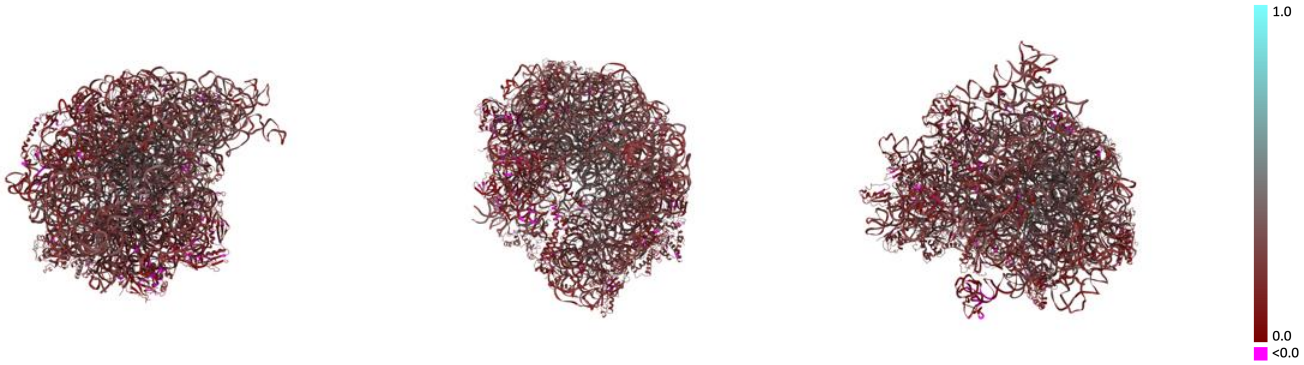
Y



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.

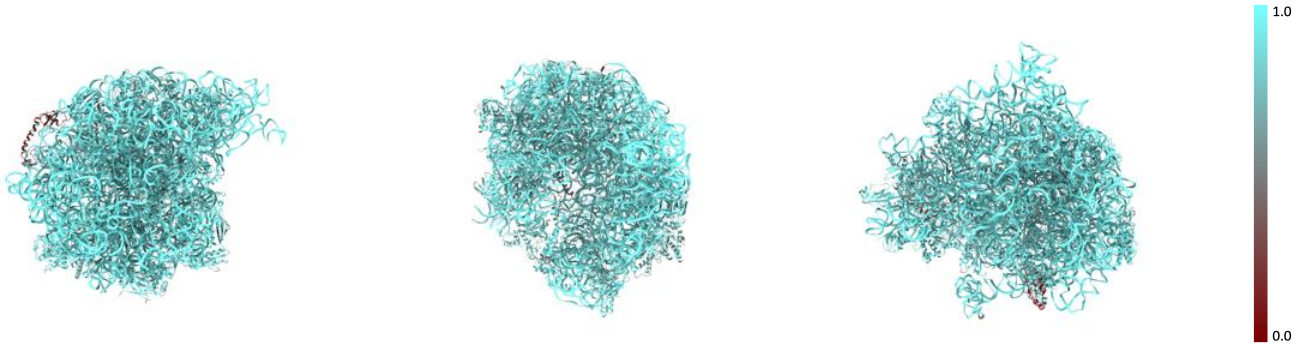
## 9.2 Q-score mapped to coordinate model (i)




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.

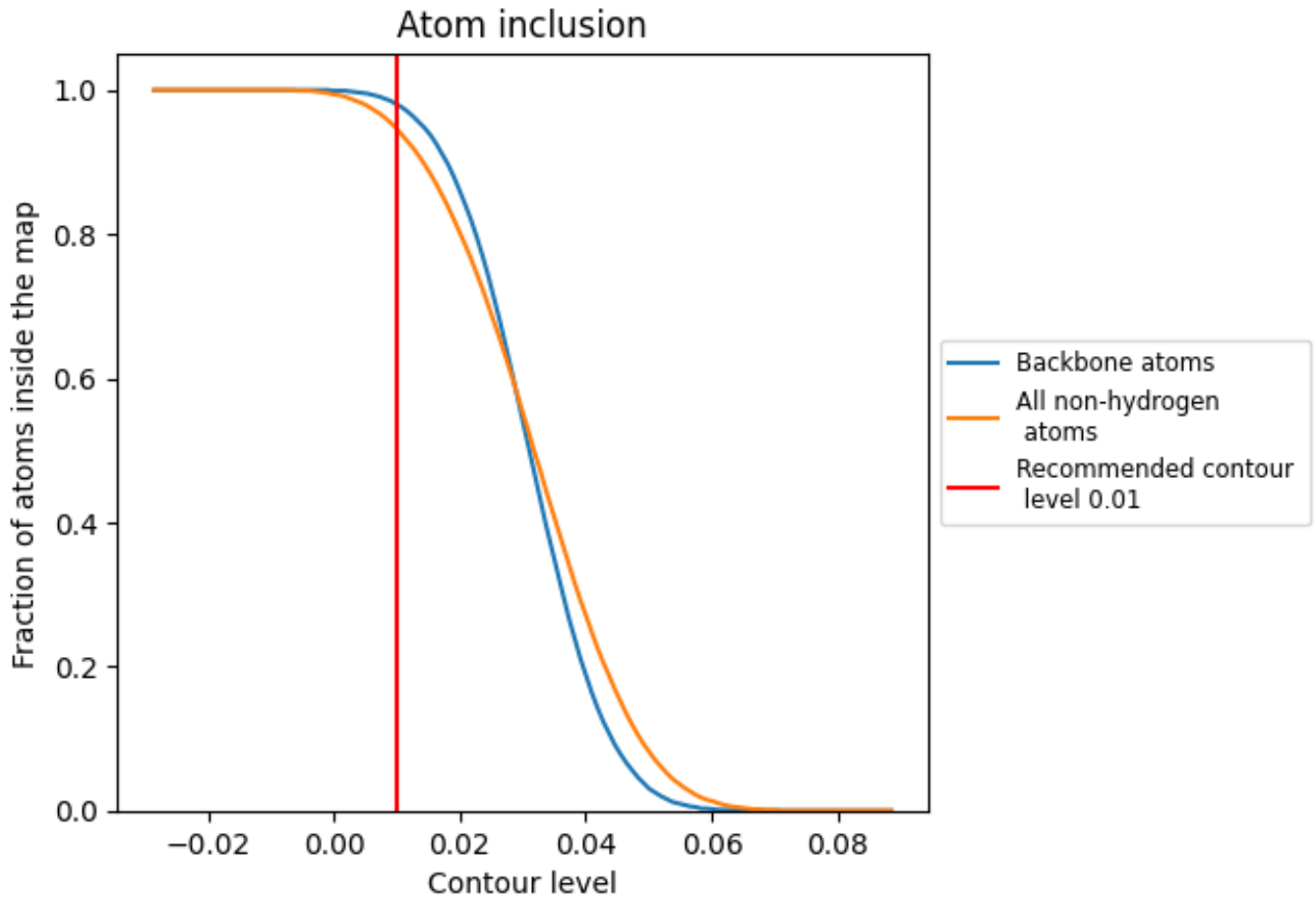
## 9.3 Atom inclusion mapped to coordinate model (i)




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, 98% of all backbone atoms, 95% 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 | 0.9460 | 0.2470 |
| 1 | 0.9870 | 0.2690 |
| 2 | 0.9910 | 0.2690 |
| 3 | 0.9860 | 0.1870 |
| 4 | 0.9840 | 0.3390 |
| 5 | 0.9670 | 0.2880 |
| A | 0.7720 | 0.1830 |
| B | 0.8420 | 0.2390 |
| C | 0.8790 | 0.2320 |
| D | 0.8940 | 0.2430 |
| E | 0.9020 | 0.1880 |
| F | 0.8590 | 0.1350 |
| G | 0.3830 | 0.1430 |
| J | 0.8440 | 0.1710 |
| K | 0.8400 | 0.2770 |
| L | 0.9050 | 0.2800 |
| M | 0.8610 | 0.1910 |
| N | 0.9100 | 0.2220 |
| O | 0.9370 | 0.1770 |
| P | 0.8720 | 0.2470 |
| Q | 0.8700 | 0.1650 |
| R | 0.8880 | 0.1620 |
| S | 0.8760 | 0.2750 |
| T | 0.8810 | 0.1940 |
| U | 0.9140 | 0.1960 |
| V | 0.8580 | 0.1450 |
| W | 0.8710 | 0.2180 |
| X | 0.8340 | 0.2310 |
| Y | 0.8670 | 0.1680 |
| Z | 0.8370 | 0.1800 |
| a | 0.8610 | 0.2030 |
| b | 0.8850 | 0.2450 |
| c | 0.9380 | 0.2860 |
| d | 0.9130 | 0.2800 |
| e | 0.8820 | 0.2890 |

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| Chain | Atom inclusion | Q-score |
|---|---|---|
| f | 0.8500 | 0.1160 |
| g | 0.7430 | 0.1740 |
| h | 0.8810 | 0.2050 |
| i | 0.8940 | 0.2100 |
| j | 0.8750 | 0.2260 |
| k | 0.8590 | 0.1670 |
| l | 0.9160 | 0.2370 |
| m | 0.8720 | 0.1770 |
| n | 0.9240 | 0.1990 |
| o | 0.8780 | 0.1870 |
| p | 0.8890 | 0.2240 |
| q | 0.8650 | 0.2650 |
| r | 0.9050 | 0.1950 |
| s | 0.9070 | 0.1920 |
| t | 0.8570 | 0.1270 |
| u | 0.8840 | 0.2020 |
| v | 0.8830 | 0.2110 |
| w | 0.8390 | 0.1670 |
| x | 0.8900 | 0.1540 |
| y | 0.9170 | 0.2160 |
| z | 0.7530 | 0.1820 |