# Full wwPDB EM Validation Report (i)

Oct 4, 2022 – 09:03 pm BST

| | | |
|---|---|---|
| PDB ID | : | 7PAI |
| EMDB ID | : | EMD-13273 |
| Title | : | 70S ribosome with P-site tRNA in Mycoplasma pneumoniae cells |
| Authors | : | Xue, L.; Lenz, S.; Rappsilber, J.; Mahamid, J. |
| Deposited on | : | 2021-07-30 |
| Resolution | : | 6.70 Å(reported) |
| Based on initial models | : | 7OOC, 7OOD, 4V7C |

This is a Full wwPDB EM Validation 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.

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

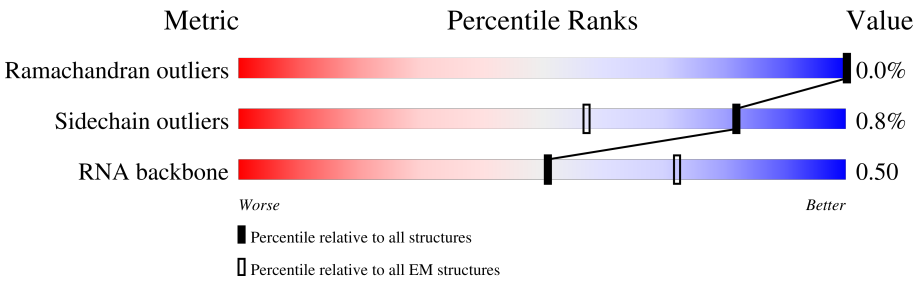
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev43 |
| MolProbity | : | 4.02b-467 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| MapQ | : | 1.9.9 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA)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

# 1 Overall quality at a glance (i)

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

The reported resolution of this entry is 6.70 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) |
|---|---|---|
| Ramachandran outliers | 154571 | 4023 |
| Sidechain outliers | 154315 | 3826 |
| RNA backbone | 4643 | 859 |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=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 | 0 | 48 | 98% |
| 2 | 1 | 59 | 98% |
| 3 | 2 | 37 | 5%, 100% |
| 4 | A | 294 | 12%, 81%, 18% |
| 5 | B | 273 | 13%, 79%, 21% |
| 6 | C | 205 | 17%, 99% |
| 7 | D | 219 | 7%, 69%, 30% |
| 8 | E | 215 | 14%, 77%, 22% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 9 | F | 155 | 14% 99% |
| 10 | G | 142 | 10% 98% |
| 11 | H | 132 | 16% 96% |
| 12 | I | 108 | 12% 94% 6% |
| 13 | J | 121 | 12% 93% 6% |
| 14 | K | 139 | 10% 95% |
| 15 | L | 124 | 10% 94% 5% |
| 16 | M | 61 | 11% 98% |
| 17 | N | 86 | 7% 97% |
| 18 | O | 94 | 5% 84% 15% |
| 19 | P | 85 | 20% 95% |
| 20 | Q | 104 | 8% 62% 38% |
| 21 | R | 87 | 17% 97% |
| 22 | S | 87 | 87% 11% |
| 23 | T | 60 | 5% 88% 12% |
| 24 | a | 287 | 6% 99% |
| 25 | b | 287 | 5% 79% 20% |
| 26 | c | 212 | 7% 99% |
| 27 | d | 180 | 10% 97% |
| 28 | e | 184 | 15% 96% |
| 29 | f | 149 | 61% 96% |
| 30 | g | 161 | 34% 72% 5% 22% |
| 31 | h | 137 | 62% 93% 7% |
| 32 | i | 146 | 7% 99% |
| 33 | j | 122 | 7% 100% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 34 | k | 151 | 9% 98% |
| 35 | l | 139 | 12% 97% |
| 36 | m | 124 | 95% |
| 37 | n | 116 | 8% 97% |
| 38 | o | 119 | 12% 95% |
| 39 | p | 127 | 90% 10% |
| 40 | q | 100 | 6% 99% |
| 41 | r | 159 | 86% 13% |
| 42 | s | 237 | 39% 61% |
| 43 | t | 111 | 23% 100% |
| 44 | u | 104 | 6% 83% 17% |
| 45 | v | 65 | 6% 95% |
| 46 | w | 111 | 6% 90% 10% |
| 47 | x | 97 | 6% 45% 55% |
| 48 | y | 57 | 5% 93% 5% |
| 49 | z | 53 | 6% 94% 6% |
| 50 | 3 | 2907 | 73% 26% |
| 51 | 4 | 108 | 63% 33% |
| 52 | 5 | 1520 | 75% 23% |
| 53 | 7 | 76 | 67% 33% |

# 2 Entry composition (i)

There are 53 unique types of molecules in this entry. The entry contains 144502 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 50S ribosomal protein L34.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 1 | 0 | 47 | 380 | 236 | 81 | 61 | 2 | 0 | 0 |

- Molecule 2 is a protein called 50S ribosomal protein L35.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 2 | 1 | 59 | 477 | 300 | 99 | 77 | 1 | 0 | 0 |

- Molecule 3 is a protein called 50S ribosomal protein L36.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 3 | 2 | 37 | 304 | 189 | 65 | 46 | 4 | 0 | 0 |

- Molecule 4 is a protein called 30S ribosomal protein S2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 4 | A | 240 | 1921 | 1226 | 334 | 352 | 9 | 0 | 0 |

- Molecule 5 is a protein called 30S ribosomal protein S3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 5 | B | 215 | 1698 | 1073 | 313 | 307 | 5 | 0 | 0 |

- Molecule 6 is a protein called 30S ribosomal protein S4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 6 | C | 203 | 1660 | 1051 | 314 | 290 | 5 | 0 | 0 |

- Molecule 7 is a protein called 30S ribosomal protein S5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 7 | D | 153 | 1173 | 742 | 226 | 202 | 3 | 0 | 0 |

- Molecule 8 is a protein called 30S ribosomal protein S6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 8 | E | 167 | 1362 | 857 | 240 | 263 | 2 | 0 | 0 |

- Molecule 9 is a protein called 30S ribosomal protein S7.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 9 | F | 154 | 1246 | 785 | 239 | 216 | 6 | 0 | 0 |

- Molecule 10 is a protein called 30S ribosomal protein S8.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 10 | G | 141 | 1110 | 723 | 193 | 192 | 2 | 0 | 0 |

- Molecule 11 is a protein called 30S ribosomal protein S9.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 11 | H | 128 | 1028 | 655 | 191 | 181 | 1 | 0 | 0 |

- Molecule 12 is a protein called 30S ribosomal protein S10.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 12 | I | 101 | 809 | 523 | 142 | 143 | 1 | 0 | 0 |

- Molecule 13 is a protein called 30S ribosomal protein S11.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 13 | J | 114 | 829 | 514 | 153 | 156 | 6 | 0 | 0 |

- Molecule 14 is a protein called 30S ribosomal protein S12.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 14 | K | 136 | 1076 | 680 | 213 | 181 | 2 | 0 | 0 |

- Molecule 15 is a protein called 30S ribosomal protein S13.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 15 | L | 118 | 951 | 594 | 191 | 166 | 0 | 0 |

- Molecule 16 is a protein called 30S ribosomal protein S14 type Z.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 16 | M | 60 | 474 | 302 | 96 | 72 | 4 | 0 | 0 |

- Molecule 17 is a protein called 30S ribosomal protein S15.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 17 | N | 83 | 673 | 428 | 125 | 120 | 0 | 0 |

- Molecule 18 is a protein called 30S ribosomal protein S16.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 18 | O | 80 | 646 | 414 | 119 | 111 | 2 | 0 | 0 |

- Molecule 19 is a protein called 30S ribosomal protein S17.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 19 | P | 83 | 675 | 425 | 135 | 115 | 0 | 0 |

- Molecule 20 is a protein called 30S ribosomal protein S18.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 20 | Q | 65 | 535 | 342 | 103 | 86 | 4 | 0 | 0 |

- Molecule 21 is a protein called 30S ribosomal protein S19.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 21 | R | 84 | 682 | 435 | 127 | 118 | 2 | 0 | 0 |

- Molecule 22 is a protein called 30S ribosomal protein S20.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 22 | S | 77 | 629 | 383 | 135 | 111 | 0 | 0 |

- Molecule 23 is a protein called 30S ribosomal protein S21.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 23 | T | 53 | 471 | 295 | 103 | 72 | 1 | 0 | 0 |

- Molecule 24 is a protein called 50S ribosomal protein L2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 24 | a | 285 | 2225 | 1385 | 437 | 397 | 6 | 0 | 0 |

- Molecule 25 is a protein called 50S ribosomal protein L3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 25 | b | 229 | 1762 | 1119 | 318 | 318 | 7 | 0 | 0 |

- Molecule 26 is a protein called 50S ribosomal protein L4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 26 | c | 210 | 1644 | 1047 | 297 | 297 | 3 | 0 | 0 |

- Molecule 27 is a protein called 50S ribosomal protein L5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 27 | d | 175 | 1388 | 893 | 245 | 246 | 4 | 0 | 0 |

- Molecule 28 is a protein called 50S ribosomal protein L6.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 28 | e | 176 | 1396 | 899 | 247 | 250 | 0 | 0 |

- Molecule 29 is a protein called 50S ribosomal protein L9.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 29 | f | 145 | 1160 | 746 | 204 | 207 | 3 | 0 | 0 |

- Molecule 30 is a protein called 50S ribosomal protein L10.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 30 | g | 126 | 960 | 612 | 167 | 178 | 3 | 0 | 0 |

- Molecule 31 is a protein called 50S ribosomal protein L11.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 31 | h | 128 | 959 | 616 | 160 | 177 | 6 | 0 | 0 |

- Molecule 32 is a protein called 50S ribosomal protein L13.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 32 | i | 144 | 1164 | 737 | 213 | 209 | 5 | 0 | 0 |

- Molecule 33 is a protein called 50S ribosomal protein L14.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 33 | j | 122 | 944 | 595 | 178 | 167 | 4 | 0 | 0 |

- Molecule 34 is a protein called 50S ribosomal protein L15.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 34 | k | 148 | 1153 | 731 | 226 | 196 | 0 | 0 |

- Molecule 35 is a protein called 50S ribosomal protein L16.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 35 | l | 136 | 1079 | 694 | 196 | 182 | 7 | 0 | 0 |

- Molecule 36 is a protein called 50S ribosomal protein L17.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 36 | m | 119 | 958 | 609 | 175 | 171 | 3 | 0 | 0 |

- Molecule 37 is a protein called 50S ribosomal protein L18.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 37 | n | 112 | 889 | 557 | 175 | 155 | 2 | 0 | 0 |

- Molecule 38 is a protein called 50S ribosomal protein L19.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 38 | o | 115 | 938 | 592 | 180 | 165 | 1 | 0 | 0 |

- Molecule 39 is a protein called 50S ribosomal protein L20.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 39 | p | 114 | 947 | 603 | 188 | 154 | 2 | 0 | 0 |

- Molecule 40 is a protein called 50S ribosomal protein L21.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 40 | q | 99 | 811 | 525 | 148 | 134 | 4 | 0 | 0 |

- Molecule 41 is a protein called 50S ribosomal protein L22.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 41 | r | 139 | 1068 | 663 | 207 | 191 | 7 | 0 | 0 |

- Molecule 42 is a protein called 50S ribosomal protein L23.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 42 | s | 92 | 720 | 475 | 122 | 122 | 1 | 0 | 0 |

- Molecule 43 is a protein called 50S ribosomal protein L24.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 43 | t | 111 | 872 | 550 | 166 | 153 | 3 | 0 | 0 |

- Molecule 44 is a protein called 50S ribosomal protein L27.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 44 | u | 86 | 657 | 409 | 130 | 117 | 1 | 0 | 0 |

- Molecule 45 is a protein called 50S ribosomal protein L28.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 45 | v | 63 | 513 | 317 | 108 | 87 | 1 | 0 | 0 |

- Molecule 46 is a protein called 50S ribosomal protein L29.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 46 | w | 100 | 818 | 517 | 153 | 148 | 0 | 0 |

- Molecule 47 is a protein called 50S ribosomal protein L31.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 47 | x | 44 | 344 | 221 | 55 | 64 | 4 | 0 | 0 |

- Molecule 48 is a protein called 50S ribosomal protein L32.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 48 | y | 56 | 452 | 274 | 98 | 75 | 5 | 0 | 0 |

- Molecule 49 is a protein called 50S ribosomal protein L33 1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 49 | z | 50 | 408 | 255 | 81 | 68 | 4 | 0 | 0 |

- Molecule 50 is a RNA chain called 23S ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 50 | 3 | 2878 | 61664 | 27558 | 11236 | 19995 | 2875 | 0 | 0 |

- Molecule 51 is a RNA chain called 5S ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 51 | 4 | 105 | 2239 | 1003 | 409 | 724 | 103 | 0 | 0 |

- Molecule 52 is a RNA chain called 16S ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 52 | 5 | 1493 | 31943 | 14279 | 5792 | 10382 | 1490 | 0 | 0 |

- Molecule 53 is a RNA chain called tRNA-Phe.

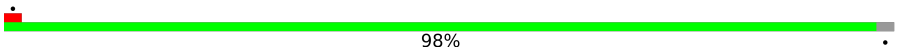
| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 53 | 7 | 76 | 1618 | 723 | 289 | 531 | 75 | 0 | 0 |

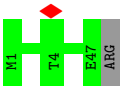
# 3 Residue-property plots (i)

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: 50S ribosomal protein L34

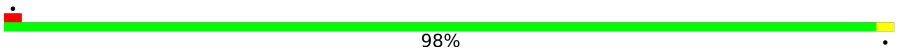
Chain 0:

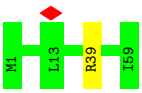



- Molecule 2: 50S ribosomal protein L35

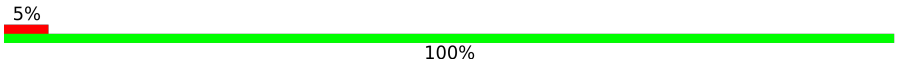
Chain 1:

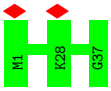



- Molecule 3: 50S ribosomal protein L36

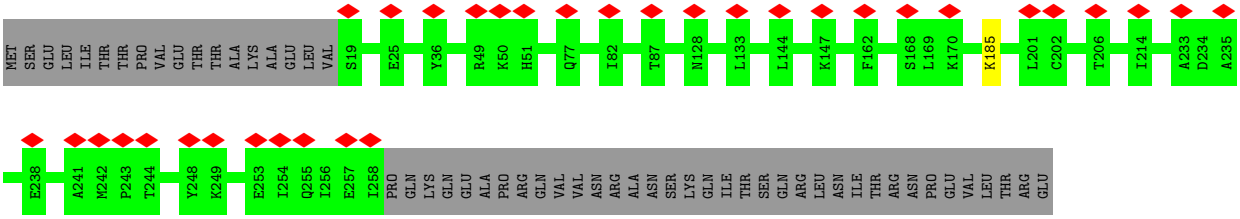
Chain 2:



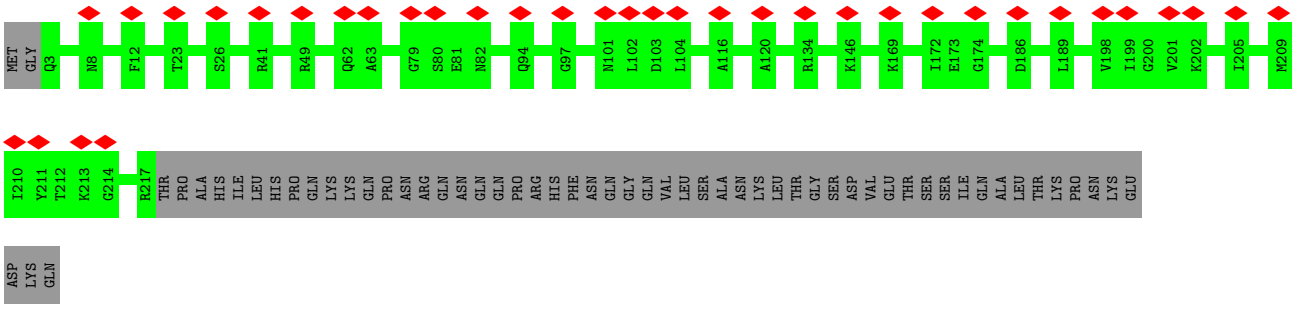

- Molecule 4: 30S ribosomal protein S2

Chain A:



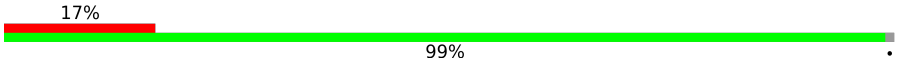

- Molecule 5: 30S ribosomal protein S3

Chain B:



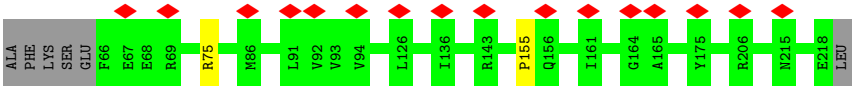

- Molecule 6: 30S ribosomal protein S4

Chain C:



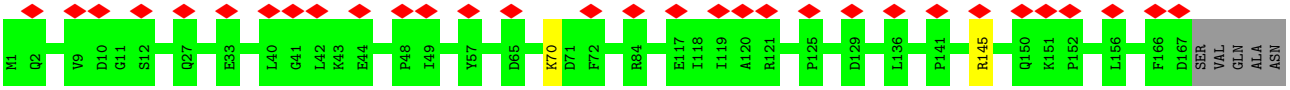
- Molecule 7: 30S ribosomal protein S5

Chain D:



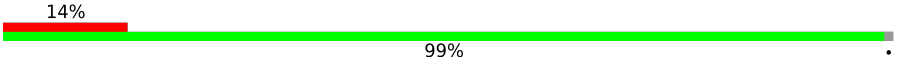

- Molecule 8: 30S ribosomal protein S6

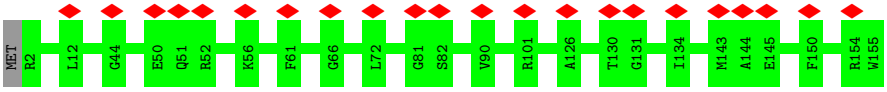
Chain E:



- Molecule 9: 30S ribosomal protein S7

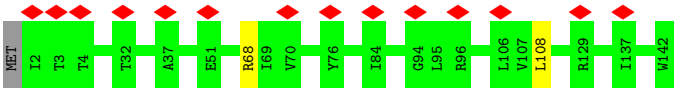
Chain F:



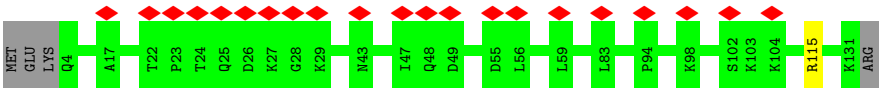

- Molecule 10: 30S ribosomal protein S8

Chain G: 10% 98%



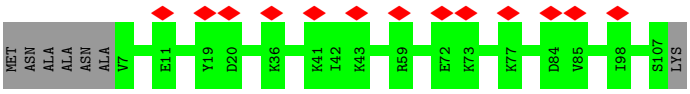

• Molecule 11: 30S ribosomal protein S9

Chain H: 16% 96%



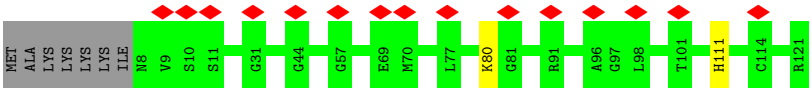

• Molecule 12: 30S ribosomal protein S10

Chain I: 12% 94% 6%



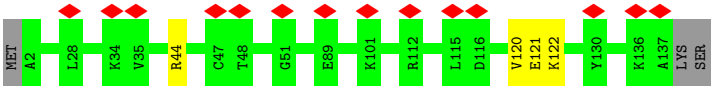

• Molecule 13: 30S ribosomal protein S11

Chain J: 12% 93% 6%



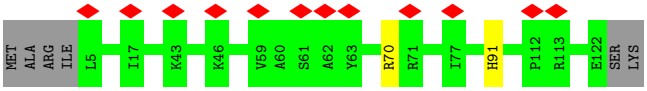

• Molecule 14: 30S ribosomal protein S12

Chain K: 10% 95%



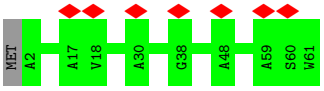

• Molecule 15: 30S ribosomal protein S13

Chain L: 10% 94% 5%



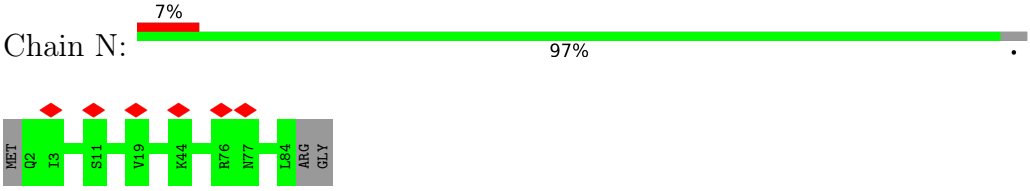

• Molecule 16: 30S ribosomal protein S14 type Z

Chain M: 11% 98%



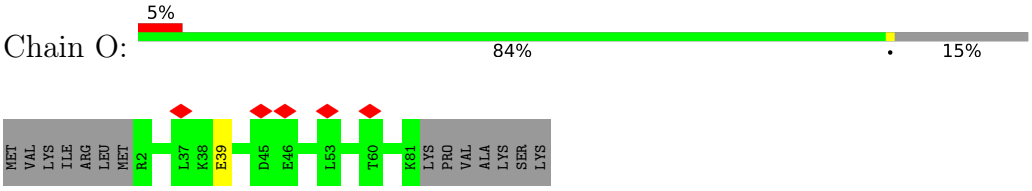
- Molecule 17: 30S ribosomal protein S15

Chain N:



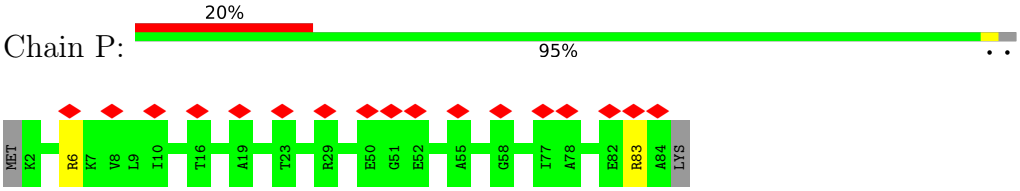

- Molecule 18: 30S ribosomal protein S16

Chain O:



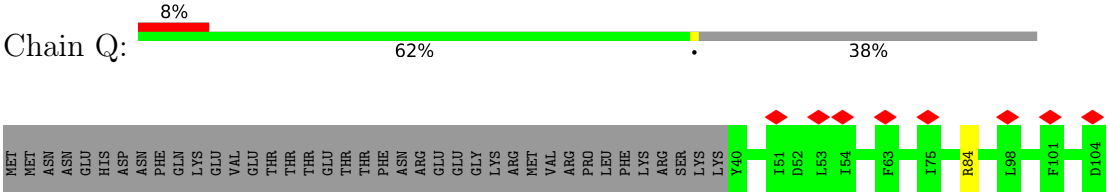

- Molecule 19: 30S ribosomal protein S17

Chain P:



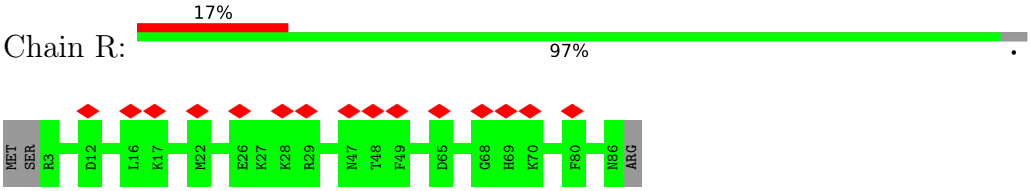

- Molecule 20: 30S ribosomal protein S18

Chain Q:



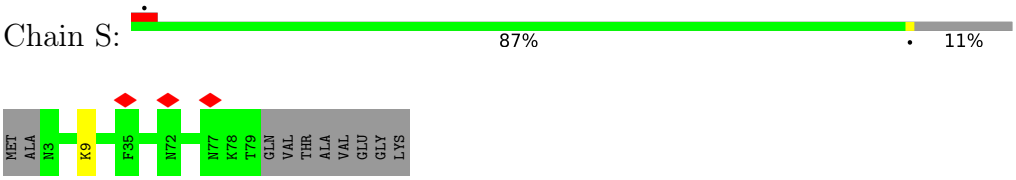

- Molecule 21: 30S ribosomal protein S19

Chain R:



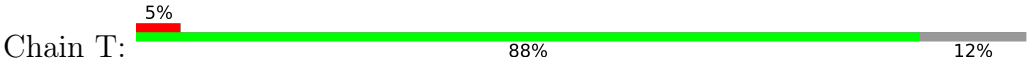

- Molecule 22: 30S ribosomal protein S20

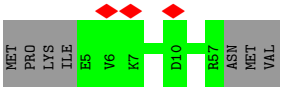
Chain S:




- Molecule 23: 30S ribosomal protein S21

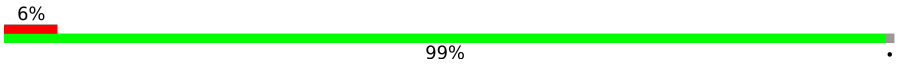
Chain T:

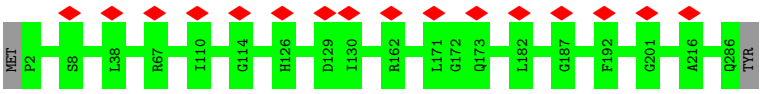





- Molecule 24: 50S ribosomal protein L2

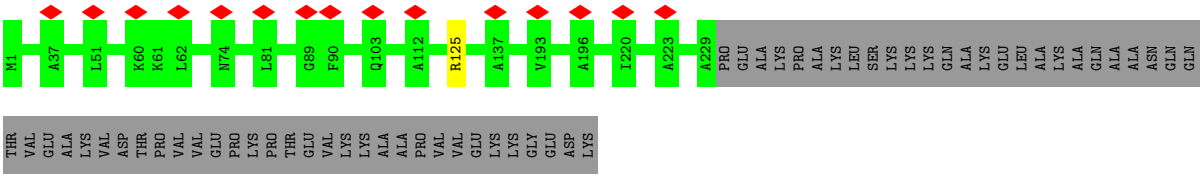
Chain a:



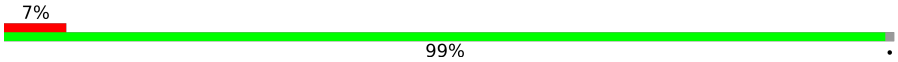

- Molecule 25: 50S ribosomal protein L3

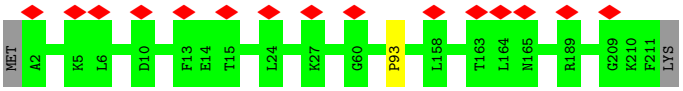
Chain b:




- Molecule 26: 50S ribosomal protein L4

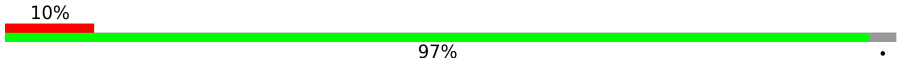
Chain c:

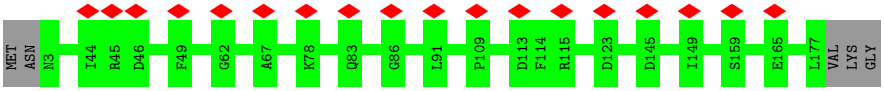



- Molecule 27: 50S ribosomal protein L5

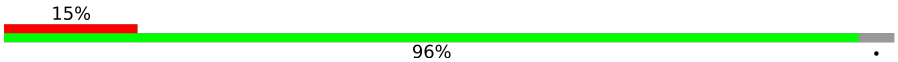
Chain d:

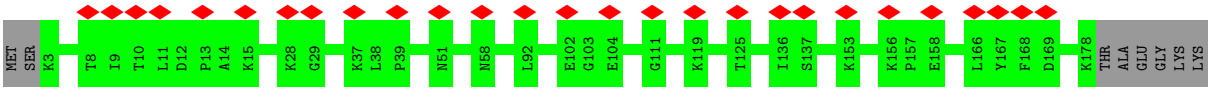



- Molecule 28: 50S ribosomal protein L6

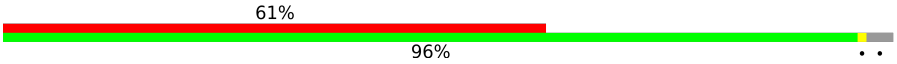
Chain e:

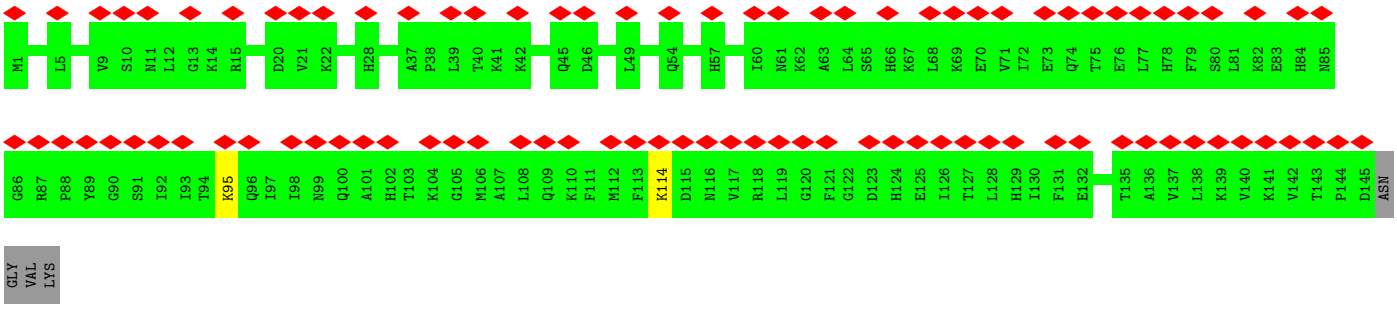



- Molecule 29: 50S ribosomal protein L9

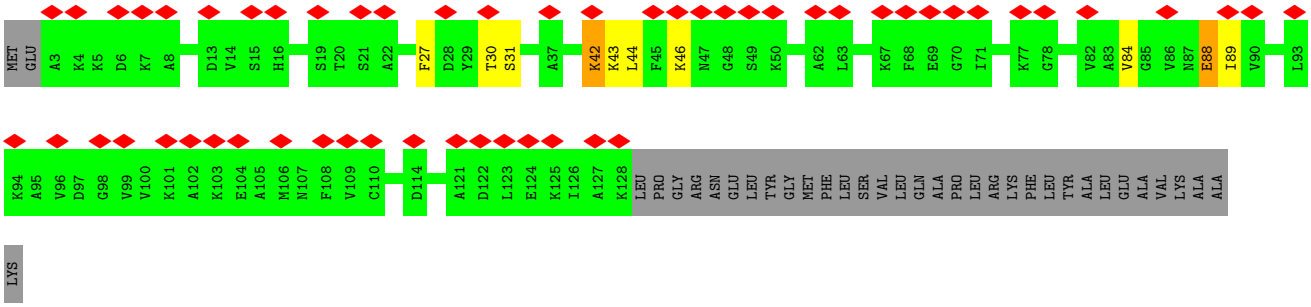
Chain f:





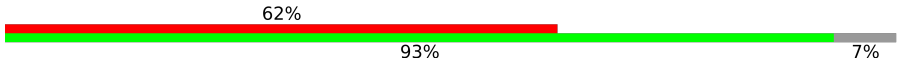

- Molecule 30: 50S ribosomal protein L10

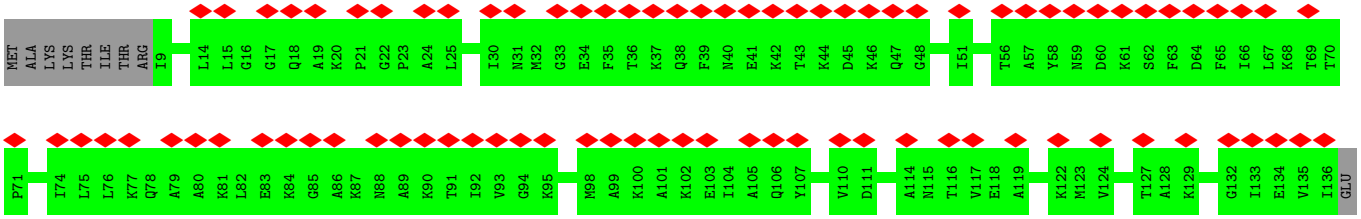
Chain g:




- Molecule 31: 50S ribosomal protein L11

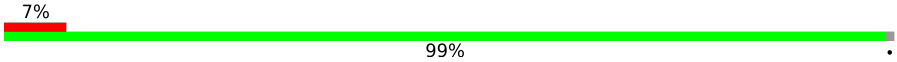
Chain h:

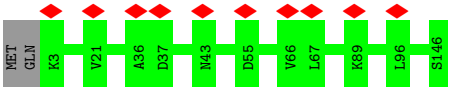



- Molecule 32: 50S ribosomal protein L13

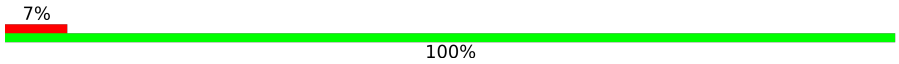
Chain i:

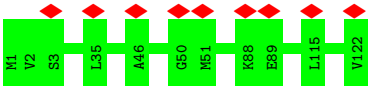



- Molecule 33: 50S ribosomal protein L14

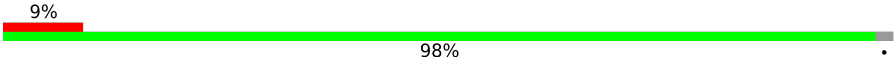
Chain j:

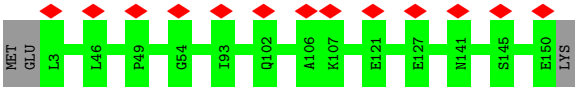


• Molecule 34: 50S ribosomal protein L15

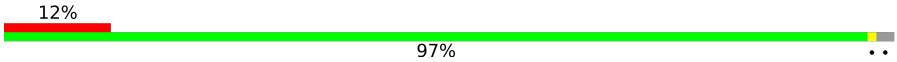
Chain k:

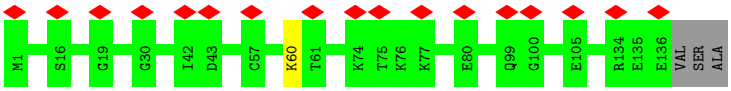



• Molecule 35: 50S ribosomal protein L16

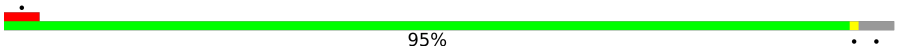
Chain l:

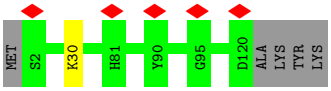



• Molecule 36: 50S ribosomal protein L17

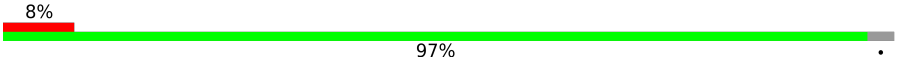
Chain m:

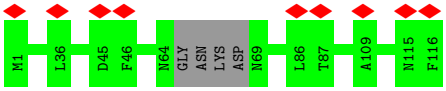



• Molecule 37: 50S ribosomal protein L18

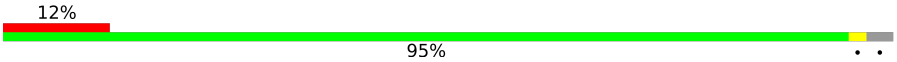
Chain n:

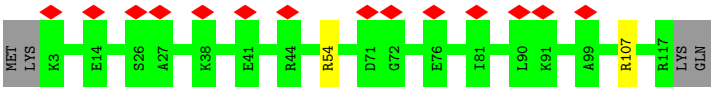



• Molecule 38: 50S ribosomal protein L19

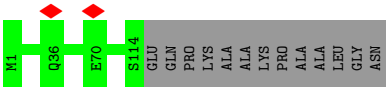
Chain o:



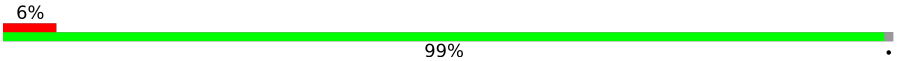

• Molecule 39: 50S ribosomal protein L20

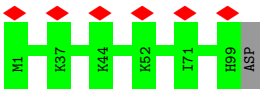
Chain p:




• Molecule 40: 50S ribosomal protein L21

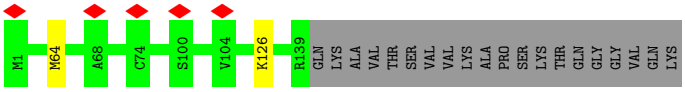
Chain q:





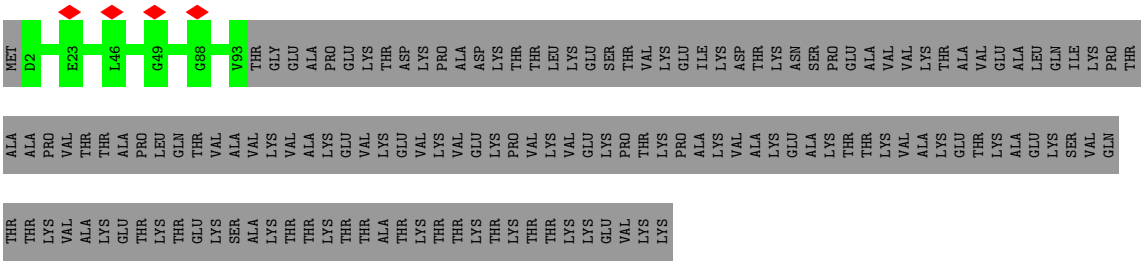

• Molecule 41: 50S ribosomal protein L22

Chain r:



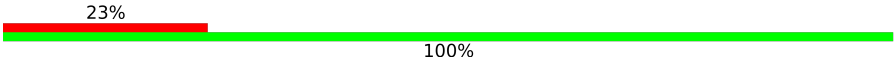

• Molecule 42: 50S ribosomal protein L23

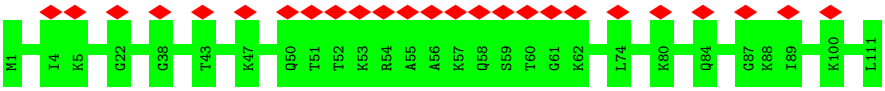
Chain s:




• Molecule 43: 50S ribosomal protein L24

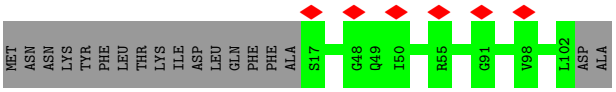
Chain t:



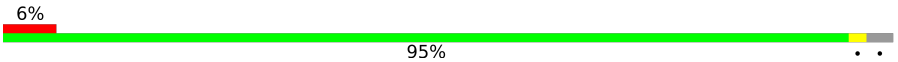

• Molecule 44: 50S ribosomal protein L27

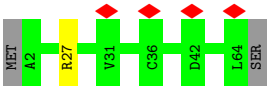
Chain u:




• Molecule 45: 50S ribosomal protein L28

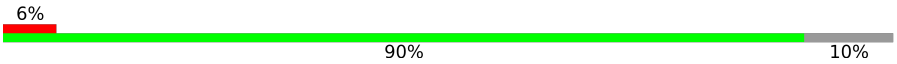
Chain v:

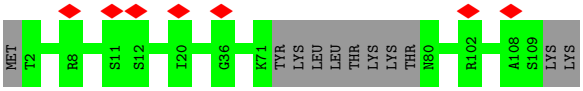



• Molecule 46: 50S ribosomal protein L29

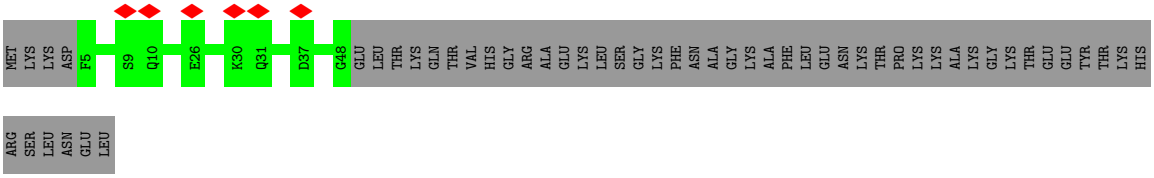
Chain w:





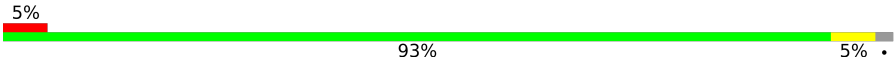

• Molecule 47: 50S ribosomal protein L31

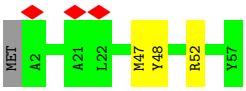
Chain x:




• Molecule 48: 50S ribosomal protein L32

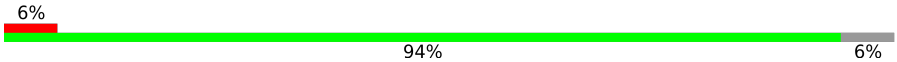
Chain y:

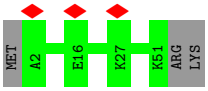



• Molecule 49: 50S ribosomal protein L33 1

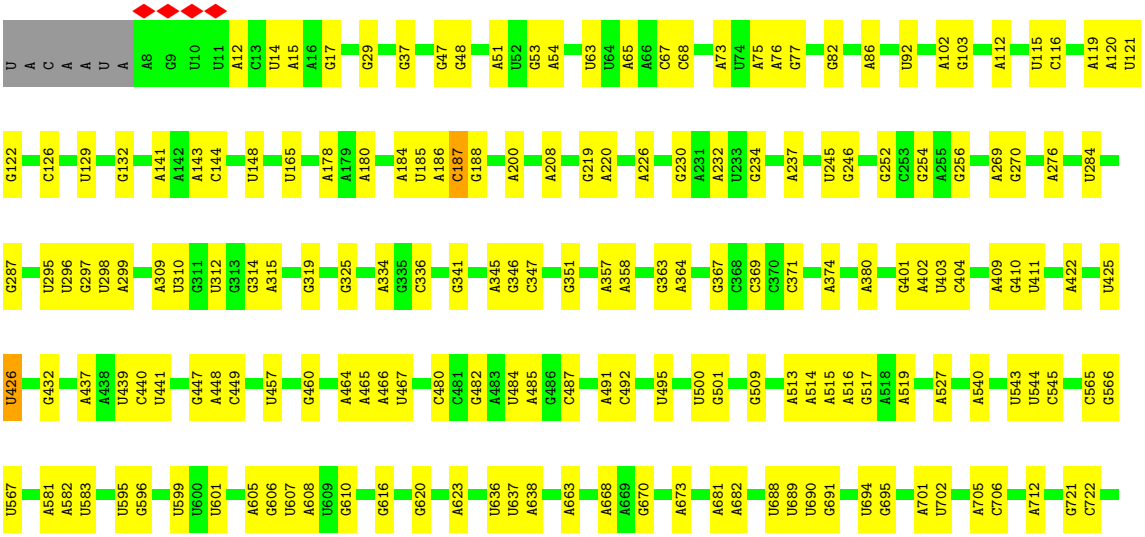
Chain z:

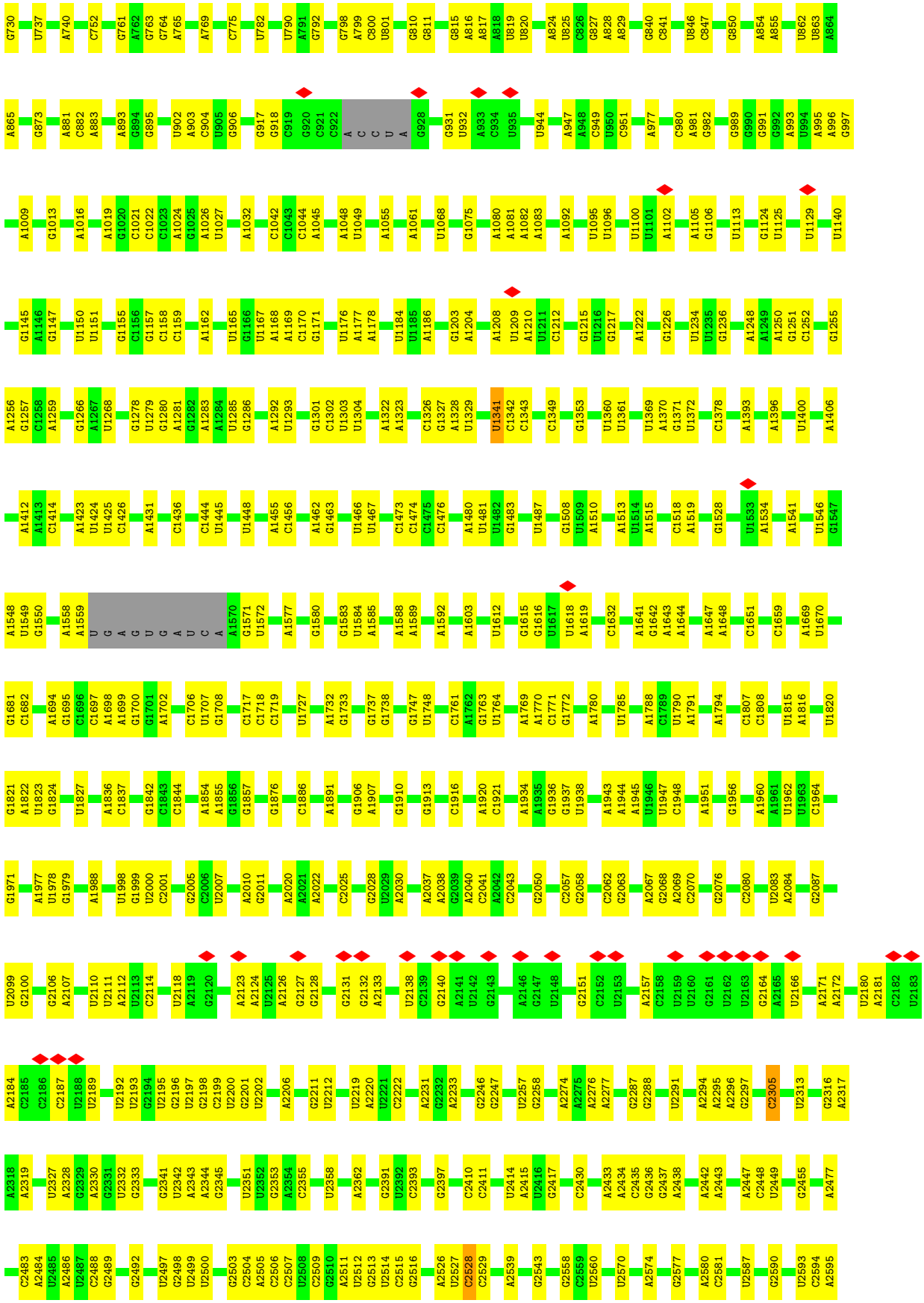


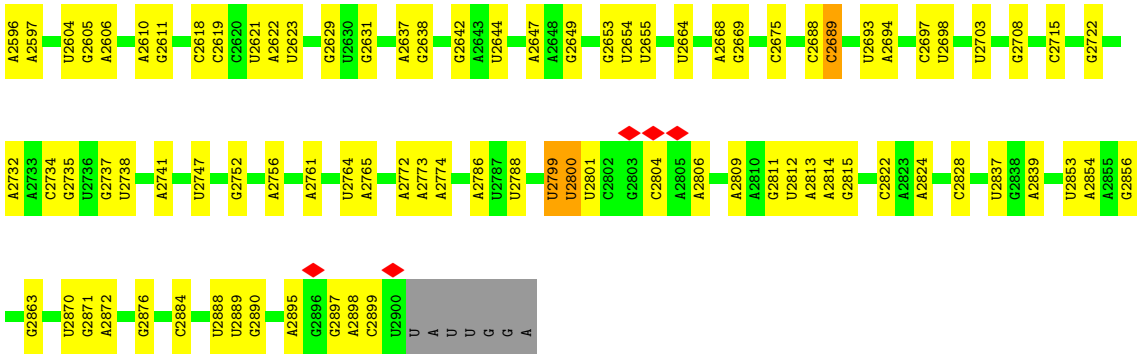




• Molecule 50: 23S ribosomal RNA

Chain 3:

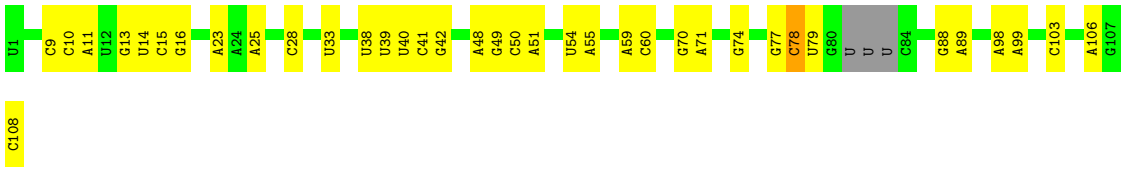



G730 U737 A740 C752 G761 A762 G763 G764 A765 A769 C775 U782 U790 A791 G792 G798 A799 C800 U801 G810 G811 G815 A816 A817 A818 U819 U820 A824 U825 C826 G827 A828 A829 G840 C841 U846 C847 G850 A854 A855 U862 U863 A864
A865 G873 A881 C882 A883 A893 G894 G895 U902 A903 C904 U905 G906 G917 G918 C919 G920 C921 C922 A C C U A G928 G931 U932 A933 C934 U935 U944 A947 A948 C949 U950 C951 A977 C980 A981 G982 G989 G990 G991 G992 A993 U994 A995 A996 G997
A1009 G1013 A1016 A1019 G1020 C1021 C1022 C1023 A1024 G1025 A1026 U1027 A1032 C1042 C1043 C1044 A1045 A1048 U1049 A1055 A1061 U1068 G1075 A1080 A1081 A1082 A1083 A1092 U1095 U1096 U1100 U1101 A1102 A1105 G1106 U1113 G1124 U1125 U1129 U1140
G1145 A1146 G1147 U1150 U1151 G1155 C1156 G1157 C1158 C1159 A1162 U1165 G1166 U1167 A1168 A1169 C1170 G1171 U1176 A1177 A1178 U1184 U1185 A1186 G1203 A1204 A1208 U1209 A1210 U1211 C1212 G1215 U1216 G1217 A1222 G1226 U1234 U1235 G1236 A1248 A1249 A1250 G1251 C1252 G1255
A1256 G1257 C1258 A1259 G1266 A1267 U1268 G1278 U1279 G1280 A1281 G1282 A1283 A1284 U1285 G1286 A1292 U1293 G1301 C1302 U1303 U1304 A1322 A1323 C1326 G1327 A1328 U1329 U1341 C1342 C1343 C1349 G1353 U1360 U1361 U1369 A1370 G1371 U1372 C1378 A1393 A1396 U1400 A1406
A1412 A1413 C1414 A1423 U1424 U1425 C1426 A1431 C1436 C1444 U1445 U1448 A1455 C1456 A1462 G1463 U1466 U1467 C1473 C1474 C1475 C1476 A1480 U1481 U1482 G1483 U1487 G1508 U1509 A1510 A1513 U1514 A1515 C1518 A1519 G1528 U1533 A1534 A1541 U1546 G1547
A1548 U1549 G1550 A1558 A1559 U G G A G U G A U C A A1570 G1571 U1572 A1577 G1580 G1583 U1584 A1585 A1588 A1589 A1592 A1603 U1612 G1615 G1616 U1617 U1618 A1619 C1632 A1641 G1642 A1643 A1644 A1647 A1648 C1651 C1659 A1669 U1670
G1681 C1682 A1694 G1695 C1696 C1697 A1698 A1699 G1700 G1701 A1702 C1706 U1707 G1708 C1717 C1718 C1719 U1727 A1732 G1733 G1737 G1738 G1747 U1748 C1761 A1762 G1763 U1764 A1769 A1770 C1771 G1772 A1780 U1785 A1788 C1789 U1790 A1791 A1794 C1807 C1808 U1815 A1816 U1820
G1821 A1822 U1823 G1824 U1827 A1836 C1837 G1842 C1843 C1844 A1854 A1855 G1856 G1857 G1876 C1886 A1891 G1906 A1907 G1910 G1913 C1916 A1920 C1921 A1934 A1935 G1936 G1937 U1938 A1943 A1944 A1945 U1946 U1947 C1948 A1951 G1956 A1960 A1961 U1962 U1963 C1964
G1971 A1977 U1978 G1979 A1988 U1998 G1999 U2000 C2001 G2005 C2006 U2007 A2010 G2011 A2020 A2021 A2022 C2025 G2028 U2029 A2030 A2037 A2038 G2039 A2040 C2041 A2042 C2043 G2050 C2057 G2058 C2062 G2063 A2067 G2068 A2069 C2070 G2076 C2080 U2083 A2084 G2087
U2099 G2100 G2106 A2107 U2110 U2111 A2112 U2113 C2114 U2118 A2119 G2120 A2123 A2124 U2125 A2126 G2127 G2128 G2131 G2132 A2133 U2138 C2139 G2140 A2141 U2142 G2143 A2146 G2147 U2148 G2151 C2152 U2153 A2157 C2158 U2159 U2160 G2161 U2162 U2163 G2164 A2165 U2166 A2171 A2172 U2180 A2181 C2182 U2183
A2184 C2185 C2186 C2187 U2188 U2189 U2192 U2193 G2194 U2195 G2196 U2197 G2198 C2199 U2200 G2201 U2202 A2206 G2211 U2212 U2219 A2220 U2221 C2222 A2231 G2232 A2233 G2246 G2247 U2257 G2258 A2274 A2275 A2276 A2277 G2287 G2288 U2291 A2294 A2295 A2296 G2297 C2305 U2313 G2316 A2317
A2318 A2319 U2327 A2328 G2329 A2330 G2331 U2332 G2333 G2341 U2342 A2343 A2344 G2345 U2351 U2352 G2353 A2354 C2355 U2358 A2362 G2391 U2392 C2393 G2397 C2410 C2411 U2414 A2415 U2416 G2417 C2430 A2433 A2434 C2435 G2436 G2437 A2438 A2442 A2443 A2447 C2448 U2449 G2455 A2477
C2483 A2484 U2485 A2486 U2487 C2488 G2489 G2492 U2497 G2498 U2499 U2500 G2503 C2504 A2505 C2506 C2507 U2508 C2509 C2510 A2511 U2512 G2513 U2514 C2515 G2516 A2526 U2527 C2528 C2529 A2539 G2543 G2558 C2559 U2560 U2570 A2574 G2577 A2580 C2581 U2587 G2590 U2593 C2594 A2595



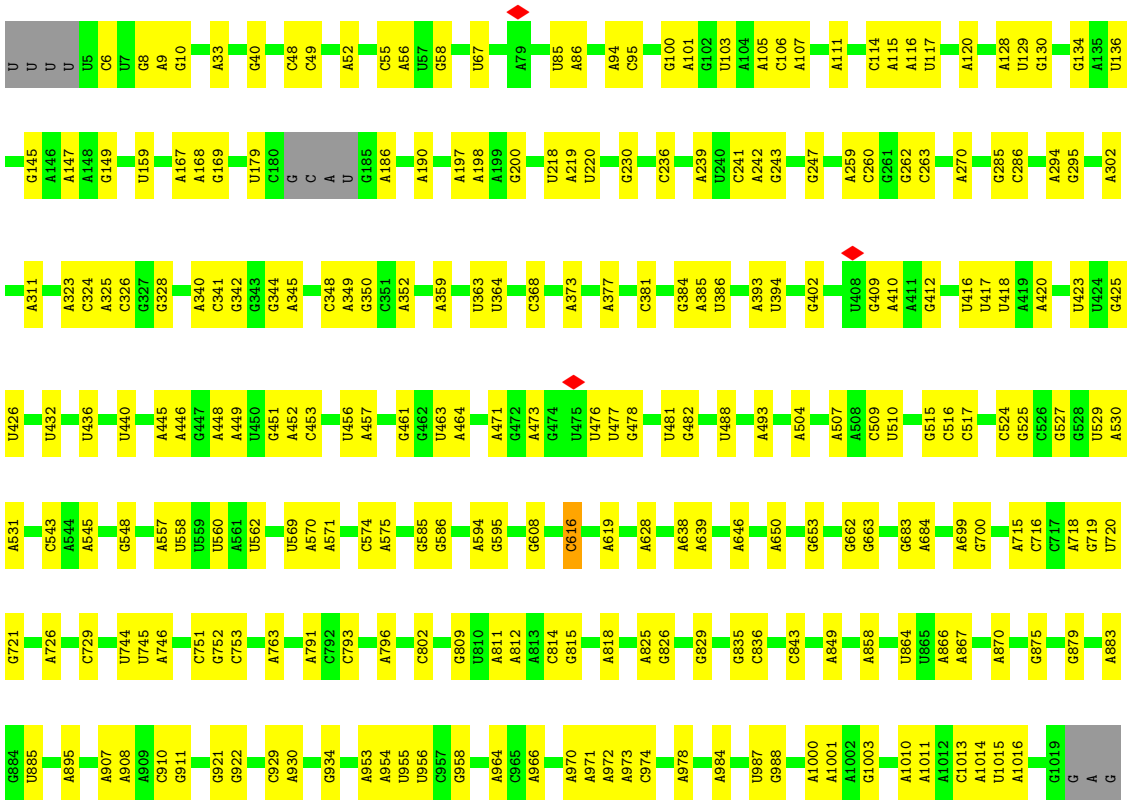

• Molecule 51: 5S ribosomal RNA

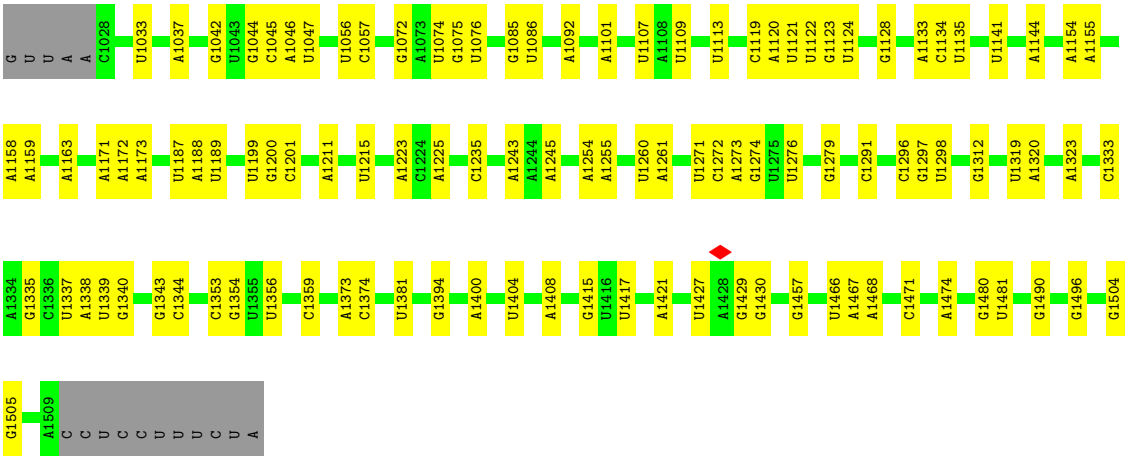
Chain 4:




• Molecule 52: 16S ribosomal RNA

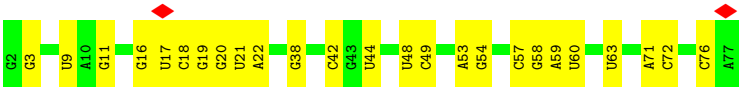
Chain 5:






- Molecule 53: tRNA-Phe

Chain 7:



# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SUBTOMOGRAM AVERAGING | Depositor |
| Imposed symmetry | POINT, C1 | Depositor |
| Number of subtomograms used | 6223 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope | FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/Å^2$) | 3.2 | Depositor |
| Minimum defocus (nm) | 1500 | Depositor |
| Maximum defocus (nm) | 3750 | Depositor |
| Magnification | 81000 | Depositor |
| Image detector | GATAN K2 SUMMIT (4k x 4k) | Depositor |
| Maximum map value | 1.902 | Depositor |
| Minimum map value | -0.783 | Depositor |
| Average map value | 0.025 | Depositor |
| Map value standard deviation | 0.128 | Depositor |
| Recommended contour level | 0.47 | Depositor |
| Map size (Å) | 435.328, 435.328, 435.328 | wwPDB |
| Map dimensions | 256, 256, 256 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 1.7005, 1.7005, 1.7005 | Depositor |

# 5 Model quality (i)

## 5.1 Standard geometry (i)

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

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | $\#\|Z\|>5$ | RMSZ | $\#\|Z\|>5$ |
| 1 | 0 | 0.23 | 0/383 | 0.41 | 0/504 |
| 2 | 1 | 0.24 | 0/484 | 0.50 | 0/637 |
| 3 | 2 | 0.23 | 0/306 | 0.48 | 0/401 |
| 4 | A | 0.24 | 0/1954 | 0.46 | 0/2642 |
| 5 | B | 0.25 | 0/1721 | 0.50 | 0/2323 |
| 6 | C | 0.25 | 0/1691 | 0.48 | 0/2267 |
| 7 | D | 0.26 | 0/1188 | 0.51 | 1/1593 (0.1%) |
| 8 | E | 0.24 | 0/1384 | 0.49 | 0/1867 |
| 9 | F | 0.26 | 0/1266 | 0.50 | 0/1700 |
| 10 | G | 0.25 | 0/1126 | 0.55 | 0/1517 |
| 11 | H | 0.24 | 0/1044 | 0.49 | 0/1395 |
| 12 | I | 0.25 | 0/820 | 0.54 | 0/1103 |
| 13 | J | 0.26 | 0/844 | 0.46 | 0/1136 |
| 14 | K | 0.27 | 0/1094 | 0.52 | 0/1468 |
| 15 | L | 0.27 | 0/962 | 0.49 | 0/1289 |
| 16 | M | 0.27 | 0/483 | 0.50 | 0/643 |
| 17 | N | 0.23 | 0/679 | 0.49 | 0/907 |
| 18 | O | 0.25 | 0/659 | 0.52 | 0/885 |
| 19 | P | 0.23 | 0/684 | 0.48 | 0/913 |
| 20 | Q | 0.27 | 0/545 | 0.54 | 0/730 |
| 21 | R | 0.26 | 0/698 | 0.47 | 0/936 |
| 22 | S | 0.25 | 0/631 | 0.49 | 0/838 |
| 23 | T | 0.27 | 0/475 | 0.52 | 0/621 |
| 24 | a | 0.23 | 0/2267 | 0.47 | 0/3044 |
| 25 | b | 0.26 | 0/1795 | 0.51 | 0/2412 |
| 26 | c | 0.26 | 0/1671 | 0.50 | 1/2246 (0.0%) |
| 27 | d | 0.25 | 0/1409 | 0.47 | 0/1894 |
| 28 | e | 0.25 | 0/1420 | 0.48 | 0/1912 |
| 29 | f | 0.27 | 0/1183 | 0.55 | 0/1587 |
| 30 | g | 0.35 | 0/969 | 0.57 | 0/1295 |
| 31 | h | 0.24 | 0/968 | 0.44 | 0/1298 |
| 32 | i | 0.24 | 0/1186 | 0.47 | 0/1592 |
| 33 | j | 0.24 | 0/953 | 0.49 | 0/1275 |
| 34 | k | 0.25 | 0/1170 | 0.50 | 0/1559 |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 35 | l | 0.26 | 0/1104 | 0.49 | 0/1481 |
| 36 | m | 0.27 | 0/973 | 0.60 | 0/1309 |
| 37 | n | 0.25 | 0/897 | 0.51 | 0/1198 |
| 38 | o | 0.26 | 0/948 | 0.50 | 0/1262 |
| 39 | p | 0.26 | 0/961 | 0.47 | 0/1278 |
| 40 | q | 0.25 | 0/828 | 0.54 | 0/1111 |
| 41 | r | 0.26 | 0/1077 | 0.51 | 0/1441 |
| 42 | s | 0.24 | 0/732 | 0.47 | 0/988 |
| 43 | t | 0.24 | 0/879 | 0.49 | 0/1165 |
| 44 | u | 0.25 | 0/665 | 0.49 | 0/884 |
| 45 | v | 0.27 | 0/519 | 0.52 | 0/695 |
| 46 | w | 0.26 | 0/826 | 0.48 | 0/1104 |
| 47 | x | 0.24 | 0/353 | 0.43 | 0/474 |
| 48 | y | 0.30 | 0/457 | 0.57 | 0/601 |
| 49 | z | 0.23 | 0/412 | 0.51 | 0/547 |
| 50 | 3 | 0.19 | 0/69073 | 0.79 | 47/107710 (0.0%) |
| 51 | 4 | 0.20 | 0/2505 | 0.81 | 4/3902 (0.1%) |
| 52 | 5 | 0.18 | 0/35768 | 0.76 | 18/55764 (0.0%) |
| 53 | 7 | 0.20 | 0/1808 | 0.83 | 0/2817 |
| All | All | 0.21 | 0/156897 | 0.71 | 71/234160 (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 |
|---|---|---|---|
| 10 | G | 0 | 1 |
| 13 | J | 0 | 1 |
| 18 | O | 0 | 1 |
| All | All | 0 | 3 |

There are no bond length outliers.

All (71) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 50 | 3 | 1718 | C | N3-C2-O2 | -11.00 | 114.20 | 121.90 |
| 50 | 3 | 2799 | U | N3-C4-O4 | -10.56 | 112.01 | 119.40 |
| 50 | 3 | 1474 | C | N3-C2-O2 | -9.37 | 115.34 | 121.90 |
| 50 | 3 | 2799 | U | C5-C4-O4 | 9.14 | 131.38 | 125.90 |
| 50 | 3 | 1159 | C | N3-C2-O2 | -8.80 | 115.74 | 121.90 |
| 52 | 5 | 843 | C | N3-C2-O2 | -8.72 | 115.80 | 121.90 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 50 | 3 | 1964 | C | N3-C2-O2 | -8.55 | 115.92 | 121.90 |
| 50 | 3 | 371 | C | N3-C2-O2 | -8.34 | 116.06 | 121.90 |
| 50 | 3 | 68 | C | N3-C2-O2 | -8.11 | 116.22 | 121.90 |
| 50 | 3 | 1719 | C | N3-C2-O2 | -7.79 | 116.45 | 121.90 |
| 51 | 4 | 78 | C | O4'-C1'-N1 | 7.79 | 114.43 | 108.20 |
| 50 | 3 | 2529 | C | N3-C2-O2 | -7.79 | 116.45 | 121.90 |
| 51 | 4 | 79 | U | C2-N1-C1' | 7.62 | 126.85 | 117.70 |
| 50 | 3 | 1718 | C | N1-C2-O2 | 7.57 | 123.44 | 118.90 |
| 50 | 3 | 2001 | C | N1-C2-O2 | 7.33 | 123.30 | 118.90 |
| 50 | 3 | 1916 | C | N3-C2-O2 | -7.05 | 116.96 | 121.90 |
| 52 | 5 | 751 | C | C2-N1-C1' | 6.80 | 126.28 | 118.80 |
| 50 | 3 | 2800 | U | C2-N1-C1' | 6.74 | 125.78 | 117.70 |
| 51 | 4 | 79 | U | N3-C2-O2 | -6.52 | 117.64 | 122.20 |
| 50 | 3 | 1474 | C | C6-N1-C2 | -6.50 | 117.70 | 120.30 |
| 51 | 4 | 79 | U | N1-C2-O2 | 6.45 | 127.32 | 122.80 |
| 50 | 3 | 2688 | C | N3-C2-O2 | -6.43 | 117.40 | 121.90 |
| 50 | 3 | 2688 | C | N1-C2-O2 | 6.41 | 122.75 | 118.90 |
| 52 | 5 | 616 | C | N1-C2-O2 | 6.29 | 122.67 | 118.90 |
| 50 | 3 | 1476 | C | N3-C2-O2 | -6.23 | 117.54 | 121.90 |
| 52 | 5 | 974 | C | C2-N1-C1' | 6.21 | 125.63 | 118.80 |
| 50 | 3 | 1159 | C | C6-N1-C2 | -6.13 | 117.85 | 120.30 |
| 52 | 5 | 974 | C | N1-C2-O2 | 6.10 | 122.56 | 118.90 |
| 50 | 3 | 371 | C | C6-N1-C2 | -5.99 | 117.90 | 120.30 |
| 52 | 5 | 463 | U | C2-N1-C1' | 5.98 | 124.87 | 117.70 |
| 50 | 3 | 2187 | C | N1-C2-O2 | 5.94 | 122.46 | 118.90 |
| 50 | 3 | 2528 | C | N1-C2-O2 | 5.92 | 122.45 | 118.90 |
| 50 | 3 | 1964 | C | N1-C2-O2 | 5.91 | 122.44 | 118.90 |
| 50 | 3 | 2735 | G | N1-C2-N2 | -5.88 | 110.91 | 116.20 |
| 50 | 3 | 1158 | C | N1-C2-O2 | 5.88 | 122.43 | 118.90 |
| 7 | D | 155 | PRO | CA-N-CD | -5.85 | 103.31 | 111.50 |
| 50 | 3 | 2305 | C | C2-N1-C1' | 5.83 | 125.22 | 118.80 |
| 50 | 3 | 1718 | C | C6-N1-C2 | -5.82 | 117.97 | 120.30 |
| 52 | 5 | 416 | U | C2-N3-C4 | -5.81 | 123.51 | 127.00 |
| 50 | 3 | 67 | C | N1-C2-O2 | 5.77 | 122.36 | 118.90 |
| 50 | 3 | 144 | C | N3-C2-O2 | -5.74 | 117.88 | 121.90 |
| 52 | 5 | 416 | U | N1-C2-N3 | 5.67 | 118.30 | 114.90 |
| 50 | 3 | 1719 | C | C6-N1-C2 | -5.64 | 118.04 | 120.30 |
| 50 | 3 | 1473 | C | N1-C2-O2 | 5.63 | 122.28 | 118.90 |
| 50 | 3 | 2800 | U | N1-C2-O2 | 5.59 | 126.71 | 122.80 |
| 50 | 3 | 1700 | G | N1-C6-O6 | -5.57 | 116.56 | 119.90 |
| 50 | 3 | 2735 | G | N3-C2-N2 | 5.53 | 123.77 | 119.90 |
| 50 | 3 | 67 | C | N3-C2-O2 | -5.53 | 118.03 | 121.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 52 | 5 | 616 | C | C2-N1-C1' | 5.50 | 124.85 | 118.80 |
| 52 | 5 | 843 | C | N1-C2-O2 | 5.49 | 122.19 | 118.90 |
| 50 | 3 | 2001 | C | N3-C2-O2 | -5.47 | 118.07 | 121.90 |
| 50 | 3 | 1717 | C | N1-C2-O2 | 5.45 | 122.17 | 118.90 |
| 52 | 5 | 463 | U | N1-C2-O2 | 5.43 | 126.60 | 122.80 |
| 50 | 3 | 426 | U | C2-N1-C1' | 5.41 | 124.19 | 117.70 |
| 52 | 5 | 751 | C | C6-N1-C1' | -5.40 | 114.32 | 120.80 |
| 52 | 5 | 835 | G | N1-C6-O6 | -5.38 | 116.67 | 119.90 |
| 52 | 5 | 835 | G | C5-C6-O6 | 5.38 | 131.83 | 128.60 |
| 52 | 5 | 751 | C | N1-C2-O2 | 5.33 | 122.10 | 118.90 |
| 50 | 3 | 2689 | C | N3-C2-O2 | -5.31 | 118.19 | 121.90 |
| 52 | 5 | 616 | C | N3-C2-O2 | -5.30 | 118.19 | 121.90 |
| 50 | 3 | 1476 | C | C6-N1-C2 | -5.18 | 118.23 | 120.30 |
| 50 | 3 | 1886 | C | N3-C2-O2 | -5.18 | 118.28 | 121.90 |
| 50 | 3 | 2005 | G | N1-C6-O6 | -5.17 | 116.80 | 119.90 |
| 52 | 5 | 1042 | G | N1-C6-O6 | -5.15 | 116.81 | 119.90 |
| 26 | c | 93 | PRO | N-CD-CG | -5.13 | 95.50 | 103.20 |
| 50 | 3 | 1738 | G | N1-C2-N2 | -5.11 | 111.61 | 116.20 |
| 50 | 3 | 187 | C | C2-N1-C1' | 5.09 | 124.40 | 118.80 |
| 50 | 3 | 2800 | U | N3-C2-O2 | -5.09 | 118.64 | 122.20 |
| 52 | 5 | 463 | U | N3-C2-O2 | -5.08 | 118.64 | 122.20 |
| 50 | 3 | 1159 | C | N1-C2-O2 | 5.03 | 121.92 | 118.90 |
| 50 | 3 | 1341 | U | C2-N1-C1' | 5.03 | 123.74 | 117.70 |

There are no chirality outliers.

All (3) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 10 | G | 108 | LEU | Peptide |
| 13 | J | 111 | HIS | Peptide |
| 18 | O | 39 | GLU | Peptide |

## 5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 5.3 Torsion angles (i)

### 5.3.1 Protein backbone (i)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 1 | 0 | 45/48 (94%) | 44 (98%) | 1 (2%) | 0 | 100 | 100 |
| 2 | 1 | 57/59 (97%) | 54 (95%) | 3 (5%) | 0 | 100 | 100 |
| 3 | 2 | 35/37 (95%) | 33 (94%) | 2 (6%) | 0 | 100 | 100 |
| 4 | A | 238/294 (81%) | 222 (93%) | 16 (7%) | 0 | 100 | 100 |
| 5 | B | 213/273 (78%) | 196 (92%) | 17 (8%) | 0 | 100 | 100 |
| 6 | C | 201/205 (98%) | 191 (95%) | 10 (5%) | 0 | 100 | 100 |
| 7 | D | 151/219 (69%) | 145 (96%) | 6 (4%) | 0 | 100 | 100 |
| 8 | E | 165/215 (77%) | 147 (89%) | 18 (11%) | 0 | 100 | 100 |
| 9 | F | 152/155 (98%) | 135 (89%) | 17 (11%) | 0 | 100 | 100 |
| 10 | G | 139/142 (98%) | 125 (90%) | 14 (10%) | 0 | 100 | 100 |
| 11 | H | 126/132 (96%) | 115 (91%) | 11 (9%) | 0 | 100 | 100 |
| 12 | I | 99/108 (92%) | 87 (88%) | 12 (12%) | 0 | 100 | 100 |
| 13 | J | 112/121 (93%) | 105 (94%) | 7 (6%) | 0 | 100 | 100 |
| 14 | K | 134/139 (96%) | 125 (93%) | 9 (7%) | 0 | 100 | 100 |
| 15 | L | 116/124 (94%) | 104 (90%) | 12 (10%) | 0 | 100 | 100 |
| 16 | M | 58/61 (95%) | 56 (97%) | 2 (3%) | 0 | 100 | 100 |
| 17 | N | 81/86 (94%) | 81 (100%) | 0 | 0 | 100 | 100 |
| 18 | O | 78/94 (83%) | 70 (90%) | 8 (10%) | 0 | 100 | 100 |
| 19 | P | 81/85 (95%) | 78 (96%) | 3 (4%) | 0 | 100 | 100 |
| 20 | Q | 63/104 (61%) | 51 (81%) | 12 (19%) | 0 | 100 | 100 |
| 21 | R | 82/87 (94%) | 73 (89%) | 9 (11%) | 0 | 100 | 100 |
| 22 | S | 75/87 (86%) | 74 (99%) | 1 (1%) | 0 | 100 | 100 |
| 23 | T | 51/60 (85%) | 50 (98%) | 1 (2%) | 0 | 100 | 100 |
| 24 | a | 283/287 (99%) | 265 (94%) | 18 (6%) | 0 | 100 | 100 |
| 25 | b | 227/287 (79%) | 214 (94%) | 13 (6%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 26 | c | 208/212 (98%) | 197 (95%) | 11 (5%) | 0 | 100 | 100 |
| 27 | d | 173/180 (96%) | 160 (92%) | 13 (8%) | 0 | 100 | 100 |
| 28 | e | 174/184 (95%) | 166 (95%) | 8 (5%) | 0 | 100 | 100 |
| 29 | f | 143/149 (96%) | 125 (87%) | 18 (13%) | 0 | 100 | 100 |
| 30 | g | 124/161 (77%) | 109 (88%) | 13 (10%) | 2 (2%) | 9 | 44 |
| 31 | h | 126/137 (92%) | 114 (90%) | 12 (10%) | 0 | 100 | 100 |
| 32 | i | 142/146 (97%) | 136 (96%) | 6 (4%) | 0 | 100 | 100 |
| 33 | j | 120/122 (98%) | 113 (94%) | 7 (6%) | 0 | 100 | 100 |
| 34 | k | 146/151 (97%) | 139 (95%) | 7 (5%) | 0 | 100 | 100 |
| 35 | l | 134/139 (96%) | 124 (92%) | 10 (8%) | 0 | 100 | 100 |
| 36 | m | 117/124 (94%) | 108 (92%) | 9 (8%) | 0 | 100 | 100 |
| 37 | n | 108/116 (93%) | 99 (92%) | 9 (8%) | 0 | 100 | 100 |
| 38 | o | 113/119 (95%) | 101 (89%) | 12 (11%) | 0 | 100 | 100 |
| 39 | p | 112/127 (88%) | 108 (96%) | 4 (4%) | 0 | 100 | 100 |
| 40 | q | 97/100 (97%) | 90 (93%) | 7 (7%) | 0 | 100 | 100 |
| 41 | r | 137/159 (86%) | 134 (98%) | 3 (2%) | 0 | 100 | 100 |
| 42 | s | 90/237 (38%) | 88 (98%) | 2 (2%) | 0 | 100 | 100 |
| 43 | t | 109/111 (98%) | 104 (95%) | 5 (5%) | 0 | 100 | 100 |
| 44 | u | 84/104 (81%) | 81 (96%) | 3 (4%) | 0 | 100 | 100 |
| 45 | v | 61/65 (94%) | 59 (97%) | 2 (3%) | 0 | 100 | 100 |
| 46 | w | 96/111 (86%) | 89 (93%) | 7 (7%) | 0 | 100 | 100 |
| 47 | x | 42/97 (43%) | 35 (83%) | 7 (17%) | 0 | 100 | 100 |
| 48 | y | 54/57 (95%) | 52 (96%) | 2 (4%) | 0 | 100 | 100 |
| 49 | z | 48/53 (91%) | 47 (98%) | 1 (2%) | 0 | 100 | 100 |
| All | All | 5820/6670 (87%) | 5418 (93%) | 400 (7%) | 2 (0%) | 100 | 100 |

All (2) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 30 | g | 88 | GLU |
| 30 | g | 42 | LYS |

### 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 | |
|---|---|---|---|---|---|---|
| 1 | 0 | 40/41 (98%) | 40 (100%) | 0 | 100 | 100 |
| 2 | 1 | 51/51 (100%) | 50 (98%) | 1 (2%) | 55 | 74 |
| 3 | 2 | 35/35 (100%) | 35 (100%) | 0 | 100 | 100 |
| 4 | A | 212/262 (81%) | 211 (100%) | 1 (0%) | 88 | 93 |
| 5 | B | 180/232 (78%) | 180 (100%) | 0 | 100 | 100 |
| 6 | C | 181/183 (99%) | 180 (99%) | 1 (1%) | 86 | 92 |
| 7 | D | 123/178 (69%) | 122 (99%) | 1 (1%) | 81 | 89 |
| 8 | E | 150/196 (76%) | 148 (99%) | 2 (1%) | 69 | 82 |
| 9 | F | 131/132 (99%) | 131 (100%) | 0 | 100 | 100 |
| 10 | G | 123/124 (99%) | 122 (99%) | 1 (1%) | 81 | 89 |
| 11 | H | 111/115 (96%) | 110 (99%) | 1 (1%) | 78 | 87 |
| 12 | I | 95/99 (96%) | 95 (100%) | 0 | 100 | 100 |
| 13 | J | 91/97 (94%) | 90 (99%) | 1 (1%) | 73 | 84 |
| 14 | K | 117/120 (98%) | 113 (97%) | 4 (3%) | 37 | 60 |
| 15 | L | 100/105 (95%) | 98 (98%) | 2 (2%) | 55 | 74 |
| 16 | M | 47/48 (98%) | 47 (100%) | 0 | 100 | 100 |
| 17 | N | 76/78 (97%) | 76 (100%) | 0 | 100 | 100 |
| 18 | O | 69/82 (84%) | 69 (100%) | 0 | 100 | 100 |
| 19 | P | 73/75 (97%) | 71 (97%) | 2 (3%) | 44 | 65 |
| 20 | Q | 56/94 (60%) | 55 (98%) | 1 (2%) | 59 | 77 |
| 21 | R | 74/77 (96%) | 74 (100%) | 0 | 100 | 100 |
| 22 | S | 70/77 (91%) | 69 (99%) | 1 (1%) | 67 | 80 |
| 23 | T | 49/56 (88%) | 49 (100%) | 0 | 100 | 100 |
| 24 | a | 241/243 (99%) | 241 (100%) | 0 | 100 | 100 |
| 25 | b | 186/233 (80%) | 185 (100%) | 1 (0%) | 88 | 93 |
| 26 | c | 182/184 (99%) | 182 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 27 | d | 150/154 (97%) | 150 (100%) | 0 | 100 | 100 |
| 28 | e | 153/159 (96%) | 153 (100%) | 0 | 100 | 100 |
| 29 | f | 123/134 (92%) | 121 (98%) | 2 (2%) | 62 | 79 |
| 30 | g | 101/129 (78%) | 91 (90%) | 10 (10%) | 8 | 26 |
| 31 | h | 102/110 (93%) | 102 (100%) | 0 | 100 | 100 |
| 32 | i | 126/128 (98%) | 126 (100%) | 0 | 100 | 100 |
| 33 | j | 103/103 (100%) | 103 (100%) | 0 | 100 | 100 |
| 34 | k | 123/126 (98%) | 123 (100%) | 0 | 100 | 100 |
| 35 | l | 113/115 (98%) | 112 (99%) | 1 (1%) | 78 | 87 |
| 36 | m | 105/109 (96%) | 104 (99%) | 1 (1%) | 76 | 86 |
| 37 | n | 96/99 (97%) | 96 (100%) | 0 | 100 | 100 |
| 38 | o | 101/105 (96%) | 99 (98%) | 2 (2%) | 55 | 74 |
| 39 | p | 100/108 (93%) | 100 (100%) | 0 | 100 | 100 |
| 40 | q | 90/91 (99%) | 90 (100%) | 0 | 100 | 100 |
| 41 | r | 116/132 (88%) | 114 (98%) | 2 (2%) | 60 | 78 |
| 42 | s | 82/208 (39%) | 82 (100%) | 0 | 100 | 100 |
| 43 | t | 96/96 (100%) | 96 (100%) | 0 | 100 | 100 |
| 44 | u | 69/85 (81%) | 69 (100%) | 0 | 100 | 100 |
| 45 | v | 58/60 (97%) | 57 (98%) | 1 (2%) | 60 | 78 |
| 46 | w | 87/98 (89%) | 87 (100%) | 0 | 100 | 100 |
| 47 | x | 41/86 (48%) | 41 (100%) | 0 | 100 | 100 |
| 48 | y | 48/49 (98%) | 45 (94%) | 3 (6%) | 18 | 43 |
| 49 | z | 47/50 (94%) | 47 (100%) | 0 | 100 | 100 |
| All | All | 5093/5751 (89%) | 5051 (99%) | 42 (1%) | 82 | 89 |

All (42) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | 1 | 39 | ARG |
| 4 | A | 185 | LYS |
| 6 | C | 41 | ARG |
| 7 | D | 75 | ARG |
| 8 | E | 70 | LYS |
| 8 | E | 145 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 10 | G | 68 | ARG |
| 11 | H | 115 | ARG |
| 13 | J | 80 | LYS |
| 14 | K | 44 | ARG |
| 14 | K | 120 | VAL |
| 14 | K | 121 | GLU |
| 14 | K | 122 | LYS |
| 15 | L | 70 | ARG |
| 15 | L | 91 | HIS |
| 19 | P | 6 | ARG |
| 19 | P | 83 | ARG |
| 20 | Q | 84 | ARG |
| 22 | S | 9 | LYS |
| 25 | b | 125 | ARG |
| 29 | f | 95 | LYS |
| 29 | f | 114 | LYS |
| 30 | g | 27 | PHE |
| 30 | g | 30 | THR |
| 30 | g | 31 | SER |
| 30 | g | 42 | LYS |
| 30 | g | 43 | LYS |
| 30 | g | 44 | LEU |
| 30 | g | 46 | LYS |
| 30 | g | 84 | VAL |
| 30 | g | 88 | GLU |
| 30 | g | 89 | ILE |
| 35 | l | 60 | LYS |
| 36 | m | 30 | LYS |
| 38 | o | 54 | ARG |
| 38 | o | 107 | ARG |
| 41 | r | 64 | MET |
| 41 | r | 126 | LYS |
| 45 | v | 27 | ARG |
| 48 | y | 47 | MET |
| 48 | y | 48 | TYR |
| 48 | y | 52 | ARG |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | 1 | 44 | GLN |
| 4 | A | 63 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 4 | A | 70 | ASN |
| 5 | B | 193 | GLN |
| 8 | E | 17 | GLN |
| 9 | F | 85 | GLN |
| 11 | H | 77 | GLN |
| 14 | K | 86 | ASN |
| 14 | K | 88 | GLN |
| 17 | N | 39 | HIS |
| 20 | Q | 82 | HIS |
| 21 | R | 47 | ASN |
| 22 | S | 20 | ASN |
| 23 | T | 8 | ASN |
| 24 | a | 62 | ASN |
| 24 | a | 159 | GLN |
| 26 | c | 104 | ASN |
| 28 | e | 68 | HIS |
| 28 | e | 72 | ASN |
| 33 | j | 18 | GLN |
| 36 | m | 117 | GLN |
| 40 | q | 79 | HIS |
| 41 | r | 52 | ASN |
| 41 | r | 94 | ASN |
| 42 | s | 19 | ASN |
| 45 | v | 6 | GLN |
| 45 | v | 16 | ASN |

### 5.3.3 RNA (i)

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|---|---|---|---|---|
| 50 | 3 | 2875/2907 (98%) | 733 (25%) | 25 (0%) |
| 51 | 4 | 103/108 (95%) | 34 (33%) | 5 (4%) |
| 52 | 5 | 1490/1520 (98%) | 349 (23%) | 6 (0%) |
| 53 | 7 | 75/76 (98%) | 25 (33%) | 2 (2%) |
| All | All | 4543/4611 (98%) | 1141 (25%) | 38 (0%) |

All (1141) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 50 | 3 | 12 | A |
| 50 | 3 | 14 | U |
| 50 | 3 | 15 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 50 | 3 | 17 | G |
| 50 | 3 | 29 | G |
| 50 | 3 | 37 | G |
| 50 | 3 | 47 | G |
| 50 | 3 | 48 | G |
| 50 | 3 | 51 | A |
| 50 | 3 | 53 | G |
| 50 | 3 | 54 | A |
| 50 | 3 | 63 | U |
| 50 | 3 | 65 | A |
| 50 | 3 | 73 | A |
| 50 | 3 | 75 | A |
| 50 | 3 | 76 | A |
| 50 | 3 | 77 | G |
| 50 | 3 | 82 | G |
| 50 | 3 | 86 | A |
| 50 | 3 | 92 | U |
| 50 | 3 | 102 | A |
| 50 | 3 | 103 | G |
| 50 | 3 | 112 | A |
| 50 | 3 | 115 | U |
| 50 | 3 | 116 | C |
| 50 | 3 | 119 | A |
| 50 | 3 | 120 | A |
| 50 | 3 | 121 | U |
| 50 | 3 | 122 | G |
| 50 | 3 | 126 | C |
| 50 | 3 | 129 | U |
| 50 | 3 | 132 | G |
| 50 | 3 | 141 | A |
| 50 | 3 | 143 | A |
| 50 | 3 | 148 | U |
| 50 | 3 | 165 | U |
| 50 | 3 | 178 | A |
| 50 | 3 | 180 | A |
| 50 | 3 | 184 | A |
| 50 | 3 | 185 | U |
| 50 | 3 | 186 | A |
| 50 | 3 | 187 | C |
| 50 | 3 | 188 | G |
| 50 | 3 | 200 | A |
| 50 | 3 | 208 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 50 | 3 | 219 | G |
| 50 | 3 | 220 | A |
| 50 | 3 | 226 | A |
| 50 | 3 | 230 | G |
| 50 | 3 | 232 | A |
| 50 | 3 | 234 | G |
| 50 | 3 | 237 | A |
| 50 | 3 | 245 | U |
| 50 | 3 | 246 | G |
| 50 | 3 | 252 | G |
| 50 | 3 | 254 | G |
| 50 | 3 | 256 | G |
| 50 | 3 | 269 | A |
| 50 | 3 | 270 | G |
| 50 | 3 | 276 | A |
| 50 | 3 | 284 | U |
| 50 | 3 | 287 | G |
| 50 | 3 | 295 | U |
| 50 | 3 | 296 | U |
| 50 | 3 | 297 | G |
| 50 | 3 | 298 | U |
| 50 | 3 | 299 | A |
| 50 | 3 | 309 | A |
| 50 | 3 | 310 | U |
| 50 | 3 | 312 | U |
| 50 | 3 | 314 | G |
| 50 | 3 | 315 | A |
| 50 | 3 | 319 | G |
| 50 | 3 | 325 | G |
| 50 | 3 | 334 | A |
| 50 | 3 | 336 | C |
| 50 | 3 | 341 | G |
| 50 | 3 | 345 | A |
| 50 | 3 | 346 | G |
| 50 | 3 | 347 | C |
| 50 | 3 | 351 | G |
| 50 | 3 | 357 | A |
| 50 | 3 | 358 | A |
| 50 | 3 | 363 | G |
| 50 | 3 | 364 | A |
| 50 | 3 | 367 | G |
| 50 | 3 | 369 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 50 | 3 | 374 | A |
| 50 | 3 | 380 | A |
| 50 | 3 | 401 | G |
| 50 | 3 | 402 | A |
| 50 | 3 | 403 | U |
| 50 | 3 | 404 | C |
| 50 | 3 | 409 | A |
| 50 | 3 | 410 | G |
| 50 | 3 | 411 | U |
| 50 | 3 | 422 | A |
| 50 | 3 | 425 | U |
| 50 | 3 | 426 | U |
| 50 | 3 | 432 | G |
| 50 | 3 | 437 | A |
| 50 | 3 | 439 | U |
| 50 | 3 | 440 | C |
| 50 | 3 | 441 | U |
| 50 | 3 | 447 | G |
| 50 | 3 | 448 | A |
| 50 | 3 | 449 | C |
| 50 | 3 | 457 | U |
| 50 | 3 | 460 | G |
| 50 | 3 | 464 | A |
| 50 | 3 | 465 | A |
| 50 | 3 | 466 | A |
| 50 | 3 | 467 | U |
| 50 | 3 | 480 | C |
| 50 | 3 | 482 | G |
| 50 | 3 | 484 | U |
| 50 | 3 | 485 | A |
| 50 | 3 | 487 | C |
| 50 | 3 | 491 | A |
| 50 | 3 | 492 | C |
| 50 | 3 | 495 | U |
| 50 | 3 | 500 | U |
| 50 | 3 | 501 | G |
| 50 | 3 | 509 | G |
| 50 | 3 | 514 | A |
| 50 | 3 | 515 | A |
| 50 | 3 | 516 | A |
| 50 | 3 | 517 | G |
| 50 | 3 | 519 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 50 | 3 | 527 | A |
| 50 | 3 | 540 | A |
| 50 | 3 | 543 | U |
| 50 | 3 | 544 | U |
| 50 | 3 | 545 | C |
| 50 | 3 | 565 | C |
| 50 | 3 | 566 | G |
| 50 | 3 | 567 | U |
| 50 | 3 | 581 | A |
| 50 | 3 | 582 | A |
| 50 | 3 | 583 | U |
| 50 | 3 | 595 | U |
| 50 | 3 | 596 | G |
| 50 | 3 | 599 | U |
| 50 | 3 | 601 | U |
| 50 | 3 | 605 | A |
| 50 | 3 | 606 | G |
| 50 | 3 | 607 | U |
| 50 | 3 | 608 | A |
| 50 | 3 | 610 | G |
| 50 | 3 | 616 | G |
| 50 | 3 | 620 | G |
| 50 | 3 | 623 | A |
| 50 | 3 | 636 | U |
| 50 | 3 | 637 | U |
| 50 | 3 | 638 | A |
| 50 | 3 | 663 | A |
| 50 | 3 | 668 | A |
| 50 | 3 | 670 | G |
| 50 | 3 | 673 | A |
| 50 | 3 | 681 | A |
| 50 | 3 | 682 | A |
| 50 | 3 | 689 | U |
| 50 | 3 | 690 | U |
| 50 | 3 | 691 | G |
| 50 | 3 | 694 | U |
| 50 | 3 | 695 | G |
| 50 | 3 | 701 | A |
| 50 | 3 | 702 | U |
| 50 | 3 | 705 | A |
| 50 | 3 | 706 | C |
| 50 | 3 | 712 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 50 | 3 | 721 | G |
| 50 | 3 | 722 | C |
| 50 | 3 | 730 | G |
| 50 | 3 | 737 | U |
| 50 | 3 | 740 | A |
| 50 | 3 | 752 | C |
| 50 | 3 | 761 | G |
| 50 | 3 | 763 | G |
| 50 | 3 | 764 | G |
| 50 | 3 | 765 | A |
| 50 | 3 | 769 | A |
| 50 | 3 | 775 | C |
| 50 | 3 | 782 | U |
| 50 | 3 | 790 | U |
| 50 | 3 | 792 | G |
| 50 | 3 | 798 | G |
| 50 | 3 | 799 | A |
| 50 | 3 | 800 | C |
| 50 | 3 | 801 | U |
| 50 | 3 | 810 | G |
| 50 | 3 | 811 | G |
| 50 | 3 | 815 | G |
| 50 | 3 | 816 | A |
| 50 | 3 | 817 | A |
| 50 | 3 | 819 | U |
| 50 | 3 | 820 | U |
| 50 | 3 | 824 | A |
| 50 | 3 | 825 | U |
| 50 | 3 | 827 | G |
| 50 | 3 | 828 | A |
| 50 | 3 | 829 | A |
| 50 | 3 | 840 | G |
| 50 | 3 | 841 | C |
| 50 | 3 | 846 | U |
| 50 | 3 | 847 | C |
| 50 | 3 | 850 | G |
| 50 | 3 | 854 | A |
| 50 | 3 | 855 | A |
| 50 | 3 | 862 | U |
| 50 | 3 | 863 | U |
| 50 | 3 | 865 | A |
| 50 | 3 | 873 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 50 | 3 | 881 | A |
| 50 | 3 | 882 | C |
| 50 | 3 | 883 | A |
| 50 | 3 | 893 | A |
| 50 | 3 | 895 | G |
| 50 | 3 | 902 | U |
| 50 | 3 | 903 | A |
| 50 | 3 | 904 | C |
| 50 | 3 | 906 | G |
| 50 | 3 | 917 | G |
| 50 | 3 | 918 | G |
| 50 | 3 | 931 | G |
| 50 | 3 | 932 | U |
| 50 | 3 | 944 | U |
| 50 | 3 | 947 | A |
| 50 | 3 | 949 | C |
| 50 | 3 | 951 | C |
| 50 | 3 | 977 | A |
| 50 | 3 | 980 | C |
| 50 | 3 | 981 | A |
| 50 | 3 | 982 | G |
| 50 | 3 | 989 | G |
| 50 | 3 | 991 | G |
| 50 | 3 | 993 | A |
| 50 | 3 | 995 | A |
| 50 | 3 | 997 | G |
| 50 | 3 | 1009 | A |
| 50 | 3 | 1013 | G |
| 50 | 3 | 1016 | A |
| 50 | 3 | 1019 | A |
| 50 | 3 | 1021 | C |
| 50 | 3 | 1022 | C |
| 50 | 3 | 1024 | A |
| 50 | 3 | 1026 | A |
| 50 | 3 | 1027 | U |
| 50 | 3 | 1032 | A |
| 50 | 3 | 1042 | C |
| 50 | 3 | 1044 | C |
| 50 | 3 | 1045 | A |
| 50 | 3 | 1049 | U |
| 50 | 3 | 1055 | A |
| 50 | 3 | 1061 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 50 | 3 | 1068 | U |
| 50 | 3 | 1075 | G |
| 50 | 3 | 1080 | A |
| 50 | 3 | 1081 | A |
| 50 | 3 | 1083 | A |
| 50 | 3 | 1092 | A |
| 50 | 3 | 1095 | U |
| 50 | 3 | 1096 | U |
| 50 | 3 | 1100 | U |
| 50 | 3 | 1102 | A |
| 50 | 3 | 1105 | A |
| 50 | 3 | 1106 | G |
| 50 | 3 | 1113 | U |
| 50 | 3 | 1124 | G |
| 50 | 3 | 1125 | U |
| 50 | 3 | 1129 | U |
| 50 | 3 | 1140 | U |
| 50 | 3 | 1145 | G |
| 50 | 3 | 1147 | G |
| 50 | 3 | 1150 | U |
| 50 | 3 | 1151 | U |
| 50 | 3 | 1155 | G |
| 50 | 3 | 1157 | G |
| 50 | 3 | 1162 | A |
| 50 | 3 | 1165 | U |
| 50 | 3 | 1167 | U |
| 50 | 3 | 1168 | A |
| 50 | 3 | 1169 | A |
| 50 | 3 | 1170 | C |
| 50 | 3 | 1171 | G |
| 50 | 3 | 1176 | U |
| 50 | 3 | 1177 | A |
| 50 | 3 | 1178 | A |
| 50 | 3 | 1184 | U |
| 50 | 3 | 1186 | A |
| 50 | 3 | 1203 | G |
| 50 | 3 | 1204 | A |
| 50 | 3 | 1208 | A |
| 50 | 3 | 1209 | U |
| 50 | 3 | 1210 | A |
| 50 | 3 | 1212 | C |
| 50 | 3 | 1215 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 50 | 3 | 1217 | G |
| 50 | 3 | 1222 | A |
| 50 | 3 | 1226 | G |
| 50 | 3 | 1234 | U |
| 50 | 3 | 1236 | G |
| 50 | 3 | 1248 | A |
| 50 | 3 | 1250 | A |
| 50 | 3 | 1251 | G |
| 50 | 3 | 1252 | C |
| 50 | 3 | 1255 | G |
| 50 | 3 | 1256 | A |
| 50 | 3 | 1257 | G |
| 50 | 3 | 1259 | A |
| 50 | 3 | 1266 | G |
| 50 | 3 | 1268 | U |
| 50 | 3 | 1278 | G |
| 50 | 3 | 1279 | U |
| 50 | 3 | 1280 | G |
| 50 | 3 | 1281 | A |
| 50 | 3 | 1283 | A |
| 50 | 3 | 1285 | U |
| 50 | 3 | 1286 | G |
| 50 | 3 | 1292 | A |
| 50 | 3 | 1293 | U |
| 50 | 3 | 1301 | G |
| 50 | 3 | 1302 | C |
| 50 | 3 | 1303 | U |
| 50 | 3 | 1304 | U |
| 50 | 3 | 1322 | A |
| 50 | 3 | 1323 | A |
| 50 | 3 | 1326 | C |
| 50 | 3 | 1328 | A |
| 50 | 3 | 1329 | U |
| 50 | 3 | 1341 | U |
| 50 | 3 | 1342 | C |
| 50 | 3 | 1343 | C |
| 50 | 3 | 1349 | C |
| 50 | 3 | 1353 | G |
| 50 | 3 | 1360 | U |
| 50 | 3 | 1361 | U |
| 50 | 3 | 1369 | U |
| 50 | 3 | 1370 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 50 | 3 | 1371 | G |
| 50 | 3 | 1372 | U |
| 50 | 3 | 1378 | C |
| 50 | 3 | 1393 | A |
| 50 | 3 | 1396 | A |
| 50 | 3 | 1400 | U |
| 50 | 3 | 1406 | A |
| 50 | 3 | 1412 | A |
| 50 | 3 | 1414 | C |
| 50 | 3 | 1423 | A |
| 50 | 3 | 1424 | U |
| 50 | 3 | 1425 | U |
| 50 | 3 | 1426 | C |
| 50 | 3 | 1431 | A |
| 50 | 3 | 1436 | C |
| 50 | 3 | 1444 | C |
| 50 | 3 | 1445 | U |
| 50 | 3 | 1448 | U |
| 50 | 3 | 1455 | A |
| 50 | 3 | 1456 | C |
| 50 | 3 | 1462 | A |
| 50 | 3 | 1463 | G |
| 50 | 3 | 1466 | U |
| 50 | 3 | 1467 | U |
| 50 | 3 | 1480 | A |
| 50 | 3 | 1481 | U |
| 50 | 3 | 1483 | G |
| 50 | 3 | 1487 | U |
| 50 | 3 | 1508 | G |
| 50 | 3 | 1510 | A |
| 50 | 3 | 1513 | A |
| 50 | 3 | 1515 | A |
| 50 | 3 | 1518 | C |
| 50 | 3 | 1519 | A |
| 50 | 3 | 1528 | G |
| 50 | 3 | 1534 | A |
| 50 | 3 | 1541 | A |
| 50 | 3 | 1546 | U |
| 50 | 3 | 1548 | A |
| 50 | 3 | 1549 | U |
| 50 | 3 | 1550 | G |
| 50 | 3 | 1558 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 50 | 3 | 1559 | A |
| 50 | 3 | 1571 | G |
| 50 | 3 | 1572 | U |
| 50 | 3 | 1577 | A |
| 50 | 3 | 1580 | G |
| 50 | 3 | 1583 | G |
| 50 | 3 | 1584 | U |
| 50 | 3 | 1585 | A |
| 50 | 3 | 1589 | A |
| 50 | 3 | 1592 | A |
| 50 | 3 | 1603 | A |
| 50 | 3 | 1612 | U |
| 50 | 3 | 1615 | G |
| 50 | 3 | 1616 | G |
| 50 | 3 | 1618 | U |
| 50 | 3 | 1619 | A |
| 50 | 3 | 1632 | C |
| 50 | 3 | 1641 | A |
| 50 | 3 | 1642 | G |
| 50 | 3 | 1643 | A |
| 50 | 3 | 1644 | A |
| 50 | 3 | 1647 | A |
| 50 | 3 | 1648 | A |
| 50 | 3 | 1651 | C |
| 50 | 3 | 1659 | C |
| 50 | 3 | 1669 | A |
| 50 | 3 | 1670 | U |
| 50 | 3 | 1681 | G |
| 50 | 3 | 1682 | C |
| 50 | 3 | 1694 | A |
| 50 | 3 | 1695 | G |
| 50 | 3 | 1697 | C |
| 50 | 3 | 1698 | A |
| 50 | 3 | 1699 | A |
| 50 | 3 | 1702 | A |
| 50 | 3 | 1706 | C |
| 50 | 3 | 1707 | U |
| 50 | 3 | 1708 | G |
| 50 | 3 | 1727 | U |
| 50 | 3 | 1732 | A |
| 50 | 3 | 1733 | G |
| 50 | 3 | 1737 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 50 | 3 | 1747 | G |
| 50 | 3 | 1748 | U |
| 50 | 3 | 1761 | C |
| 50 | 3 | 1763 | G |
| 50 | 3 | 1764 | U |
| 50 | 3 | 1769 | A |
| 50 | 3 | 1770 | A |
| 50 | 3 | 1771 | C |
| 50 | 3 | 1772 | G |
| 50 | 3 | 1780 | A |
| 50 | 3 | 1785 | U |
| 50 | 3 | 1788 | A |
| 50 | 3 | 1790 | U |
| 50 | 3 | 1791 | A |
| 50 | 3 | 1794 | A |
| 50 | 3 | 1807 | C |
| 50 | 3 | 1808 | C |
| 50 | 3 | 1815 | U |
| 50 | 3 | 1816 | A |
| 50 | 3 | 1821 | G |
| 50 | 3 | 1822 | A |
| 50 | 3 | 1823 | U |
| 50 | 3 | 1824 | G |
| 50 | 3 | 1827 | U |
| 50 | 3 | 1836 | A |
| 50 | 3 | 1837 | C |
| 50 | 3 | 1842 | G |
| 50 | 3 | 1844 | C |
| 50 | 3 | 1854 | A |
| 50 | 3 | 1855 | A |
| 50 | 3 | 1857 | G |
| 50 | 3 | 1876 | G |
| 50 | 3 | 1891 | A |
| 50 | 3 | 1906 | G |
| 50 | 3 | 1907 | A |
| 50 | 3 | 1910 | G |
| 50 | 3 | 1913 | G |
| 50 | 3 | 1920 | A |
| 50 | 3 | 1921 | C |
| 50 | 3 | 1934 | A |
| 50 | 3 | 1936 | G |
| 50 | 3 | 1937 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 50 | 3 | 1938 | U |
| 50 | 3 | 1943 | A |
| 50 | 3 | 1944 | A |
| 50 | 3 | 1945 | A |
| 50 | 3 | 1947 | U |
| 50 | 3 | 1948 | C |
| 50 | 3 | 1951 | A |
| 50 | 3 | 1956 | G |
| 50 | 3 | 1960 | A |
| 50 | 3 | 1962 | U |
| 50 | 3 | 1971 | G |
| 50 | 3 | 1977 | A |
| 50 | 3 | 1978 | U |
| 50 | 3 | 1979 | G |
| 50 | 3 | 1988 | A |
| 50 | 3 | 1998 | U |
| 50 | 3 | 1999 | G |
| 50 | 3 | 2000 | U |
| 50 | 3 | 2007 | U |
| 50 | 3 | 2010 | A |
| 50 | 3 | 2011 | G |
| 50 | 3 | 2020 | A |
| 50 | 3 | 2022 | A |
| 50 | 3 | 2025 | C |
| 50 | 3 | 2028 | G |
| 50 | 3 | 2030 | A |
| 50 | 3 | 2037 | A |
| 50 | 3 | 2038 | A |
| 50 | 3 | 2040 | A |
| 50 | 3 | 2041 | C |
| 50 | 3 | 2043 | C |
| 50 | 3 | 2050 | G |
| 50 | 3 | 2057 | C |
| 50 | 3 | 2058 | G |
| 50 | 3 | 2062 | C |
| 50 | 3 | 2063 | G |
| 50 | 3 | 2067 | A |
| 50 | 3 | 2068 | G |
| 50 | 3 | 2069 | A |
| 50 | 3 | 2070 | C |
| 50 | 3 | 2076 | G |
| 50 | 3 | 2080 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 50 | 3 | 2083 | U |
| 50 | 3 | 2084 | A |
| 50 | 3 | 2087 | G |
| 50 | 3 | 2099 | U |
| 50 | 3 | 2100 | G |
| 50 | 3 | 2106 | G |
| 50 | 3 | 2107 | A |
| 50 | 3 | 2110 | U |
| 50 | 3 | 2111 | U |
| 50 | 3 | 2112 | A |
| 50 | 3 | 2114 | C |
| 50 | 3 | 2118 | U |
| 50 | 3 | 2123 | A |
| 50 | 3 | 2124 | A |
| 50 | 3 | 2126 | A |
| 50 | 3 | 2127 | G |
| 50 | 3 | 2128 | G |
| 50 | 3 | 2131 | G |
| 50 | 3 | 2132 | G |
| 50 | 3 | 2133 | A |
| 50 | 3 | 2138 | U |
| 50 | 3 | 2140 | G |
| 50 | 3 | 2151 | G |
| 50 | 3 | 2157 | A |
| 50 | 3 | 2164 | G |
| 50 | 3 | 2166 | U |
| 50 | 3 | 2171 | A |
| 50 | 3 | 2172 | A |
| 50 | 3 | 2180 | U |
| 50 | 3 | 2181 | A |
| 50 | 3 | 2184 | A |
| 50 | 3 | 2189 | U |
| 50 | 3 | 2192 | U |
| 50 | 3 | 2193 | U |
| 50 | 3 | 2195 | U |
| 50 | 3 | 2196 | G |
| 50 | 3 | 2197 | U |
| 50 | 3 | 2198 | G |
| 50 | 3 | 2199 | C |
| 50 | 3 | 2200 | U |
| 50 | 3 | 2201 | G |
| 50 | 3 | 2202 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 50 | 3 | 2206 | A |
| 50 | 3 | 2211 | G |
| 50 | 3 | 2212 | U |
| 50 | 3 | 2219 | U |
| 50 | 3 | 2220 | A |
| 50 | 3 | 2222 | C |
| 50 | 3 | 2231 | A |
| 50 | 3 | 2233 | A |
| 50 | 3 | 2246 | G |
| 50 | 3 | 2247 | G |
| 50 | 3 | 2257 | U |
| 50 | 3 | 2258 | G |
| 50 | 3 | 2274 | A |
| 50 | 3 | 2276 | A |
| 50 | 3 | 2277 | A |
| 50 | 3 | 2287 | G |
| 50 | 3 | 2288 | G |
| 50 | 3 | 2291 | U |
| 50 | 3 | 2294 | A |
| 50 | 3 | 2295 | A |
| 50 | 3 | 2296 | A |
| 50 | 3 | 2297 | G |
| 50 | 3 | 2305 | C |
| 50 | 3 | 2313 | U |
| 50 | 3 | 2316 | G |
| 50 | 3 | 2317 | A |
| 50 | 3 | 2319 | A |
| 50 | 3 | 2327 | U |
| 50 | 3 | 2328 | A |
| 50 | 3 | 2330 | A |
| 50 | 3 | 2332 | U |
| 50 | 3 | 2333 | G |
| 50 | 3 | 2341 | G |
| 50 | 3 | 2342 | U |
| 50 | 3 | 2343 | A |
| 50 | 3 | 2344 | A |
| 50 | 3 | 2345 | G |
| 50 | 3 | 2351 | U |
| 50 | 3 | 2353 | G |
| 50 | 3 | 2355 | C |
| 50 | 3 | 2358 | U |
| 50 | 3 | 2362 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 50 | 3 | 2391 | G |
| 50 | 3 | 2393 | C |
| 50 | 3 | 2397 | G |
| 50 | 3 | 2410 | C |
| 50 | 3 | 2411 | C |
| 50 | 3 | 2414 | U |
| 50 | 3 | 2415 | A |
| 50 | 3 | 2417 | G |
| 50 | 3 | 2430 | C |
| 50 | 3 | 2433 | A |
| 50 | 3 | 2434 | A |
| 50 | 3 | 2435 | C |
| 50 | 3 | 2436 | G |
| 50 | 3 | 2437 | G |
| 50 | 3 | 2438 | A |
| 50 | 3 | 2442 | A |
| 50 | 3 | 2443 | A |
| 50 | 3 | 2447 | A |
| 50 | 3 | 2448 | C |
| 50 | 3 | 2449 | U |
| 50 | 3 | 2455 | G |
| 50 | 3 | 2477 | A |
| 50 | 3 | 2483 | C |
| 50 | 3 | 2484 | A |
| 50 | 3 | 2486 | A |
| 50 | 3 | 2488 | C |
| 50 | 3 | 2489 | G |
| 50 | 3 | 2492 | G |
| 50 | 3 | 2497 | U |
| 50 | 3 | 2498 | G |
| 50 | 3 | 2499 | U |
| 50 | 3 | 2500 | U |
| 50 | 3 | 2503 | G |
| 50 | 3 | 2505 | A |
| 50 | 3 | 2506 | C |
| 50 | 3 | 2507 | C |
| 50 | 3 | 2509 | C |
| 50 | 3 | 2511 | A |
| 50 | 3 | 2512 | U |
| 50 | 3 | 2513 | G |
| 50 | 3 | 2514 | U |
| 50 | 3 | 2515 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 50 | 3 | 2516 | G |
| 50 | 3 | 2526 | A |
| 50 | 3 | 2527 | U |
| 50 | 3 | 2528 | C |
| 50 | 3 | 2539 | A |
| 50 | 3 | 2543 | G |
| 50 | 3 | 2558 | G |
| 50 | 3 | 2560 | U |
| 50 | 3 | 2570 | U |
| 50 | 3 | 2574 | A |
| 50 | 3 | 2577 | G |
| 50 | 3 | 2580 | A |
| 50 | 3 | 2581 | C |
| 50 | 3 | 2587 | U |
| 50 | 3 | 2590 | G |
| 50 | 3 | 2593 | U |
| 50 | 3 | 2594 | C |
| 50 | 3 | 2595 | A |
| 50 | 3 | 2596 | A |
| 50 | 3 | 2597 | A |
| 50 | 3 | 2605 | G |
| 50 | 3 | 2606 | A |
| 50 | 3 | 2610 | A |
| 50 | 3 | 2611 | G |
| 50 | 3 | 2618 | C |
| 50 | 3 | 2619 | C |
| 50 | 3 | 2621 | U |
| 50 | 3 | 2622 | A |
| 50 | 3 | 2623 | U |
| 50 | 3 | 2629 | G |
| 50 | 3 | 2631 | G |
| 50 | 3 | 2637 | A |
| 50 | 3 | 2638 | G |
| 50 | 3 | 2642 | G |
| 50 | 3 | 2644 | U |
| 50 | 3 | 2647 | A |
| 50 | 3 | 2649 | G |
| 50 | 3 | 2653 | G |
| 50 | 3 | 2654 | U |
| 50 | 3 | 2655 | U |
| 50 | 3 | 2664 | U |
| 50 | 3 | 2668 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 50 | 3 | 2669 | G |
| 50 | 3 | 2675 | C |
| 50 | 3 | 2689 | C |
| 50 | 3 | 2693 | U |
| 50 | 3 | 2694 | A |
| 50 | 3 | 2697 | C |
| 50 | 3 | 2698 | U |
| 50 | 3 | 2703 | U |
| 50 | 3 | 2708 | G |
| 50 | 3 | 2715 | C |
| 50 | 3 | 2722 | G |
| 50 | 3 | 2732 | A |
| 50 | 3 | 2734 | C |
| 50 | 3 | 2737 | G |
| 50 | 3 | 2738 | U |
| 50 | 3 | 2741 | A |
| 50 | 3 | 2747 | U |
| 50 | 3 | 2752 | G |
| 50 | 3 | 2756 | A |
| 50 | 3 | 2761 | A |
| 50 | 3 | 2765 | A |
| 50 | 3 | 2772 | A |
| 50 | 3 | 2773 | A |
| 50 | 3 | 2774 | A |
| 50 | 3 | 2786 | A |
| 50 | 3 | 2788 | U |
| 50 | 3 | 2799 | U |
| 50 | 3 | 2800 | U |
| 50 | 3 | 2801 | U |
| 50 | 3 | 2804 | C |
| 50 | 3 | 2806 | A |
| 50 | 3 | 2809 | A |
| 50 | 3 | 2811 | G |
| 50 | 3 | 2812 | U |
| 50 | 3 | 2813 | A |
| 50 | 3 | 2814 | A |
| 50 | 3 | 2815 | G |
| 50 | 3 | 2822 | C |
| 50 | 3 | 2824 | A |
| 50 | 3 | 2828 | C |
| 50 | 3 | 2837 | U |
| 50 | 3 | 2839 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 50 | 3 | 2853 | U |
| 50 | 3 | 2854 | A |
| 50 | 3 | 2856 | G |
| 50 | 3 | 2863 | G |
| 50 | 3 | 2870 | U |
| 50 | 3 | 2871 | G |
| 50 | 3 | 2872 | A |
| 50 | 3 | 2876 | G |
| 50 | 3 | 2884 | C |
| 50 | 3 | 2888 | U |
| 50 | 3 | 2889 | U |
| 50 | 3 | 2890 | G |
| 50 | 3 | 2895 | A |
| 50 | 3 | 2897 | G |
| 50 | 3 | 2898 | A |
| 50 | 3 | 2899 | C |
| 51 | 4 | 9 | C |
| 51 | 4 | 10 | C |
| 51 | 4 | 11 | A |
| 51 | 4 | 13 | G |
| 51 | 4 | 14 | U |
| 51 | 4 | 15 | C |
| 51 | 4 | 16 | G |
| 51 | 4 | 23 | A |
| 51 | 4 | 25 | A |
| 51 | 4 | 28 | C |
| 51 | 4 | 33 | U |
| 51 | 4 | 38 | U |
| 51 | 4 | 39 | U |
| 51 | 4 | 40 | U |
| 51 | 4 | 41 | C |
| 51 | 4 | 42 | G |
| 51 | 4 | 48 | A |
| 51 | 4 | 49 | G |
| 51 | 4 | 50 | C |
| 51 | 4 | 51 | A |
| 51 | 4 | 54 | U |
| 51 | 4 | 55 | A |
| 51 | 4 | 60 | C |
| 51 | 4 | 71 | A |
| 51 | 4 | 74 | G |
| 51 | 4 | 77 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 51 | 4 | 78 | C |
| 51 | 4 | 88 | G |
| 51 | 4 | 89 | A |
| 51 | 4 | 98 | A |
| 51 | 4 | 99 | A |
| 51 | 4 | 103 | C |
| 51 | 4 | 106 | A |
| 51 | 4 | 108 | C |
| 52 | 5 | 6 | C |
| 52 | 5 | 8 | G |
| 52 | 5 | 9 | A |
| 52 | 5 | 10 | G |
| 52 | 5 | 33 | A |
| 52 | 5 | 40 | G |
| 52 | 5 | 48 | C |
| 52 | 5 | 49 | C |
| 52 | 5 | 52 | A |
| 52 | 5 | 55 | C |
| 52 | 5 | 56 | A |
| 52 | 5 | 58 | G |
| 52 | 5 | 67 | U |
| 52 | 5 | 85 | U |
| 52 | 5 | 86 | A |
| 52 | 5 | 94 | A |
| 52 | 5 | 95 | C |
| 52 | 5 | 100 | G |
| 52 | 5 | 101 | A |
| 52 | 5 | 103 | U |
| 52 | 5 | 105 | A |
| 52 | 5 | 106 | C |
| 52 | 5 | 107 | A |
| 52 | 5 | 111 | A |
| 52 | 5 | 114 | C |
| 52 | 5 | 115 | A |
| 52 | 5 | 116 | A |
| 52 | 5 | 117 | U |
| 52 | 5 | 120 | A |
| 52 | 5 | 128 | A |
| 52 | 5 | 129 | U |
| 52 | 5 | 130 | G |
| 52 | 5 | 134 | G |
| 52 | 5 | 136 | U |

*Continued on next page...*

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 52 | 5 | 145 | G |
| 52 | 5 | 147 | A |
| 52 | 5 | 149 | G |
| 52 | 5 | 159 | U |
| 52 | 5 | 167 | A |
| 52 | 5 | 168 | A |
| 52 | 5 | 169 | G |
| 52 | 5 | 179 | U |
| 52 | 5 | 186 | A |
| 52 | 5 | 190 | A |
| 52 | 5 | 197 | A |
| 52 | 5 | 198 | A |
| 52 | 5 | 200 | G |
| 52 | 5 | 218 | U |
| 52 | 5 | 219 | A |
| 52 | 5 | 220 | U |
| 52 | 5 | 230 | G |
| 52 | 5 | 236 | C |
| 52 | 5 | 239 | A |
| 52 | 5 | 241 | C |
| 52 | 5 | 242 | A |
| 52 | 5 | 243 | G |
| 52 | 5 | 247 | G |
| 52 | 5 | 259 | A |
| 52 | 5 | 260 | C |
| 52 | 5 | 262 | G |
| 52 | 5 | 263 | C |
| 52 | 5 | 270 | A |
| 52 | 5 | 285 | G |
| 52 | 5 | 286 | C |
| 52 | 5 | 294 | A |
| 52 | 5 | 295 | G |
| 52 | 5 | 302 | A |
| 52 | 5 | 311 | A |
| 52 | 5 | 323 | A |
| 52 | 5 | 324 | C |
| 52 | 5 | 325 | A |
| 52 | 5 | 326 | C |
| 52 | 5 | 328 | G |
| 52 | 5 | 340 | A |
| 52 | 5 | 341 | C |
| 52 | 5 | 342 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 52 | 5 | 344 | G |
| 52 | 5 | 345 | A |
| 52 | 5 | 348 | C |
| 52 | 5 | 349 | A |
| 52 | 5 | 350 | G |
| 52 | 5 | 352 | A |
| 52 | 5 | 359 | A |
| 52 | 5 | 363 | U |
| 52 | 5 | 364 | U |
| 52 | 5 | 368 | C |
| 52 | 5 | 373 | A |
| 52 | 5 | 377 | A |
| 52 | 5 | 381 | C |
| 52 | 5 | 384 | G |
| 52 | 5 | 385 | A |
| 52 | 5 | 386 | U |
| 52 | 5 | 393 | A |
| 52 | 5 | 394 | U |
| 52 | 5 | 402 | G |
| 52 | 5 | 409 | G |
| 52 | 5 | 410 | A |
| 52 | 5 | 412 | G |
| 52 | 5 | 417 | U |
| 52 | 5 | 418 | U |
| 52 | 5 | 420 | A |
| 52 | 5 | 423 | U |
| 52 | 5 | 425 | G |
| 52 | 5 | 426 | U |
| 52 | 5 | 432 | U |
| 52 | 5 | 436 | U |
| 52 | 5 | 440 | U |
| 52 | 5 | 445 | A |
| 52 | 5 | 446 | A |
| 52 | 5 | 449 | A |
| 52 | 5 | 451 | G |
| 52 | 5 | 452 | A |
| 52 | 5 | 453 | C |
| 52 | 5 | 456 | U |
| 52 | 5 | 457 | A |
| 52 | 5 | 461 | G |
| 52 | 5 | 464 | A |
| 52 | 5 | 471 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 52 | 5 | 473 | A |
| 52 | 5 | 476 | U |
| 52 | 5 | 477 | U |
| 52 | 5 | 478 | G |
| 52 | 5 | 481 | U |
| 52 | 5 | 482 | G |
| 52 | 5 | 488 | U |
| 52 | 5 | 493 | A |
| 52 | 5 | 504 | A |
| 52 | 5 | 507 | A |
| 52 | 5 | 509 | C |
| 52 | 5 | 510 | U |
| 52 | 5 | 515 | G |
| 52 | 5 | 516 | C |
| 52 | 5 | 517 | C |
| 52 | 5 | 524 | C |
| 52 | 5 | 525 | G |
| 52 | 5 | 527 | G |
| 52 | 5 | 529 | U |
| 52 | 5 | 530 | A |
| 52 | 5 | 531 | A |
| 52 | 5 | 543 | C |
| 52 | 5 | 545 | A |
| 52 | 5 | 548 | G |
| 52 | 5 | 557 | A |
| 52 | 5 | 558 | U |
| 52 | 5 | 560 | U |
| 52 | 5 | 562 | U |
| 52 | 5 | 569 | U |
| 52 | 5 | 570 | A |
| 52 | 5 | 571 | A |
| 52 | 5 | 574 | C |
| 52 | 5 | 575 | A |
| 52 | 5 | 585 | G |
| 52 | 5 | 586 | G |
| 52 | 5 | 594 | A |
| 52 | 5 | 595 | G |
| 52 | 5 | 608 | G |
| 52 | 5 | 616 | C |
| 52 | 5 | 619 | A |
| 52 | 5 | 628 | A |
| 52 | 5 | 638 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 52 | 5 | 639 | A |
| 52 | 5 | 646 | A |
| 52 | 5 | 650 | A |
| 52 | 5 | 653 | G |
| 52 | 5 | 662 | G |
| 52 | 5 | 663 | G |
| 52 | 5 | 683 | G |
| 52 | 5 | 684 | A |
| 52 | 5 | 699 | A |
| 52 | 5 | 700 | G |
| 52 | 5 | 715 | A |
| 52 | 5 | 716 | C |
| 52 | 5 | 718 | A |
| 52 | 5 | 719 | G |
| 52 | 5 | 720 | U |
| 52 | 5 | 721 | G |
| 52 | 5 | 726 | A |
| 52 | 5 | 729 | C |
| 52 | 5 | 744 | U |
| 52 | 5 | 745 | U |
| 52 | 5 | 746 | A |
| 52 | 5 | 752 | G |
| 52 | 5 | 753 | C |
| 52 | 5 | 763 | A |
| 52 | 5 | 791 | A |
| 52 | 5 | 793 | C |
| 52 | 5 | 796 | A |
| 52 | 5 | 802 | C |
| 52 | 5 | 809 | G |
| 52 | 5 | 811 | A |
| 52 | 5 | 812 | A |
| 52 | 5 | 814 | C |
| 52 | 5 | 815 | G |
| 52 | 5 | 818 | A |
| 52 | 5 | 825 | A |
| 52 | 5 | 826 | G |
| 52 | 5 | 829 | G |
| 52 | 5 | 836 | C |
| 52 | 5 | 849 | A |
| 52 | 5 | 858 | A |
| 52 | 5 | 864 | U |
| 52 | 5 | 866 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 52 | 5 | 867 | A |
| 52 | 5 | 870 | A |
| 52 | 5 | 875 | G |
| 52 | 5 | 879 | G |
| 52 | 5 | 883 | A |
| 52 | 5 | 885 | U |
| 52 | 5 | 895 | A |
| 52 | 5 | 907 | A |
| 52 | 5 | 908 | A |
| 52 | 5 | 910 | C |
| 52 | 5 | 911 | G |
| 52 | 5 | 921 | G |
| 52 | 5 | 922 | G |
| 52 | 5 | 929 | C |
| 52 | 5 | 930 | A |
| 52 | 5 | 934 | G |
| 52 | 5 | 953 | A |
| 52 | 5 | 954 | A |
| 52 | 5 | 955 | U |
| 52 | 5 | 956 | U |
| 52 | 5 | 958 | G |
| 52 | 5 | 964 | A |
| 52 | 5 | 966 | A |
| 52 | 5 | 970 | A |
| 52 | 5 | 971 | A |
| 52 | 5 | 972 | A |
| 52 | 5 | 973 | A |
| 52 | 5 | 978 | A |
| 52 | 5 | 984 | A |
| 52 | 5 | 987 | U |
| 52 | 5 | 988 | G |
| 52 | 5 | 1000 | A |
| 52 | 5 | 1001 | A |
| 52 | 5 | 1003 | G |
| 52 | 5 | 1010 | A |
| 52 | 5 | 1011 | A |
| 52 | 5 | 1013 | C |
| 52 | 5 | 1014 | A |
| 52 | 5 | 1015 | U |
| 52 | 5 | 1016 | A |
| 52 | 5 | 1033 | U |
| 52 | 5 | 1037 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 52 | 5 | 1044 | G |
| 52 | 5 | 1045 | C |
| 52 | 5 | 1046 | A |
| 52 | 5 | 1047 | U |
| 52 | 5 | 1056 | U |
| 52 | 5 | 1057 | C |
| 52 | 5 | 1072 | G |
| 52 | 5 | 1074 | U |
| 52 | 5 | 1075 | G |
| 52 | 5 | 1076 | U |
| 52 | 5 | 1085 | G |
| 52 | 5 | 1086 | U |
| 52 | 5 | 1092 | A |
| 52 | 5 | 1101 | A |
| 52 | 5 | 1107 | U |
| 52 | 5 | 1109 | U |
| 52 | 5 | 1113 | U |
| 52 | 5 | 1119 | C |
| 52 | 5 | 1120 | A |
| 52 | 5 | 1121 | U |
| 52 | 5 | 1122 | U |
| 52 | 5 | 1123 | G |
| 52 | 5 | 1124 | U |
| 52 | 5 | 1128 | G |
| 52 | 5 | 1133 | A |
| 52 | 5 | 1134 | C |
| 52 | 5 | 1135 | U |
| 52 | 5 | 1141 | U |
| 52 | 5 | 1144 | A |
| 52 | 5 | 1154 | A |
| 52 | 5 | 1155 | A |
| 52 | 5 | 1158 | A |
| 52 | 5 | 1159 | A |
| 52 | 5 | 1163 | A |
| 52 | 5 | 1171 | A |
| 52 | 5 | 1172 | A |
| 52 | 5 | 1173 | A |
| 52 | 5 | 1187 | U |
| 52 | 5 | 1188 | A |
| 52 | 5 | 1189 | U |
| 52 | 5 | 1199 | U |
| 52 | 5 | 1200 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 52 | 5 | 1201 | C |
| 52 | 5 | 1211 | A |
| 52 | 5 | 1215 | U |
| 52 | 5 | 1223 | A |
| 52 | 5 | 1225 | A |
| 52 | 5 | 1235 | C |
| 52 | 5 | 1243 | A |
| 52 | 5 | 1245 | A |
| 52 | 5 | 1254 | A |
| 52 | 5 | 1255 | A |
| 52 | 5 | 1260 | U |
| 52 | 5 | 1261 | A |
| 52 | 5 | 1271 | U |
| 52 | 5 | 1272 | C |
| 52 | 5 | 1273 | A |
| 52 | 5 | 1274 | G |
| 52 | 5 | 1276 | U |
| 52 | 5 | 1279 | G |
| 52 | 5 | 1291 | C |
| 52 | 5 | 1296 | C |
| 52 | 5 | 1297 | G |
| 52 | 5 | 1298 | U |
| 52 | 5 | 1312 | G |
| 52 | 5 | 1319 | U |
| 52 | 5 | 1320 | A |
| 52 | 5 | 1323 | A |
| 52 | 5 | 1333 | C |
| 52 | 5 | 1335 | G |
| 52 | 5 | 1337 | U |
| 52 | 5 | 1338 | A |
| 52 | 5 | 1339 | U |
| 52 | 5 | 1340 | G |
| 52 | 5 | 1343 | G |
| 52 | 5 | 1344 | C |
| 52 | 5 | 1353 | C |
| 52 | 5 | 1354 | G |
| 52 | 5 | 1356 | U |
| 52 | 5 | 1359 | C |
| 52 | 5 | 1373 | A |
| 52 | 5 | 1374 | C |
| 52 | 5 | 1381 | U |
| 52 | 5 | 1394 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 52 | 5 | 1400 | A |
| 52 | 5 | 1404 | U |
| 52 | 5 | 1408 | A |
| 52 | 5 | 1415 | G |
| 52 | 5 | 1417 | U |
| 52 | 5 | 1421 | A |
| 52 | 5 | 1427 | U |
| 52 | 5 | 1429 | G |
| 52 | 5 | 1430 | G |
| 52 | 5 | 1457 | G |
| 52 | 5 | 1466 | U |
| 52 | 5 | 1467 | A |
| 52 | 5 | 1468 | A |
| 52 | 5 | 1471 | C |
| 52 | 5 | 1474 | A |
| 52 | 5 | 1480 | G |
| 52 | 5 | 1481 | U |
| 52 | 5 | 1490 | G |
| 52 | 5 | 1496 | G |
| 52 | 5 | 1504 | G |
| 52 | 5 | 1505 | G |
| 53 | 7 | 3 | G |
| 53 | 7 | 9 | U |
| 53 | 7 | 11 | G |
| 53 | 7 | 16 | G |
| 53 | 7 | 17 | U |
| 53 | 7 | 18 | C |
| 53 | 7 | 19 | G |
| 53 | 7 | 20 | G |
| 53 | 7 | 21 | U |
| 53 | 7 | 22 | A |
| 53 | 7 | 38 | G |
| 53 | 7 | 42 | C |
| 53 | 7 | 44 | U |
| 53 | 7 | 48 | U |
| 53 | 7 | 49 | C |
| 53 | 7 | 53 | A |
| 53 | 7 | 54 | G |
| 53 | 7 | 57 | C |
| 53 | 7 | 58 | G |
| 53 | 7 | 59 | A |
| 53 | 7 | 60 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 53 | 7 | 63 | U |
| 53 | 7 | 71 | A |
| 53 | 7 | 72 | C |
| 53 | 7 | 76 | C |

All (38) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 50 | 3 | 309 | A |
| 50 | 3 | 410 | G |
| 50 | 3 | 425 | U |
| 50 | 3 | 500 | U |
| 50 | 3 | 513 | A |
| 50 | 3 | 688 | U |
| 50 | 3 | 881 | A |
| 50 | 3 | 996 | A |
| 50 | 3 | 1048 | A |
| 50 | 3 | 1082 | A |
| 50 | 3 | 1209 | U |
| 50 | 3 | 1255 | G |
| 50 | 3 | 1327 | G |
| 50 | 3 | 1583 | G |
| 50 | 3 | 1588 | A |
| 50 | 3 | 1820 | U |
| 50 | 3 | 1920 | A |
| 50 | 3 | 2180 | U |
| 50 | 3 | 2504 | C |
| 50 | 3 | 2506 | C |
| 50 | 3 | 2513 | G |
| 50 | 3 | 2604 | U |
| 50 | 3 | 2668 | A |
| 50 | 3 | 2764 | U |
| 50 | 3 | 2897 | G |
| 51 | 4 | 10 | C |
| 51 | 4 | 50 | C |
| 51 | 4 | 54 | U |
| 51 | 4 | 59 | A |
| 51 | 4 | 70 | G |
| 52 | 5 | 294 | A |
| 52 | 5 | 417 | U |
| 52 | 5 | 448 | A |
| 52 | 5 | 1075 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 52 | 5 | 1123 | G |
| 52 | 5 | 1373 | A |
| 53 | 7 | 16 | G |
| 53 | 7 | 19 | G |

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

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

## 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry (i)

There are no ligands in this entry.

## 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

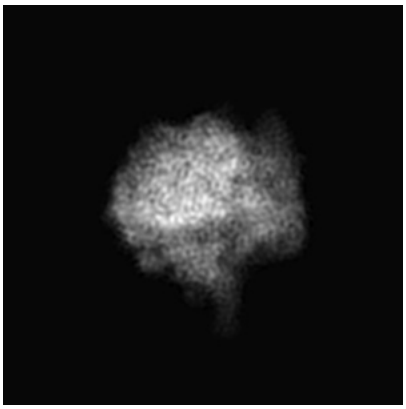
# 6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-13273. These allow visual inspection of the internal detail of the map and identification of artifacts.

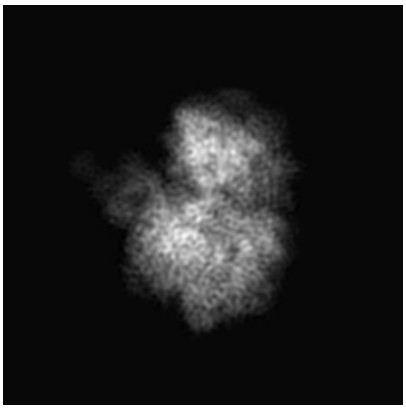
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

## 6.1 Orthogonal projections (i)

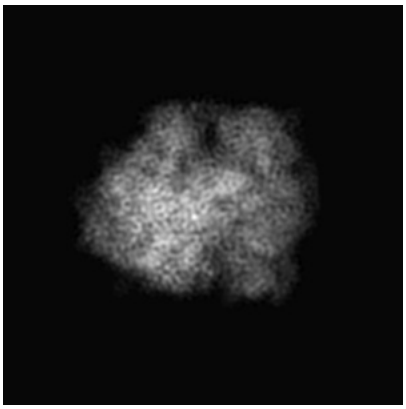
### 6.1.1 Primary map



X

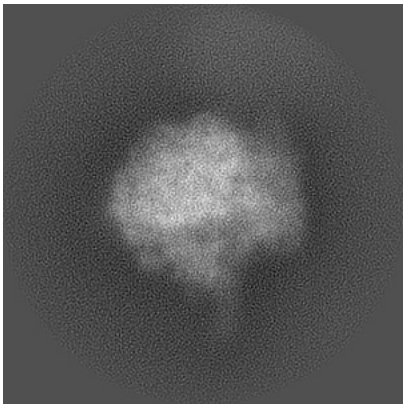


Y

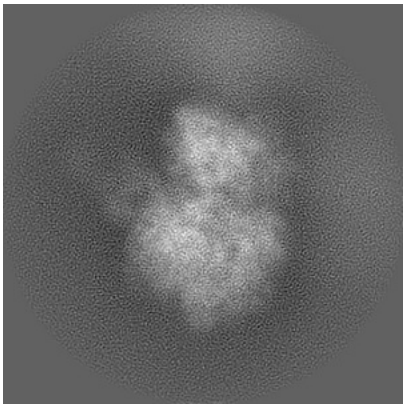


Z

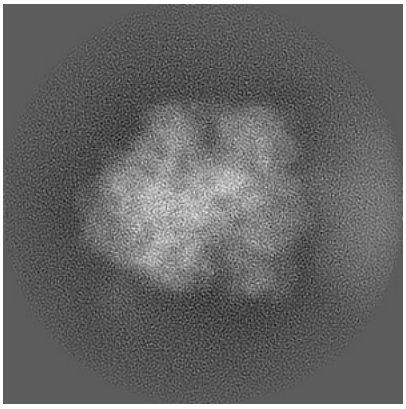
### 6.1.2 Raw map



X



Y



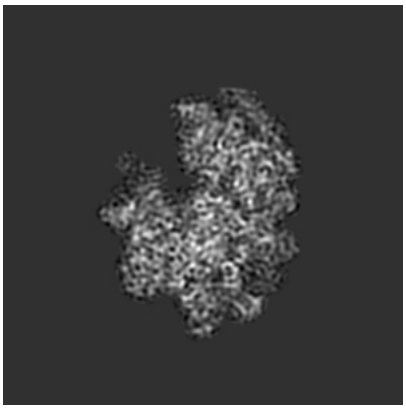
Z

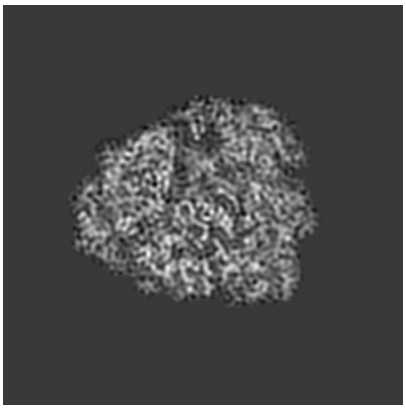
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices (i)

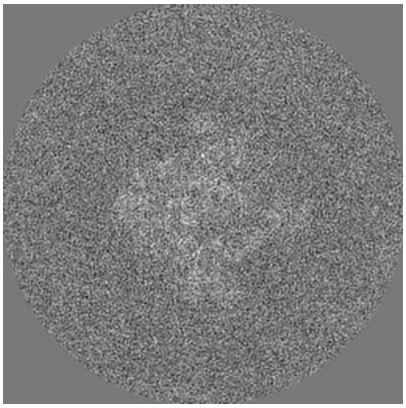
### 6.2.1 Primary map

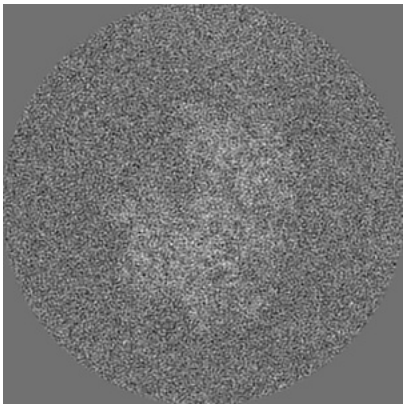
X Index: 128

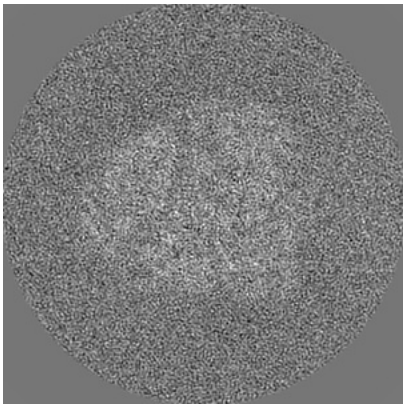

Y Index: 128


Z Index: 128

### 6.2.2 Raw map


X Index: 128

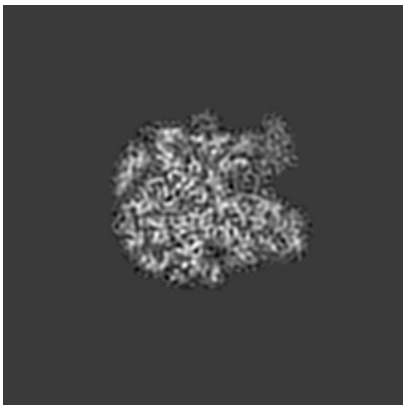

Y Index: 128


Z Index: 128

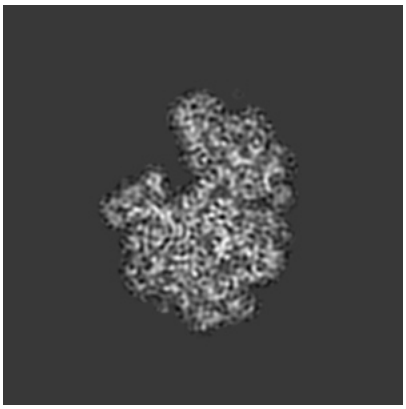
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices (i)

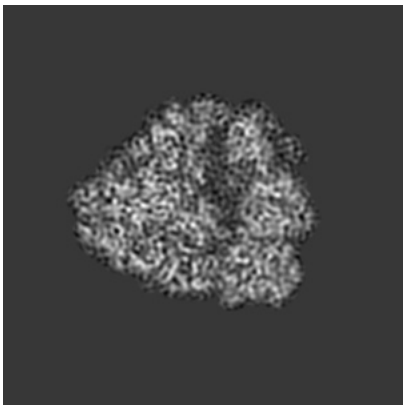
### 6.3.1 Primary map



X Index: 104

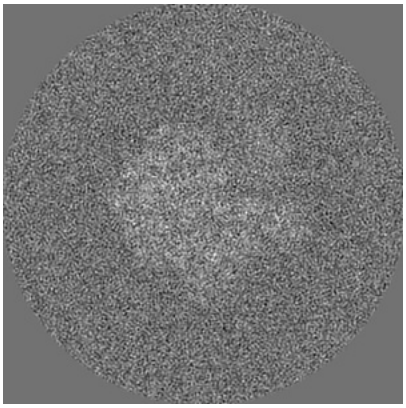


Y Index: 120

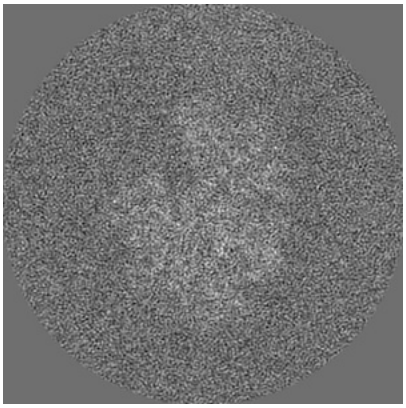


Z Index: 122

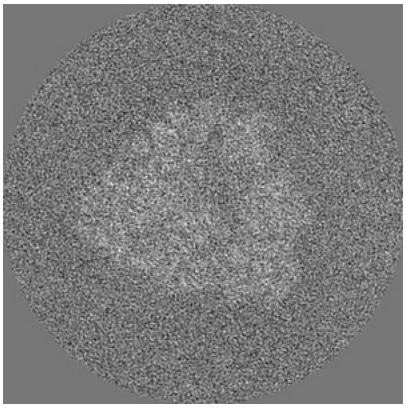
### 6.3.2 Raw map



X Index: 119



Y Index: 120

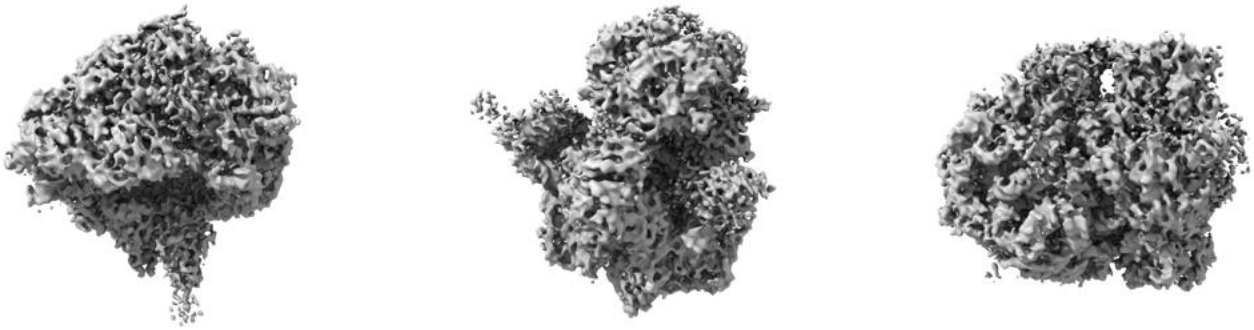


Z Index: 122

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

## 6.4 Orthogonal surface views (i)

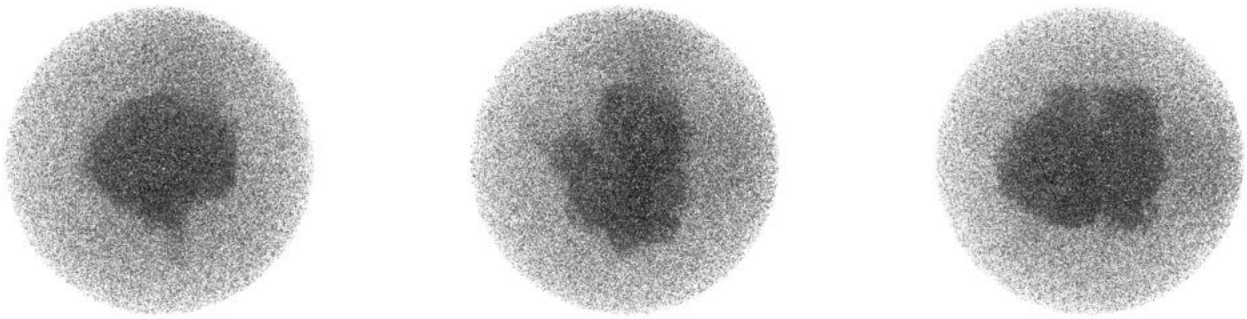
### 6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.47. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.4.2 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.

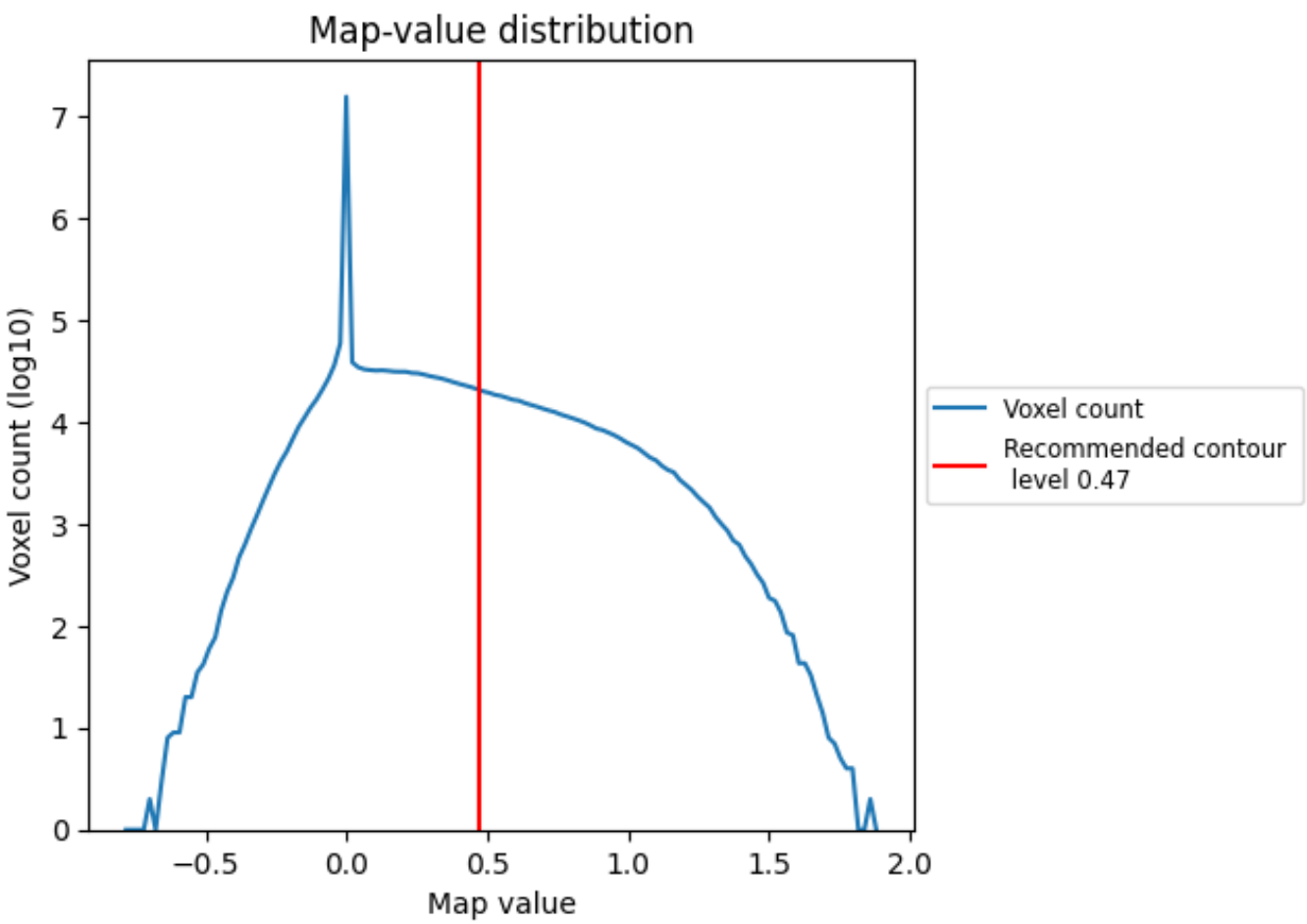
## 6.5 Mask visualisation (i)

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

# 7 Map analysis (i)

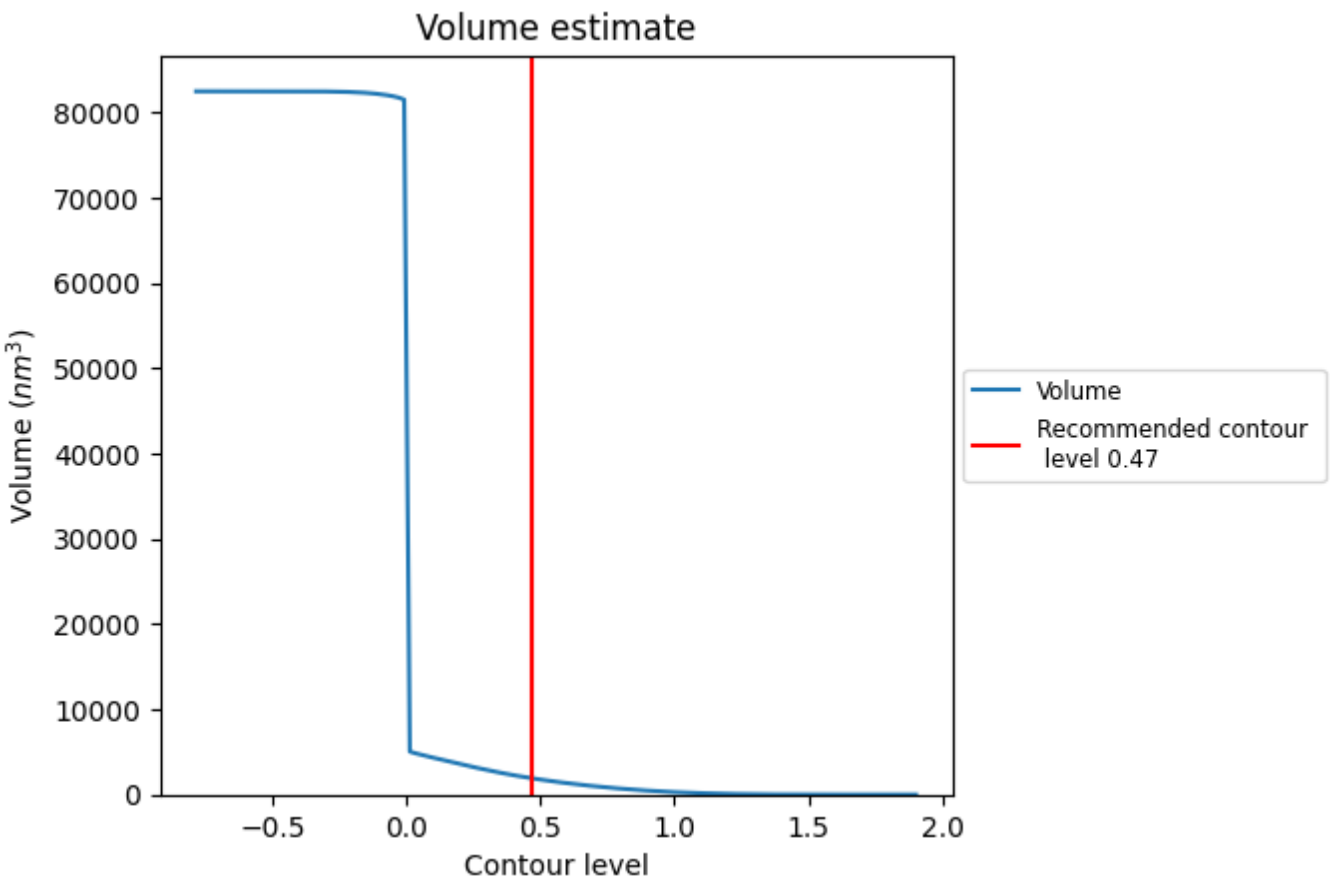
This section contains the results of statistical analysis of the map.

## 7.1 Map-value distribution (i)




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

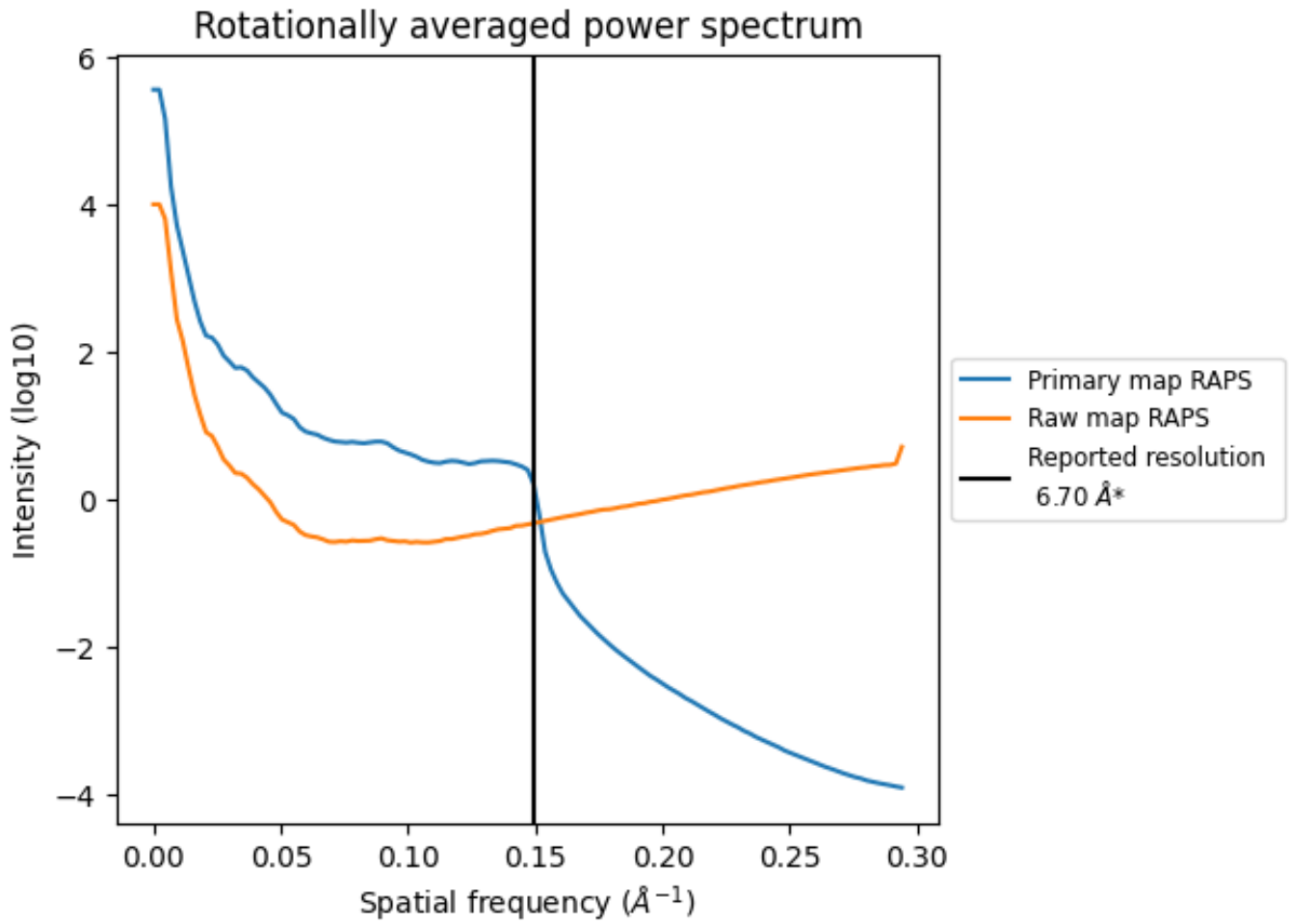
## 7.2 Volume estimate (i)




The volume at the recommended contour level is 1908 $nm^3$; this corresponds to an approximate mass of 1723 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)

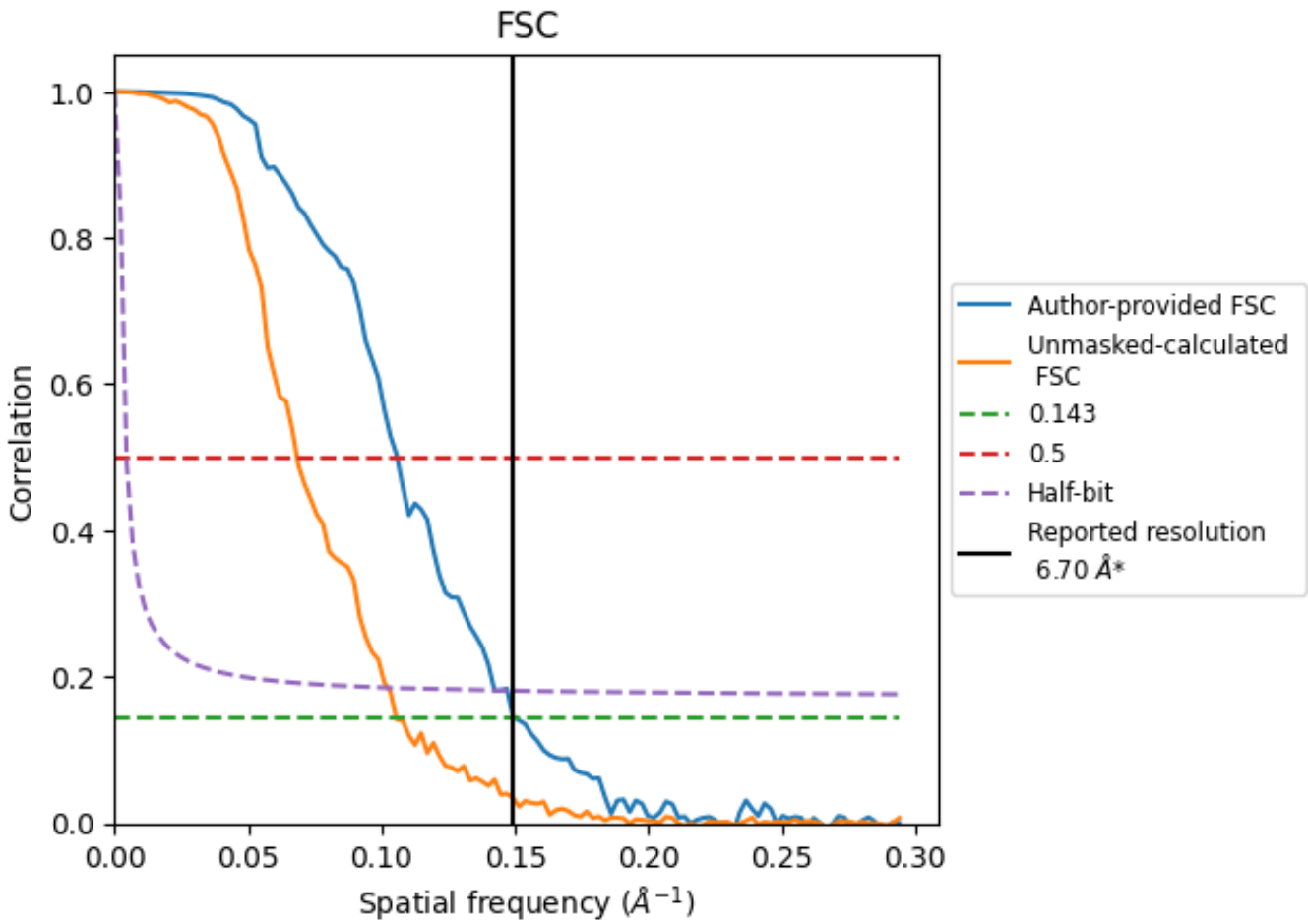



*Reported resolution corresponds to spatial frequency of 0.149 Å$^{-1}$

# 8 Fourier-Shell correlation (i)

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

## 8.1 FSC (i)




*Reported resolution corresponds to spatial frequency of 0.149 Å$^{-1}$

## 8.2 Resolution estimates (i)

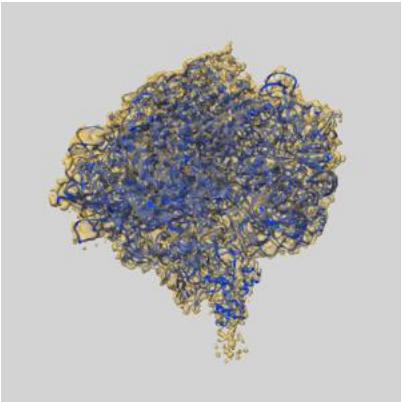
| Resolution estimate (Å) | Estimation criterion (FSC cut-off) | | |
|---|---|---|---|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | 6.70 | - | - |
| Author-provided FSC curve | 6.65 | 9.44 | 7.02 |
| Unmasked-calculated* | 9.47 | 14.62 | 9.77 |

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 9.47 differs from the reported value 6.7 by more than 10 %

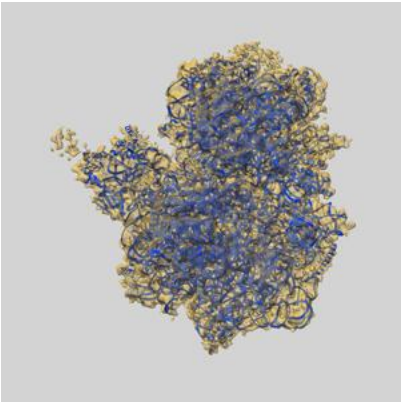
# 9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-13273 and PDB model 7PAI. Per-residue inclusion information can be found in section 3 on page 13.

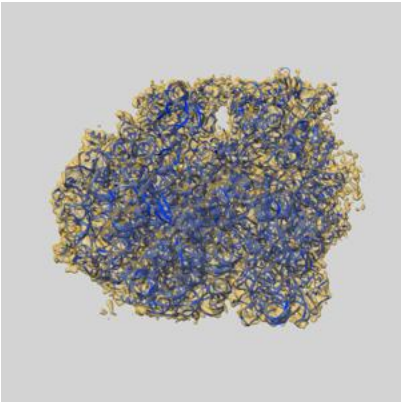
## 9.1 Map-model overlay (i)



X



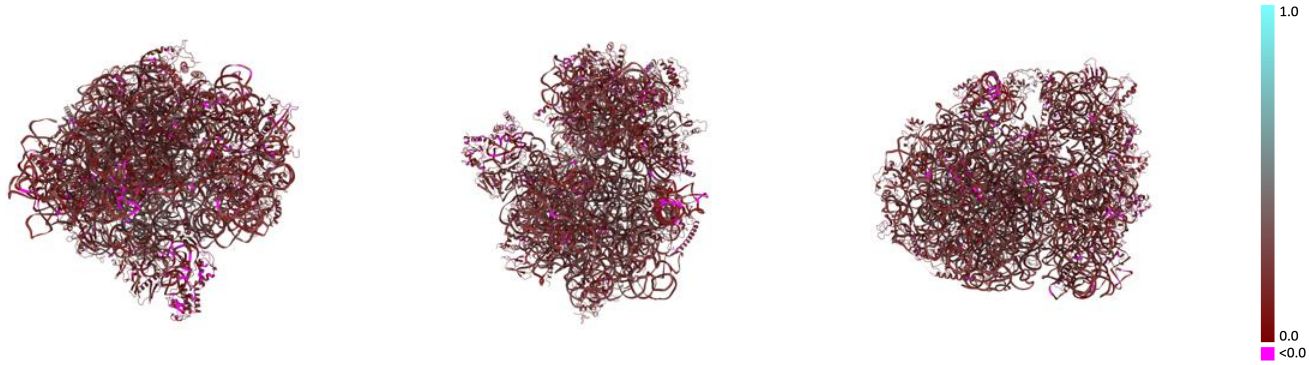
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.47 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.

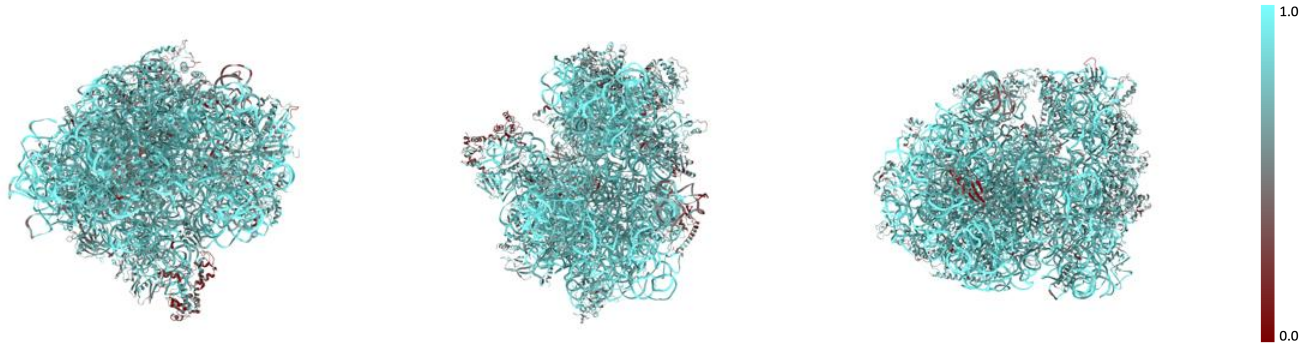
## 9.2 Q-score mapped to coordinate model (i)




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.

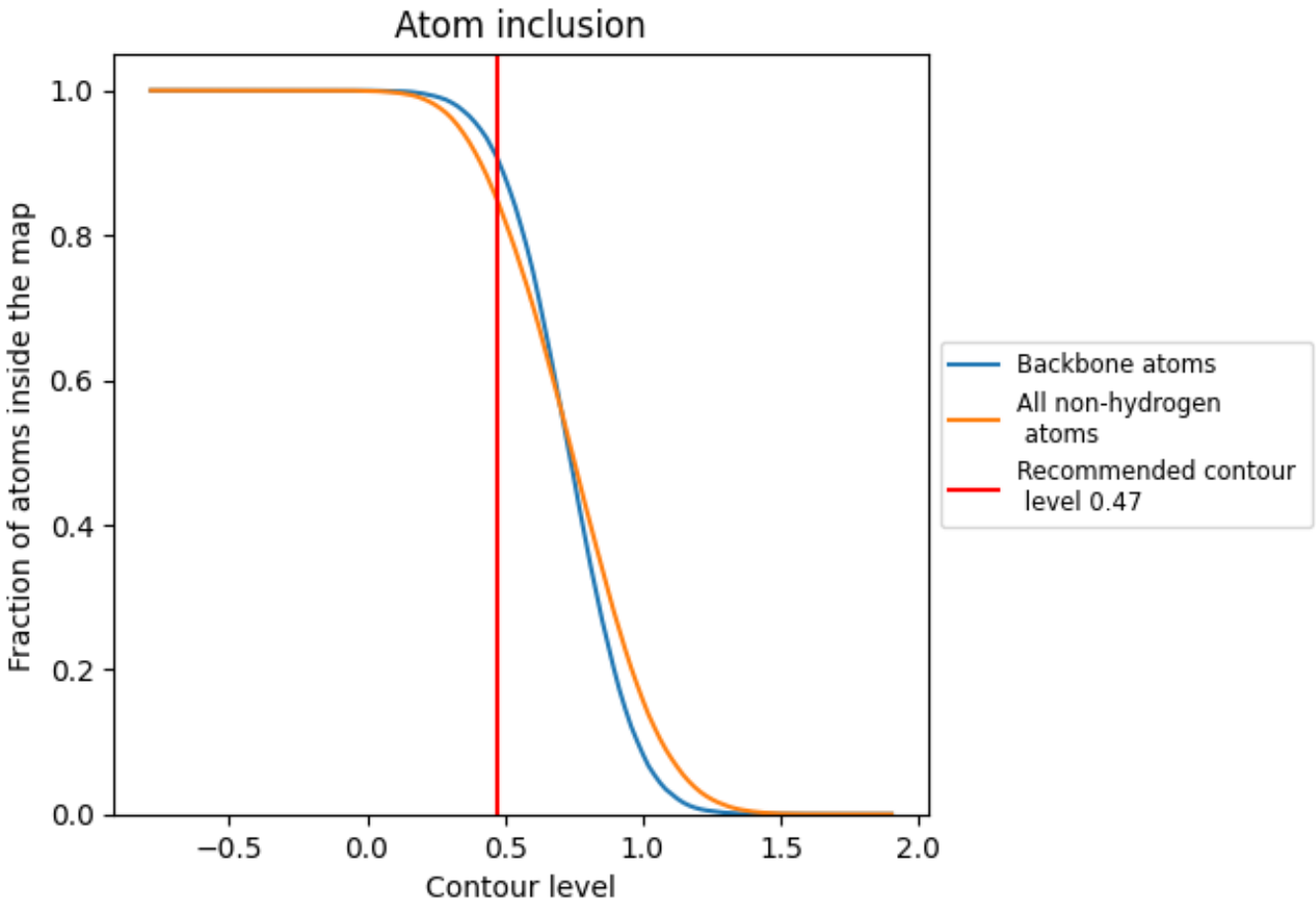
## 9.3 Atom inclusion mapped to coordinate model (i)




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 (0.47).

## 9.4 Atom inclusion (i)




At the recommended contour level, 91% of all backbone atoms, 85% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.47) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|---|---|---|
| All | 0.8512 | 0.2110 |
| 0 | 0.7836 | 0.1880 |
| 1 | 0.7768 | 0.2000 |
| 2 | 0.7635 | 0.1700 |
| 3 | 0.9358 | 0.2240 |
| 4 | 0.9294 | 0.2270 |
| 5 | 0.9368 | 0.2140 |
| 7 | 0.8857 | 0.2070 |
| A | 0.6429 | 0.1980 |
| B | 0.6504 | 0.1880 |
| C | 0.6509 | 0.1760 |
| D | 0.6611 | 0.1840 |
| E | 0.6168 | 0.2090 |
| F | 0.6554 | 0.1850 |
| G | 0.6700 | 0.1770 |
| H | 0.6793 | 0.1690 |
| I | 0.6465 | 0.1810 |
| J | 0.6891 | 0.1930 |
| K | 0.7155 | 0.2000 |
| L | 0.6852 | 0.2000 |
| M | 0.7363 | 0.1620 |
| N | 0.6843 | 0.1980 |
| O | 0.7281 | 0.1710 |
| P | 0.6591 | 0.1890 |
| Q | 0.6957 | 0.1780 |
| R | 0.6403 | 0.1800 |
| S | 0.7393 | 0.1850 |
| T | 0.6897 | 0.1980 |
| a | 0.7537 | 0.1940 |
| b | 0.7200 | 0.1870 |
| c | 0.7236 | 0.2140 |
| d | 0.6878 | 0.1920 |
| e | 0.6461 | 0.2040 |
| f | 0.3307 | 0.1710 |
| g | 0.4421 | 0.1380 |

*Continued on next page...*

*Continued from previous page...*

| Chain | Atom inclusion | Q-score |
|---|---|---|
| h | 0.3083 | 0.1460 |
| i | 0.7388 | 0.1980 |
| j | 0.6880 | 0.2040 |
| k | 0.7237 | 0.2010 |
| l | 0.7204 | 0.2110 |
| m | 0.7308 | 0.2010 |
| n | 0.7220 | 0.1960 |
| o | 0.6707 | 0.1970 |
| p | 0.7530 | 0.1730 |
| q | 0.6821 | 0.1940 |
| r | 0.7464 | 0.1950 |
| s | 0.7546 | 0.2250 |
| t | 0.6214 | 0.1950 |
| u | 0.7484 | 0.1990 |
| v | 0.7475 | 0.1930 |
| w | 0.6841 | 0.1920 |
| x | 0.6706 | 0.2290 |
| y | 0.7558 | 0.2130 |
| z | 0.7935 | 0.2150 |