



wwPDB EM Validation Summary Report ⓘ

May 14, 2025 – 11:03 AM EDT

PDB ID : 9CN3 / pdb_00009cn3
EMDB ID : EMD-45757
Title : Human 39S mitoribosome in complex with antibiotic Linezolid
Authors : Raskar, T.; Bibel, B.; Galonic Fujimori, D.; Fraser, J.
Deposited on : 2024-07-15
Resolution : 2.62 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

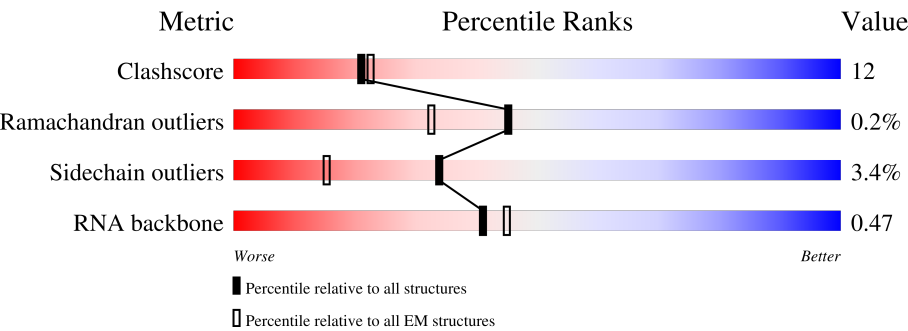
EMDB validation analysis : 0.0.1.dev118
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0rc1
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.62 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) |
|-----------------------|--------------------------|--------------------------|
| Clashscore | 210492 | 15764 |
| Ramachandran outliers | 207382 | 16835 |
| Sidechain outliers | 206894 | 16415 |
| RNA backbone | 6643 | 2191 |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|-----------------------------------|
| 1 | 0 | 188 | <div><div>40%16%43%</div></div> |
| 2 | 1 | 65 | <div><div>55%25%20%</div></div> |
| 3 | 2 | 92 | <div><div>42%8%50%</div></div> |
| 4 | 3 | 188 | <div><div>39%11%49%</div></div> |
| 5 | 4 | 103 | <div><div>23%14%63%</div></div> |
| 6 | 5 | 423 | <div><div>65%25%7%</div></div> |
| 7 | 6 | 380 | <div><div>14%55%36%7%</div></div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 8 | 7 | 338 | |
| 9 | 8 | 206 | |
| 10 | 9 | 137 | |
| 11 | A | 1559 | |
| 12 | B | 72 | |
| 13 | D | 305 | |
| 14 | E | 348 | |
| 15 | F | 311 | |
| 16 | H | 267 | |
| 17 | I | 261 | |
| 18 | J | 192 | |
| 19 | K | 178 | |
| 20 | L | 145 | |
| 21 | M | 296 | |
| 22 | N | 251 | |
| 23 | O | 175 | |
| 24 | P | 179 | |
| 25 | Q | 292 | |
| 26 | R | 149 | |
| 27 | S | 205 | |
| 28 | T | 212 | |
| 29 | U | 153 | |
| 30 | V | 216 | |
| 31 | W | 148 | |
| 32 | X | 256 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 33 | Y | 250 | |
| 34 | Z | 161 | |
| 35 | a | 142 | |
| 36 | b | 155 | |
| 37 | c | 332 | |
| 38 | d | 306 | |
| 39 | e | 279 | |
| 40 | f | 194 | |
| 41 | g | 166 | |
| 42 | h | 158 | |
| 43 | i | 128 | |
| 44 | j | 123 | |
| 45 | k | 112 | |
| 46 | l | 138 | |
| 47 | m | 128 | |
| 48 | o | 102 | |
| 49 | p | 206 | |
| 50 | q | 222 | |
| 51 | r | 196 | |
| 52 | s | 439 | |
| 53 | u | 710 | |
| 54 | TA | 198 | |
| 54 | TB | 198 | |
| 54 | TC | 198 | |

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 107417 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 39S ribosomal protein L32, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 1 | 0 | 108 | Total | C | N | O | S | 0 | 0 |
| | | | 880 | 545 | 172 | 157 | 6 | | |

- Molecule 2 is a protein called 39S ribosomal protein L33, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 2 | 1 | 52 | Total | C | N | O | S | 0 | 0 |
| | | | 433 | 278 | 83 | 70 | 2 | | |

- Molecule 3 is a protein called 39S ribosomal protein L34, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 3 | 2 | 46 | Total | C | N | O | S | 0 | 0 |
| | | | 376 | 233 | 83 | 59 | 1 | | |

- Molecule 4 is a protein called 39S ribosomal protein L35, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 4 | 3 | 95 | Total | C | N | O | S | 0 | 0 |
| | | | 831 | 539 | 162 | 127 | 3 | | |

- Molecule 5 is a protein called 39S ribosomal protein L36, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 5 | 4 | 38 | Total | C | N | O | S | 0 | 0 |
| | | | 342 | 217 | 72 | 49 | 4 | | |

- Molecule 6 is a protein called 39S ribosomal protein L37, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 6 | 5 | 393 | Total | C | N | O | S | 0 | 0 |
| | | | 3205 | 2070 | 559 | 565 | 11 | | |

- Molecule 7 is a protein called 39S ribosomal protein L38, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 7 | 6 | 354 | Total | C | N | O | S | 0 | 0 |
| | | | 2948 | 1881 | 525 | 533 | 9 | | |

- Molecule 8 is a protein called 39S ribosomal protein L39, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 8 | 7 | 297 | Total | C | N | O | S | 0 | 0 |
| | | | 2410 | 1540 | 409 | 443 | 18 | | |

- Molecule 9 is a protein called 39S ribosomal protein L40, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 9 | 8 | 99 | Total | C | N | O | S | 0 | 0 |
| | | | 836 | 535 | 144 | 155 | 2 | | |

- Molecule 10 is a protein called 39S ribosomal protein L41, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 10 | 9 | 124 | Total | C | N | O | S | 0 | 0 |
| | | | 997 | 644 | 170 | 181 | 2 | | |

- Molecule 11 is a RNA chain called 16S rRNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|-------|
| 11 | A | 1527 | Total | C | N | O | P | 0 | 0 |
| | | | 32395 | 14536 | 5844 | 10488 | 1527 | | |

- Molecule 12 is a RNA chain called tRNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 12 | B | 56 | Total | C | N | O | P | 0 | 0 |
| | | | 1191 | 534 | 214 | 387 | 56 | | |

- Molecule 13 is a protein called 39S ribosomal protein L2, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 13 | D | 239 | Total | C | N | O | S | 0 | 0 |
| | | | 1866 | 1162 | 377 | 318 | 9 | | |

- Molecule 14 is a protein called 39S ribosomal protein L3, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 14 | E | 306 | Total | C | N | O | S | 0 | 0 |
| | | | 2410 | 1547 | 419 | 433 | 11 | | |

- Molecule 15 is a protein called 39S ribosomal protein L4, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 15 | F | 250 | Total | C | N | O | S | 0 | 0 |
| | | | 2013 | 1294 | 365 | 348 | 6 | | |

- Molecule 16 is a protein called 39S ribosomal protein L9, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|-------|
| 16 | H | 98 | Total | C | N | O | | 0 | 0 |
| | | | 806 | 510 | 156 | 140 | | | |

- Molecule 17 is a protein called 39S ribosomal protein L10, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 17 | I | 179 | Total | C | N | O | S | 0 | 0 |
| | | | 1435 | 925 | 258 | 242 | 10 | | |

- Molecule 18 is a protein called 39S ribosomal protein L11, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 18 | J | 175 | Total | C | N | O | S | 0 | 0 |
| | | | 1330 | 847 | 237 | 244 | 2 | | |

- Molecule 19 is a protein called 39S ribosomal protein L13, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 19 | K | 177 | Total | C | N | O | S | 0 | 0 |
| | | | 1451 | 934 | 259 | 251 | 7 | | |

- Molecule 20 is a protein called 39S ribosomal protein L14, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 20 | L | 115 | Total | C | N | O | S | 0 | 0 |
| | | | 889 | 559 | 171 | 154 | 5 | | |

- Molecule 21 is a protein called 39S ribosomal protein L15, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 21 | M | 287 | Total | C | N | O | S | 0 | 0 |
| | | | 2305 | 1472 | 425 | 402 | 6 | | |

- Molecule 22 is a protein called 39S ribosomal protein L16, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 22 | N | 222 | Total | C | N | O | S | 0 | 0 |
| | | | 1786 | 1143 | 326 | 307 | 10 | | |

- Molecule 23 is a protein called 39S ribosomal protein L17, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 23 | O | 152 | Total | C | N | O | S | 0 | 0 |
| | | | 1245 | 784 | 239 | 215 | 7 | | |

- Molecule 24 is a protein called Mitochondrial ribosomal protein L18, isoform CRA_b.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 24 | P | 143 | Total | C | N | O | S | 0 | 0 |
| | | | 1165 | 729 | 223 | 208 | 5 | | |

- Molecule 25 is a protein called 39S ribosomal protein L19, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 25 | Q | 220 | Total | C | N | O | S | 0 | 0 |
| | | | 1834 | 1174 | 326 | 325 | 9 | | |

- Molecule 26 is a protein called 39S ribosomal protein L20, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 26 | R | 140 | Total | C | N | O | S | 0 | 0 |
| | | | 1153 | 732 | 231 | 186 | 4 | | |

- Molecule 27 is a protein called 39S ribosomal protein L21, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 27 | S | 156 | Total | C | N | O | S | 0 | 0 |
| | | | 1251 | 806 | 222 | 219 | 4 | | |

- Molecule 28 is a protein called 39S ribosomal protein L22, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 28 | T | 166 | Total | C | N | O | S | 0 | 0 |
| | | | 1368 | 875 | 254 | 232 | 7 | | |

- Molecule 29 is a protein called 39S ribosomal protein L23, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 29 | U | 152 | Total | C | N | O | S | 0 | 0 |
| | | | 1222 | 773 | 233 | 213 | 3 | | |

- Molecule 30 is a protein called 39S ribosomal protein L24, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 30 | V | 206 | Total | C | N | O | S | 0 | 0 |
| | | | 1682 | 1071 | 299 | 304 | 8 | | |

- Molecule 31 is a protein called 39S ribosomal protein L27, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 31 | W | 111 | Total | C | N | O | S | 0 | 0 |
| | | | 871 | 558 | 164 | 146 | 3 | | |

- Molecule 32 is a protein called 39S ribosomal protein L28, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 32 | X | 243 | Total | C | N | O | S | 0 | 0 |
| | | | 2035 | 1317 | 351 | 362 | 5 | | |

- Molecule 33 is a protein called 39S ribosomal protein L47, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 33 | Y | 176 | Total | C | N | O | S | 0 | 0 |
| | | | 1517 | 970 | 291 | 252 | 4 | | |

- Molecule 34 is a protein called 39S ribosomal protein L30, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 34 | Z | 120 | Total | C | N | O | S | 0 | 0 |
| | | | 978 | 626 | 183 | 166 | 3 | | |

- Molecule 35 is a protein called 39S ribosomal protein L42, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 35 | a | 108 | Total | C | N | O | S | 0 | 0 |
| | | | 896 | 560 | 162 | 169 | 5 | | |

- Molecule 36 is a protein called 39S ribosomal protein L43, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 36 | b | 148 | Total | C | N | O | S | 0 | 0 |
| | | | 1178 | 733 | 229 | 213 | 3 | | |

- Molecule 37 is a protein called 39S ribosomal protein L44, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 37 | c | 289 | Total | C | N | O | S | 0 | 0 |
| | | | 2322 | 1483 | 400 | 430 | 9 | | |

- Molecule 38 is a protein called 39S ribosomal protein L45, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 38 | d | 257 | Total | C | N | O | S | 0 | 0 |
| | | | 2075 | 1326 | 363 | 372 | 14 | | |

- Molecule 39 is a protein called 39S ribosomal protein L46, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 39 | e | 217 | Total | C | N | O | S | 0 | 0 |
| | | | 1762 | 1124 | 310 | 323 | 5 | | |

- Molecule 40 is a protein called 39S ribosomal protein L48, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 40 | f | 146 | Total | C | N | O | S | 0 | 0 |
| | | | 1126 | 714 | 186 | 222 | 4 | | |

- Molecule 41 is a protein called 39S ribosomal protein L49, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 41 | g | 132 | Total | C | N | O | S | 0 | 0 |
| | | | 1096 | 709 | 191 | 194 | 2 | | |

- Molecule 42 is a protein called 39S ribosomal protein L50, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 42 | h | 110 | Total | C | N | O | S | 0 | 0 |
| | | | 894 | 568 | 156 | 167 | 3 | | |

- Molecule 43 is a protein called 39S ribosomal protein L51, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 43 | i | 97 | Total | C | N | O | S | 0 | 0 |
| | | | 827 | 532 | 165 | 126 | 4 | | |

- Molecule 44 is a protein called cDNA FLJ76418, highly similar to Homo sapiens mitochondrial ribosomal protein L52 (MRPL52), transcript variant 1, mRNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 44 | j | 93 | Total | C | N | O | S | 0 | 0 |
| | | | 740 | 460 | 143 | 135 | 2 | | |

- Molecule 45 is a protein called 39S ribosomal protein L53, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 45 | k | 96 | Total | C | N | O | S | 0 | 0 |
| | | | 743 | 462 | 143 | 133 | 5 | | |

- Molecule 46 is a protein called 39S ribosomal protein L54, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 46 | l | 72 | Total | C | N | O | S | 0 | 0 |
| | | | 619 | 394 | 112 | 111 | 2 | | |

- Molecule 47 is a protein called 39S ribosomal protein L55, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 47 | m | 45 | Total | C | N | O | S | 0 | 0 |
| | | | 372 | 232 | 76 | 62 | 2 | | |

- Molecule 48 is a protein called Ribosomal protein 63, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 48 | o | 94 | Total | C | N | O | S | 0 | 0 |
| | | | 797 | 501 | 165 | 128 | 3 | | |

- Molecule 49 is a protein called Peptidyl-tRNA hydrolase ICT1, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 49 | p | 152 | Total | C | N | O | S | 0 | 0 |
| | | | 1227 | 762 | 232 | 229 | 4 | | |

- Molecule 50 is a protein called Growth arrest and DNA damage-inducible proteins-interacting protein 1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 50 | q | 168 | Total | C | N | O | S | 0 | 0 |
| | | | 1294 | 801 | 255 | 233 | 5 | | |

- Molecule 51 is a protein called 39S ribosomal protein S18a, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 51 | r | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 1322 | 839 | 252 | 223 | 8 | | |

- Molecule 52 is a protein called 39S ribosomal protein S30, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 52 | s | 393 | Total | C | N | O | S | 0 | 0 |
| | | | 3178 | 2036 | 565 | 563 | 14 | | |

- Molecule 53 is a protein called P-site finger.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 53 | u | 65 | Total | C | N | O | 0 | 0 |
| | | | 325 | 195 | 65 | 65 | | |

- Molecule 54 is a protein called 39S ribosomal protein L12, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 54 | TA | 45 | Total | C | N | O | 0 | 0 |
| | | | 345 | 222 | 54 | 69 | | |
| 54 | TB | 27 | Total | C | N | O | 0 | 0 |
| | | | 213 | 137 | 33 | 43 | | |
| 54 | TC | 71 | Total | C | N | O | 0 | 0 |
| | | | 352 | 210 | 71 | 71 | | |

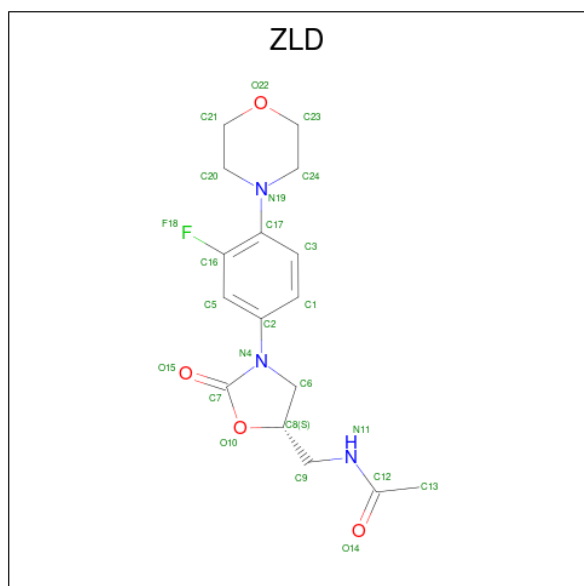
- Molecule 55 is ZINC ION (CCD ID: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|----|---------|
| 55 | 0 | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |
| 55 | 4 | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |
| 55 | r | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |

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

| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|-----|---------|
| 56 | A | 100 | Total | Mg | 0 |
| | | | 100 | 100 | |
| 56 | D | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 56 | g | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |

- Molecule 57 is N-{[(5S)-3-(3-fluoro-4-morpholin-4-ylphenyl)-2-oxo-1,3-oxazolidin-5-yl]methyl}acetamide (CCD ID: ZLD) (formula: C₁₆H₂₀FN₃O₄).



| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 57 | A | 1 | Total | C | F | N | O | 0 |
| | | | 24 | 16 | 1 | 3 | 4 | |

- Molecule 58 is water.

| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|---------------|-----------|---------|
| 58 | 0 | 16 | Total 16 | O 16 | 0 |
| 58 | 1 | 8 | Total 8 | O 8 | 0 |
| 58 | 2 | 10 | Total 10 | O 10 | 0 |
| 58 | 3 | 15 | Total 15 | O 15 | 0 |
| 58 | 4 | 7 | Total 7 | O 7 | 0 |
| 58 | 5 | 63 | Total 63 | O 63 | 0 |
| 58 | 6 | 99 | Total 99 | O 99 | 0 |
| 58 | 7 | 96 | Total 96 | O 96 | 0 |
| 58 | 8 | 44 | Total 44 | O 44 | 0 |
| 58 | 9 | 23 | Total 23 | O 23 | 0 |
| 58 | A | 1975 | Total 1975 | O 1975 | 0 |
| 58 | B | 99 | Total 99 | O 99 | 0 |
| 58 | D | 31 | Total 31 | O 31 | 0 |
| 58 | E | 51 | Total 51 | O 51 | 0 |
| 58 | F | 24 | Total 24 | O 24 | 0 |
| 58 | H | 29 | Total 29 | O 29 | 0 |
| 58 | I | 62 | Total 62 | O 62 | 0 |
| 58 | J | 107 | Total 107 | O 107 | 0 |
| 58 | K | 28 | Total 28 | O 28 | 0 |
| 58 | L | 14 | Total 14 | O 14 | 0 |
| 58 | M | 39 | Total 39 | O 39 | 0 |
| 58 | N | 49 | Total 49 | O 49 | 0 |

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| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|--------------|----------|---------|
| 58 | O | 26 | Total 26 | O 26 | 0 |
| 58 | P | 34 | Total 34 | O 34 | 0 |
| 58 | Q | 50 | Total 50 | O 50 | 0 |
| 58 | R | 20 | Total 20 | O 20 | 0 |
| 58 | S | 27 | Total 27 | O 27 | 0 |
| 58 | T | 29 | Total 29 | O 29 | 0 |
| 58 | U | 35 | Total 35 | O 35 | 0 |
| 58 | V | 37 | Total 37 | O 37 | 0 |
| 58 | W | 19 | Total 19 | O 19 | 0 |
| 58 | X | 30 | Total 30 | O 30 | 0 |
| 58 | Y | 22 | Total 22 | O 22 | 0 |
| 58 | Z | 27 | Total 27 | O 27 | 0 |
| 58 | a | 18 | Total 18 | O 18 | 0 |
| 58 | b | 34 | Total 34 | O 34 | 0 |
| 58 | c | 21 | Total 21 | O 21 | 0 |
| 58 | d | 10 | Total 10 | O 10 | 0 |
| 58 | e | 196 | Total 196 | O 196 | 0 |
| 58 | f | 59 | Total 59 | O 59 | 0 |
| 58 | g | 27 | Total 27 | O 27 | 0 |
| 58 | h | 36 | Total 36 | O 36 | 0 |
| 58 | i | 28 | Total 28 | O 28 | 0 |

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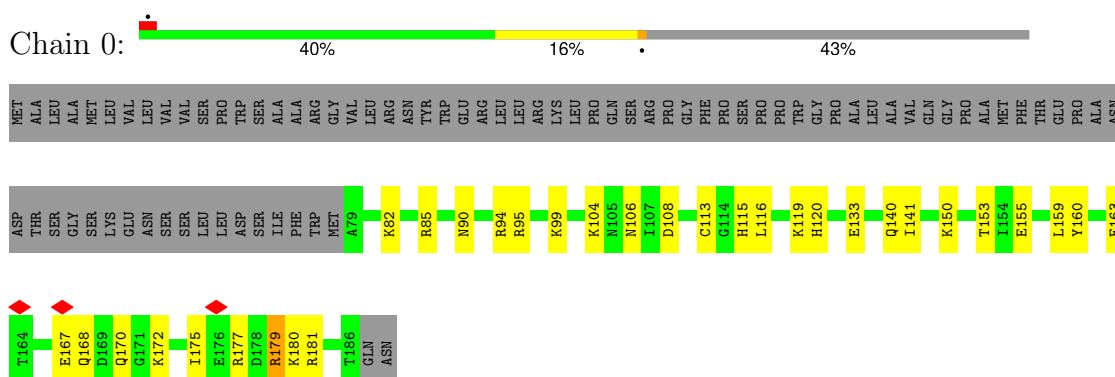
Continued from previous page...

| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------------|---------|---------|
| 58 | j | 24 | Total 24 | O 24 | 0 |
| 58 | k | 32 | Total 32 | O 32 | 0 |
| 58 | l | 50 | Total 50 | O 50 | 0 |
| 58 | m | 33 | Total 33 | O 33 | 0 |
| 58 | o | 18 | Total 18 | O 18 | 0 |
| 58 | p | 57 | Total 57 | O 57 | 0 |
| 58 | q | 6 | Total 6 | O 6 | 0 |
| 58 | r | 44 | Total 44 | O 44 | 0 |
| 58 | s | 57 | Total 57 | O 57 | 0 |
| 58 | u | 32 | Total 32 | O 32 | 0 |
| 58 | TA | 43 | Total 43 | O 43 | 0 |
| 58 | TB | 22 | Total 22 | O 22 | 0 |
| 58 | TC | 37 | Total 37 | O 37 | 0 |

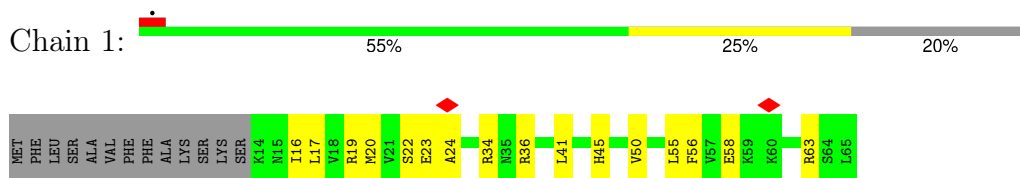
3 Residue-property plots [i](#)

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.

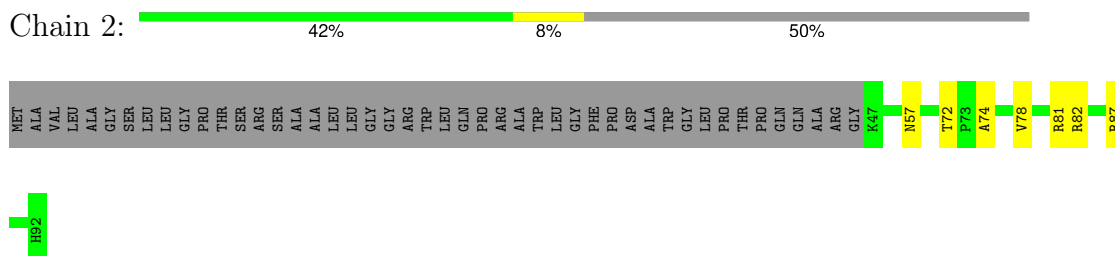
- Molecule 1: 39S ribosomal protein L32, mitochondrial



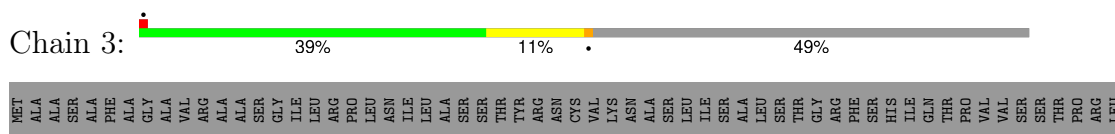
- Molecule 2: 39S ribosomal protein L33, mitochondrial

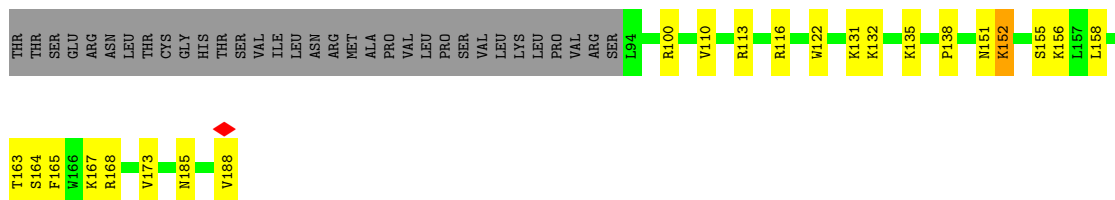


- Molecule 3: 39S ribosomal protein L34, mitochondrial



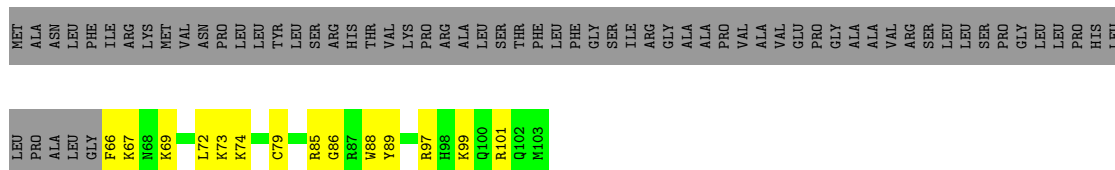
- Molecule 4: 39S ribosomal protein L35, mitochondrial





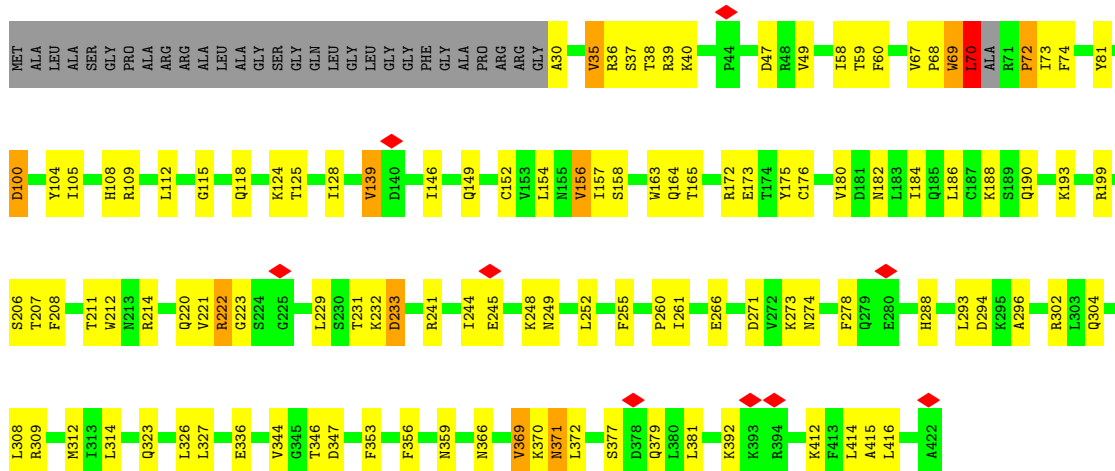
- Molecule 5: 39S ribosomal protein L36, mitochondrial

Chain 4: 23% 14% 63%



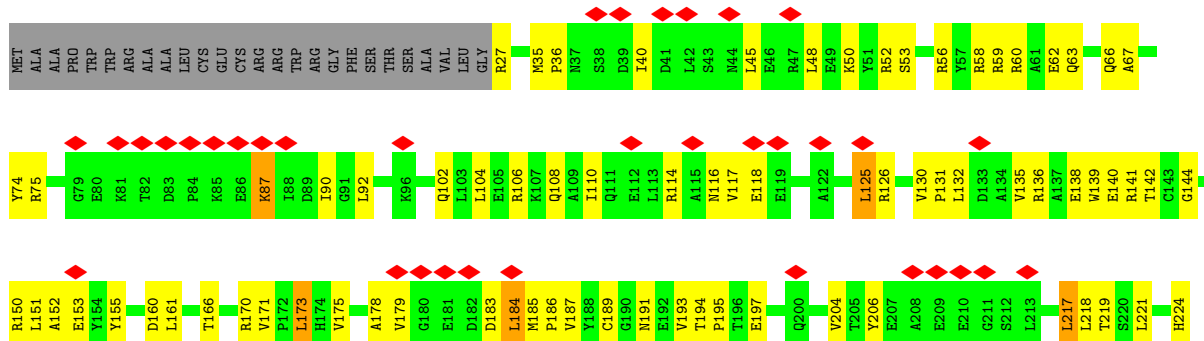
- Molecule 6: 39S ribosomal protein L37, mitochondrial

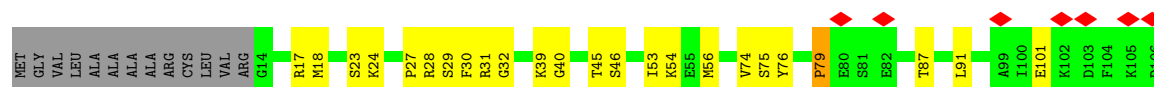
Chain 5: 65% 25% 7%

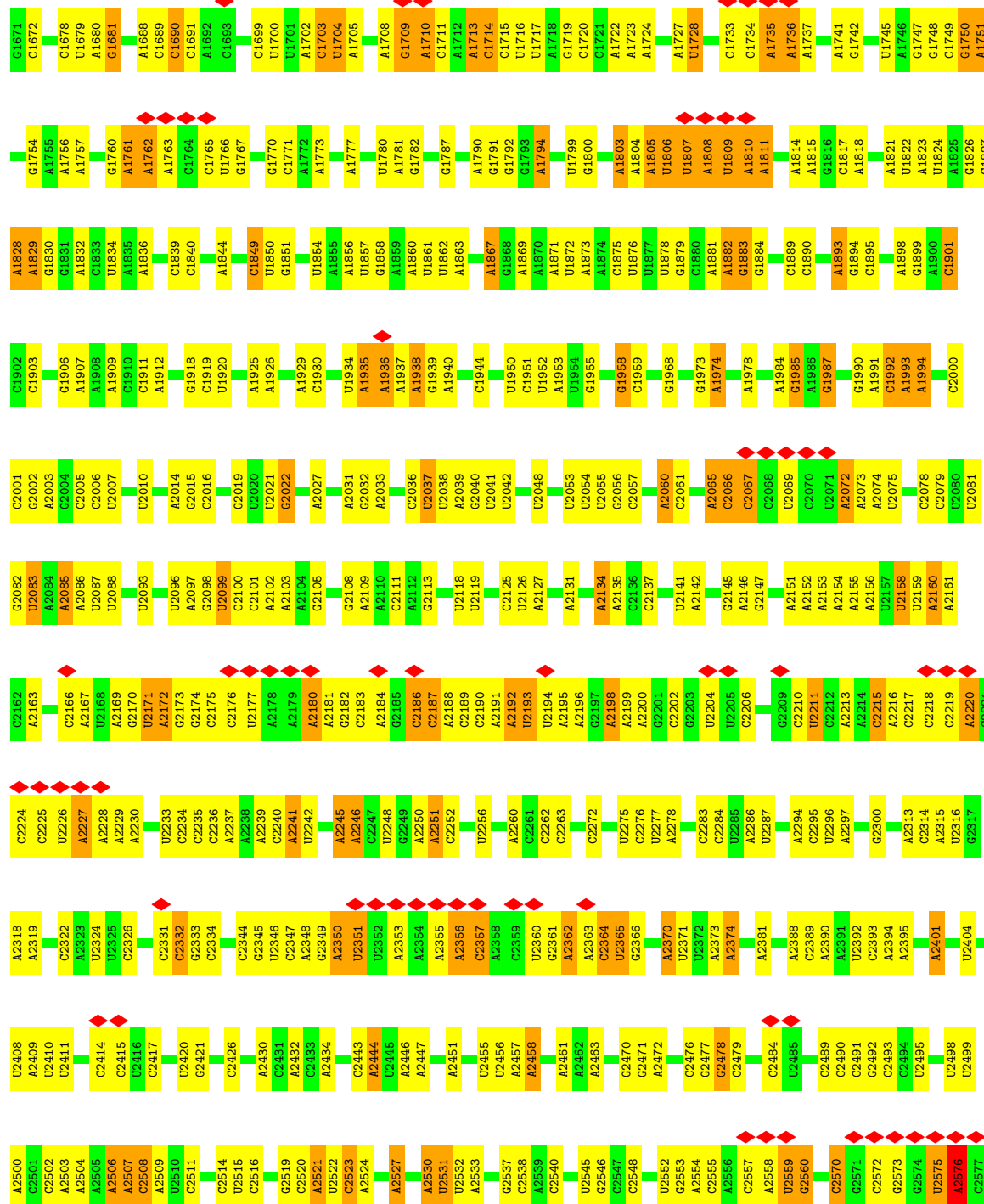


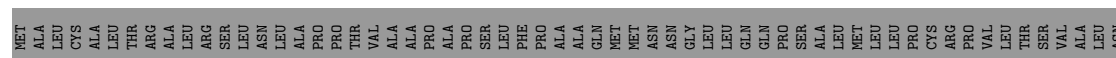
- Molecule 7: 39S ribosomal protein L38, mitochondrial

Chain 6: 14% 55% 36% 7%

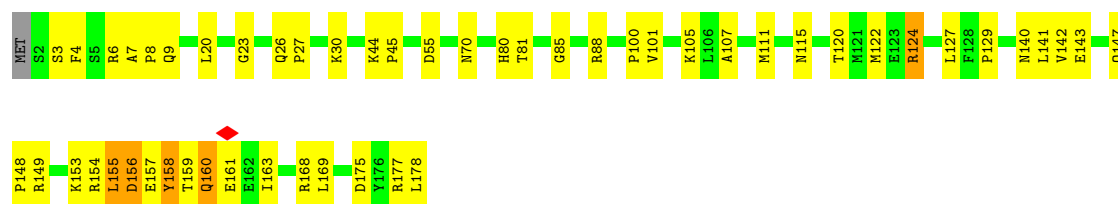






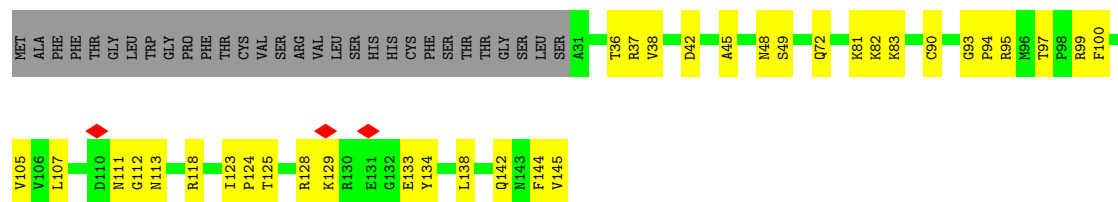


Chain K:  70% 26% ..



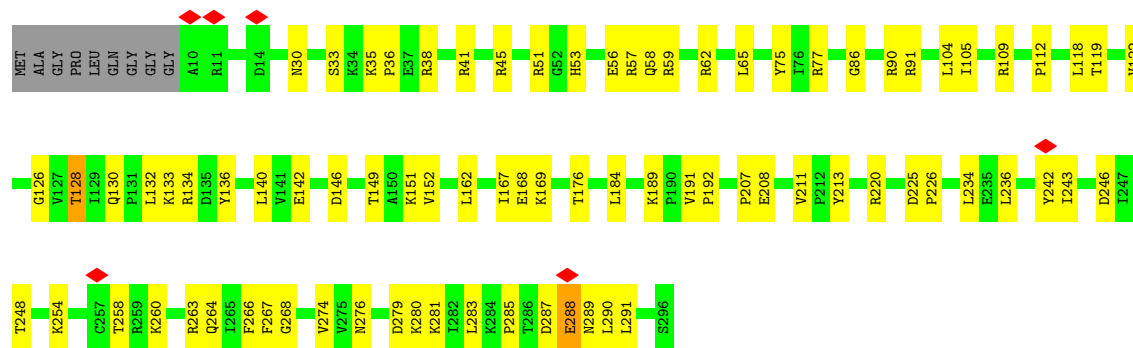
- Molecule 20: 39S ribosomal protein L14, mitochondrial

Chain L:  55% 24% 21%



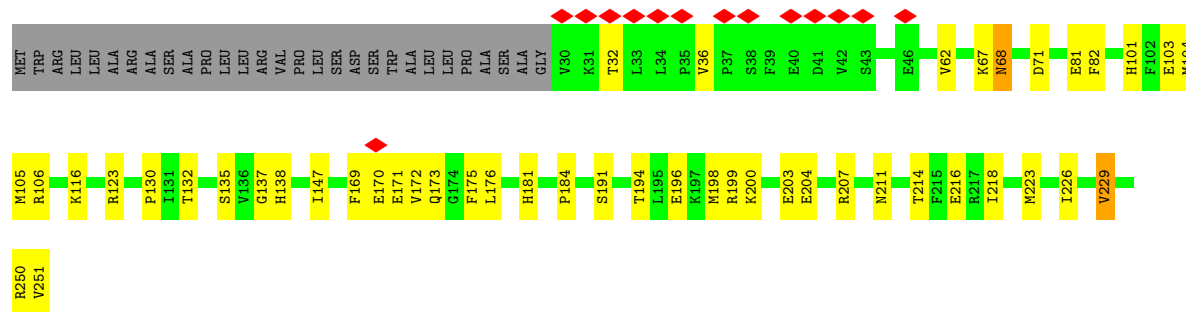
- Molecule 21: 39S ribosomal protein L15, mitochondrial

Chain M:  69% 27% ..



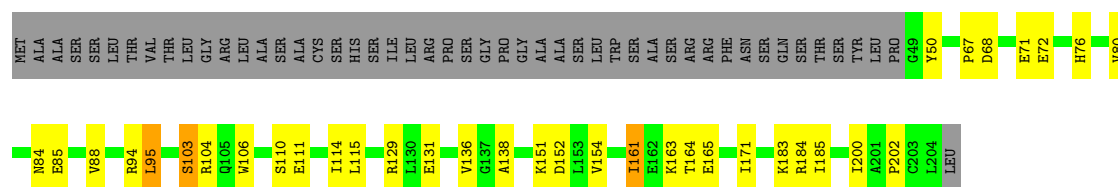
- Molecule 22: 39S ribosomal protein L16, mitochondrial

Chain N:  6% 69% 18% 12%



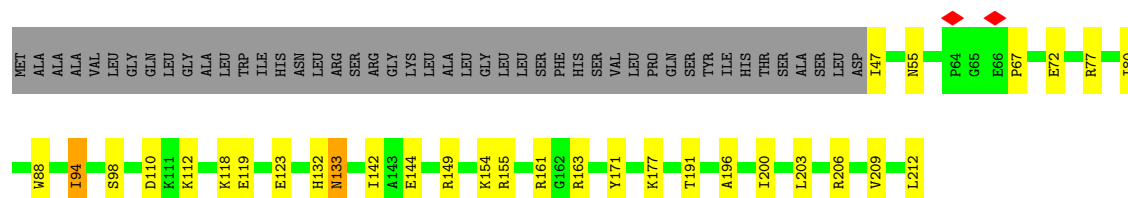
- Molecule 23: 39S ribosomal protein L17, mitochondrial

Chain S: 




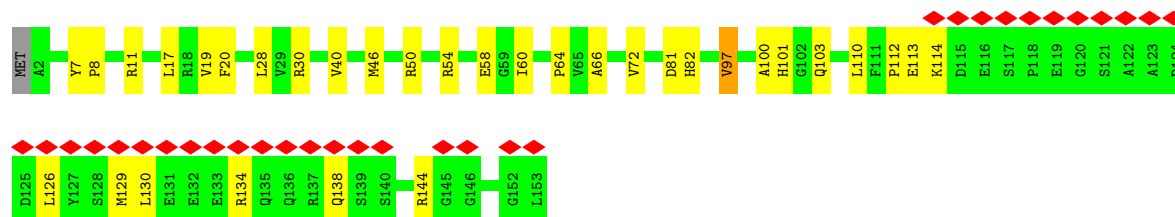
- Molecule 28: 39S ribosomal protein L22, mitochondrial

Chain T: 



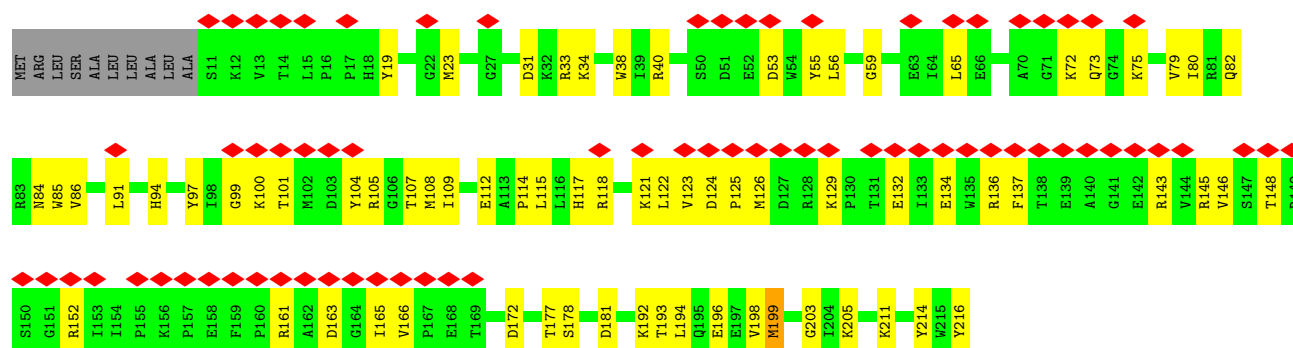
- Molecule 29: 39S ribosomal protein L23, mitochondrial

Chain U: 



- Molecule 30: 39S ribosomal protein L24, mitochondrial

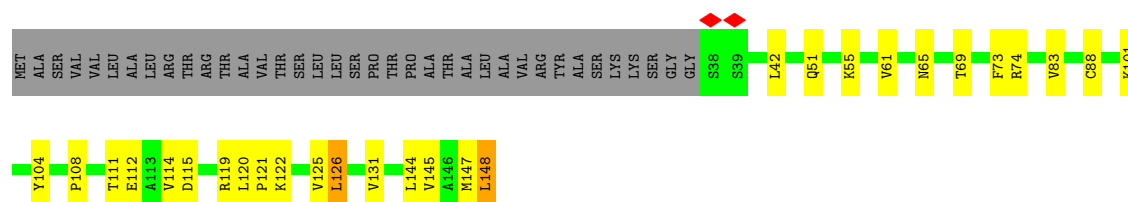
Chain V: 



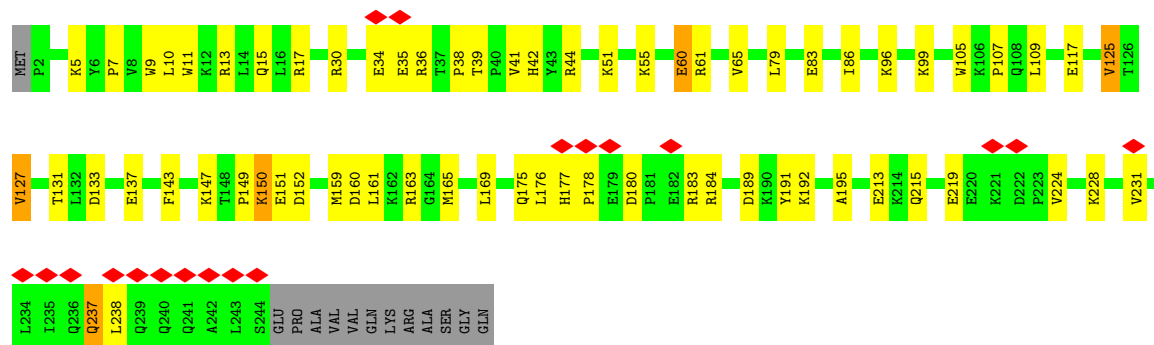
- Molecule 31: 39S ribosomal protein L27, mitochondrial

Chain W: 

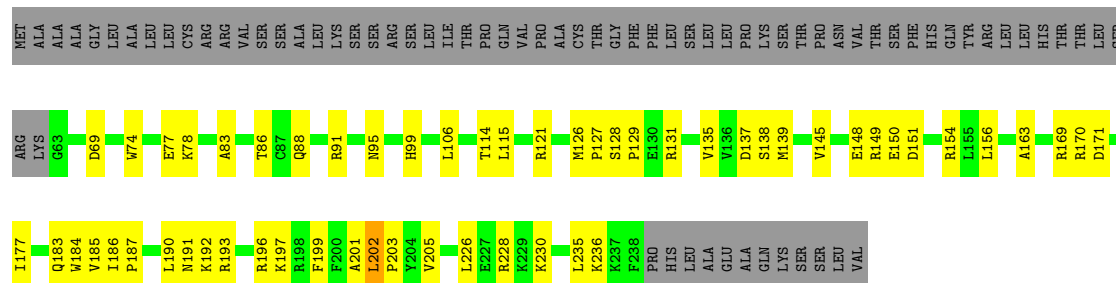




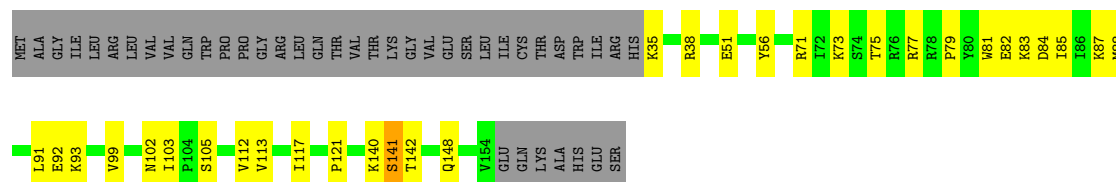
- Molecule 32: 39S ribosomal protein L28, mitochondrial



- Molecule 33: 39S ribosomal protein L47, mitochondrial

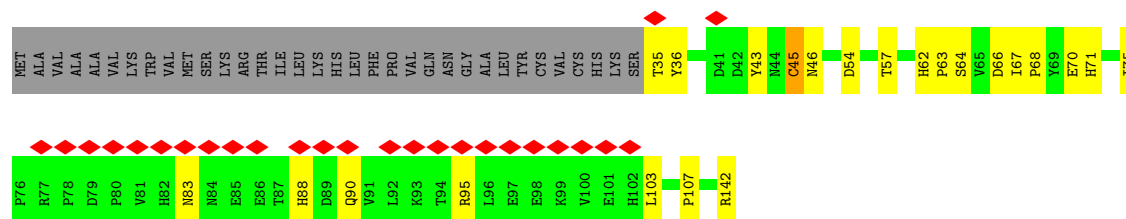


- Molecule 34: 39S ribosomal protein L30, mitochondrial



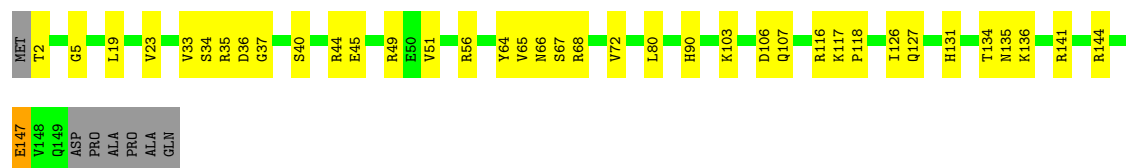
- Molecule 35: 39S ribosomal protein L42, mitochondrial





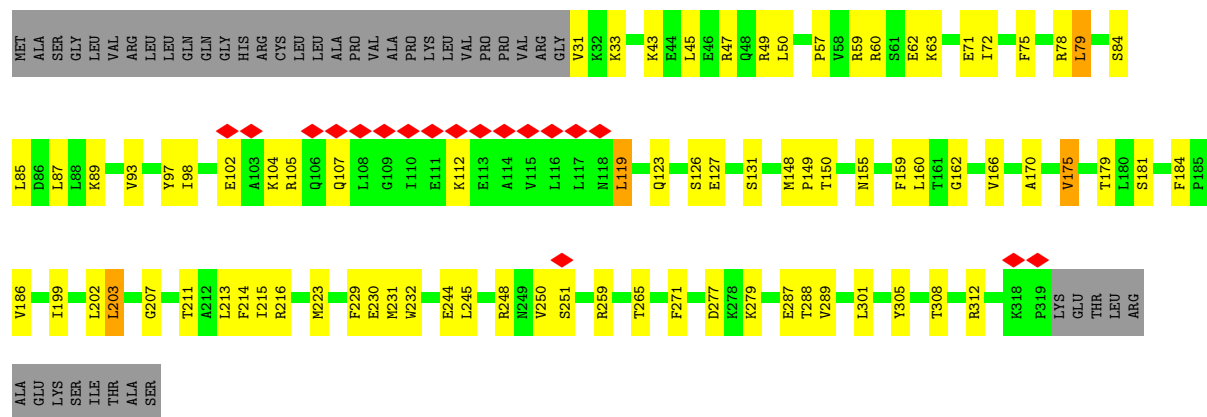
- Molecule 36: 39S ribosomal protein L43, mitochondrial

Chain b: 71% 24% 5%



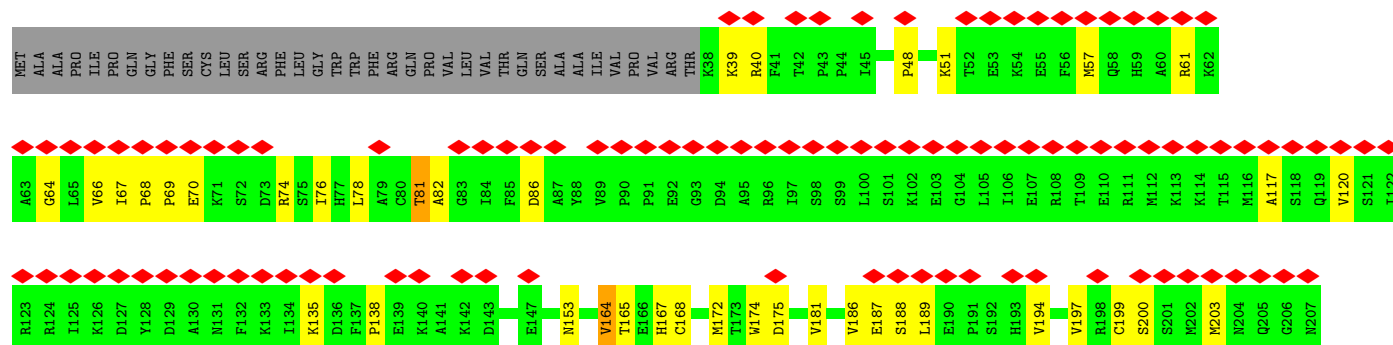
- Molecule 37: 39S ribosomal protein L44, mitochondrial

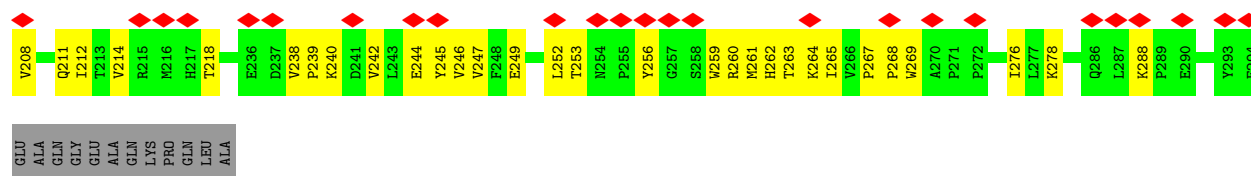
Chain c: 5% 63% 23% 13%



- Molecule 38: 39S ribosomal protein L45, mitochondrial

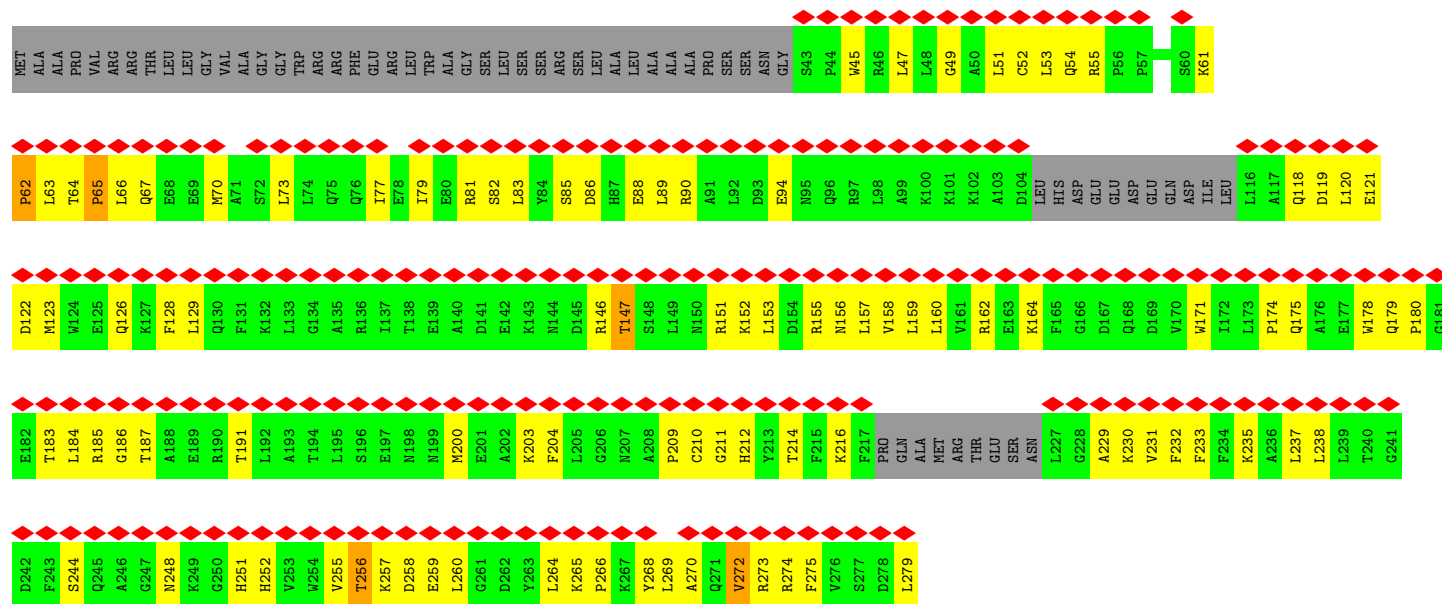
Chain d: 42% 61% 22% 16%





• Molecule 39: 39S ribosomal protein L46, mitochondrial

Chain e:



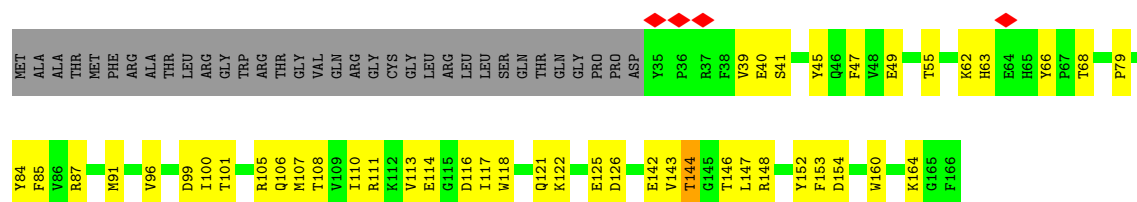
• Molecule 40: 39S ribosomal protein L48, mitochondrial

Chain f:

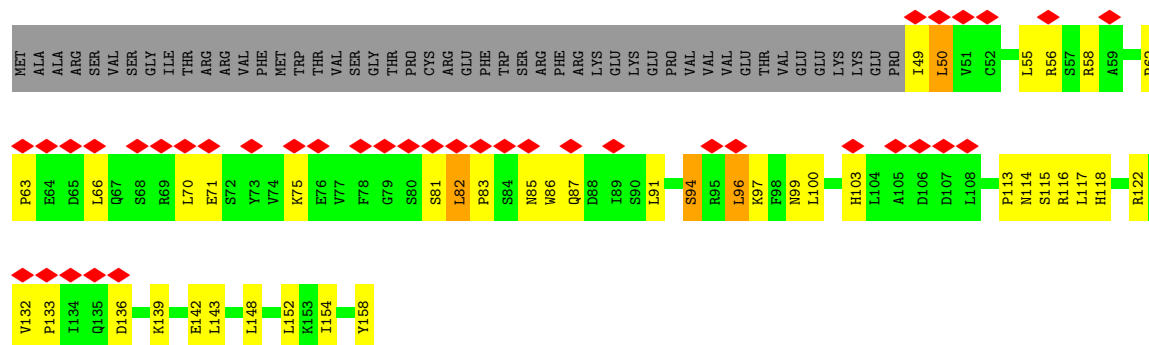


• Molecule 41: 39S ribosomal protein L49, mitochondrial

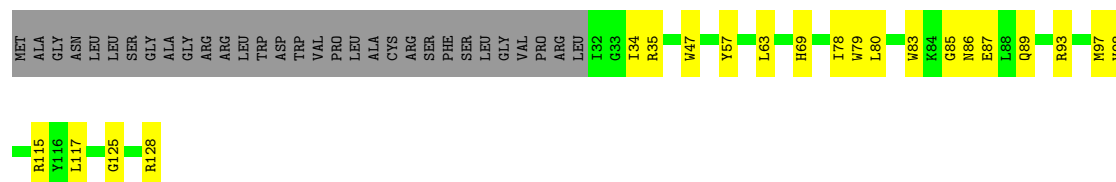
Chain g:



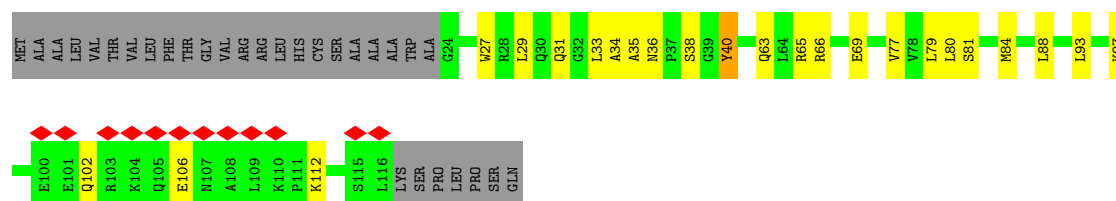
- Molecule 42: 39S ribosomal protein L50, mitochondrial



- Molecule 43: 39S ribosomal protein L51, mitochondrial

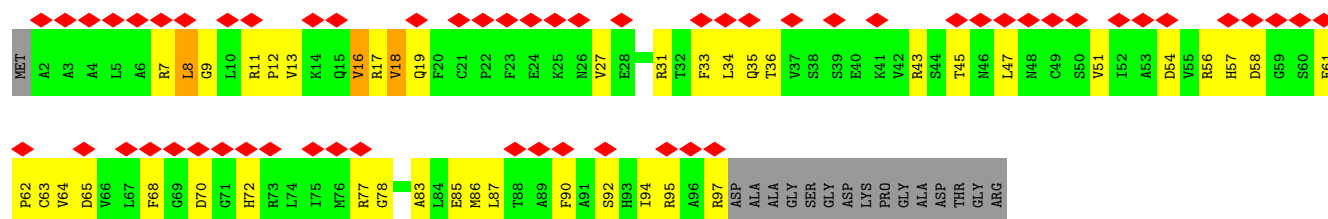


- Molecule 44: cDNA FLJ76418, highly similar to Homo sapiens mitochondrial ribosomal protein L52 (MRPL52), transcript variant 1, mRNA

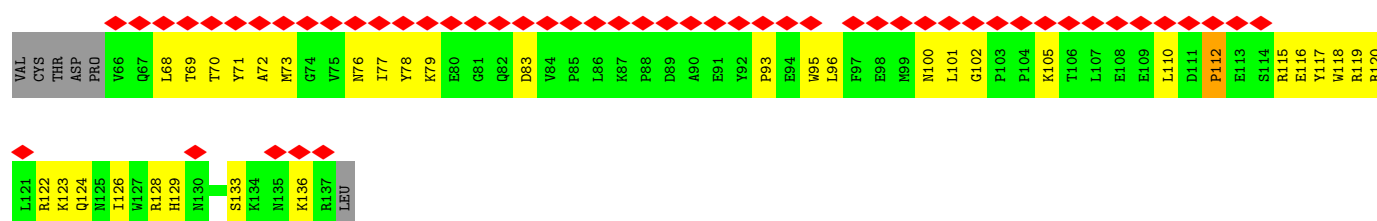
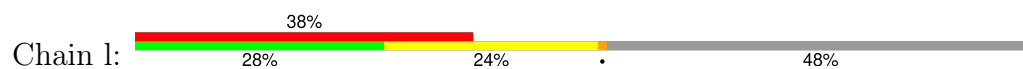


- Molecule 45: 39S ribosomal protein L53, mitochondrial

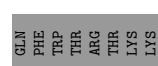
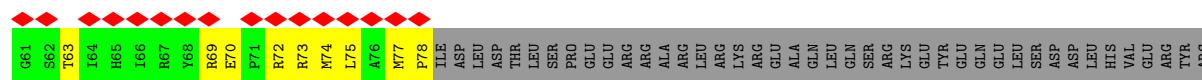
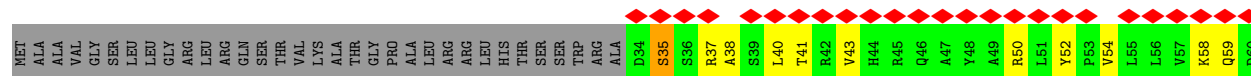




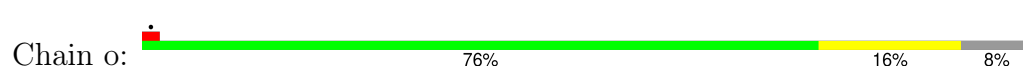
• Molecule 46: 39S ribosomal protein L54, mitochondrial



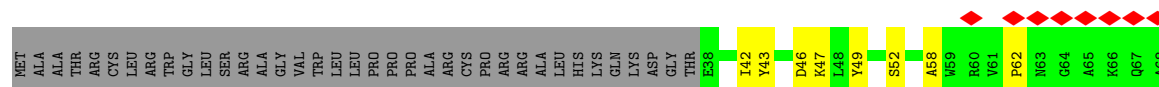
• Molecule 47: 39S ribosomal protein L55, mitochondrial



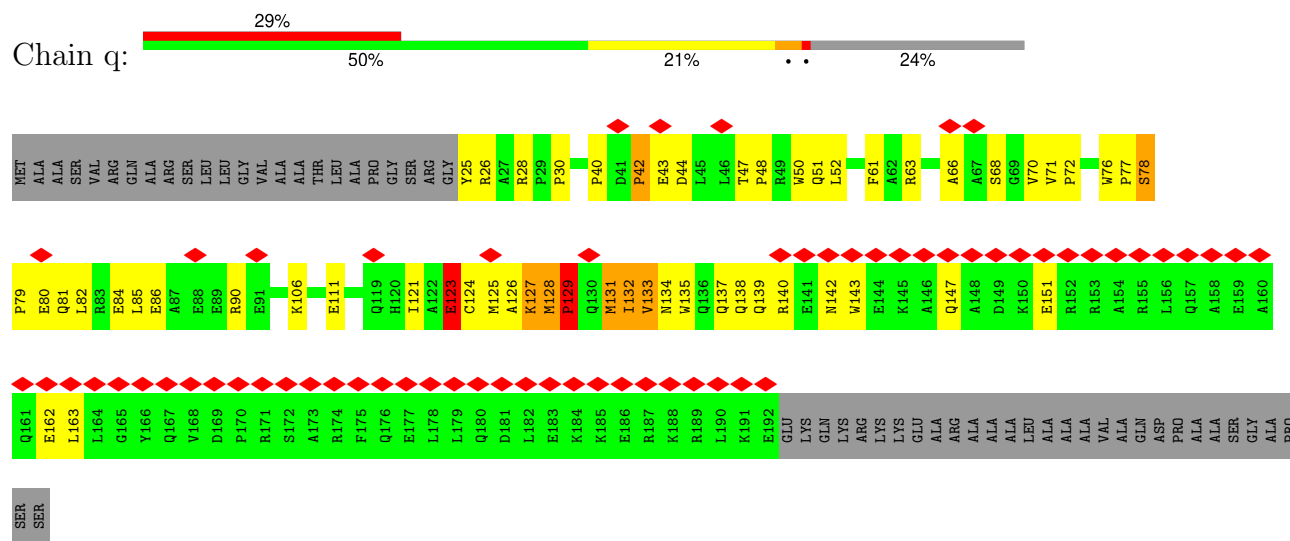
• Molecule 48: Ribosomal protein 63, mitochondrial



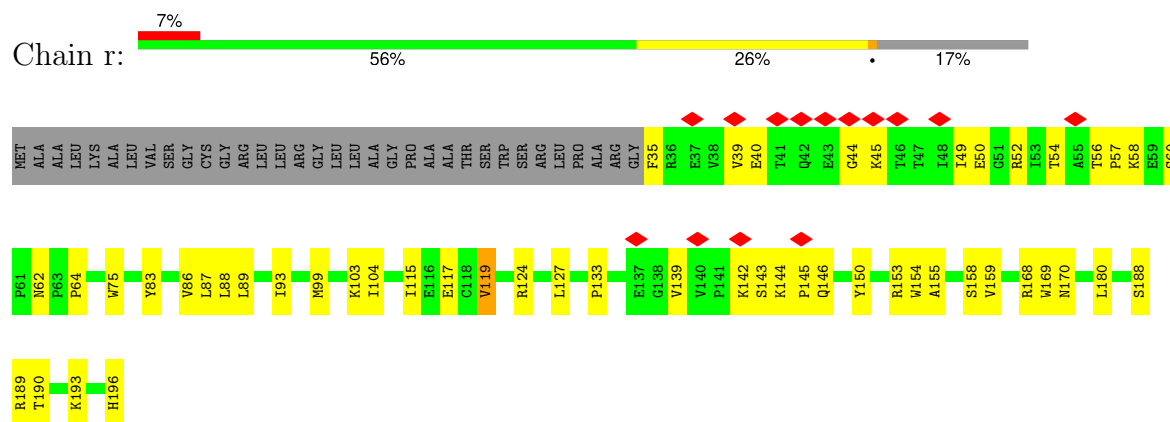
• Molecule 49: Peptidyl-tRNA hydrolase ICT1, mitochondrial



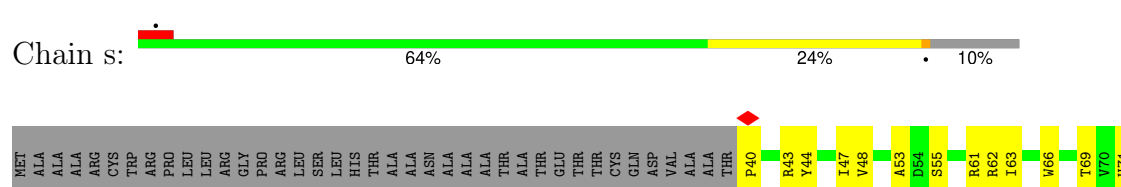
- Molecule 50: Growth arrest and DNA damage-inducible proteins-interacting protein 1

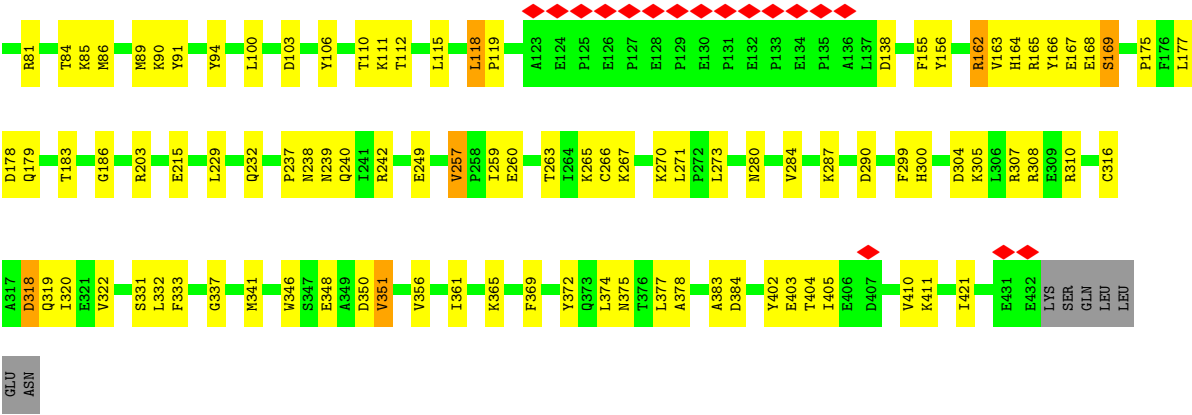


- Molecule 51: 39S ribosomal protein S18a, mitochondrial

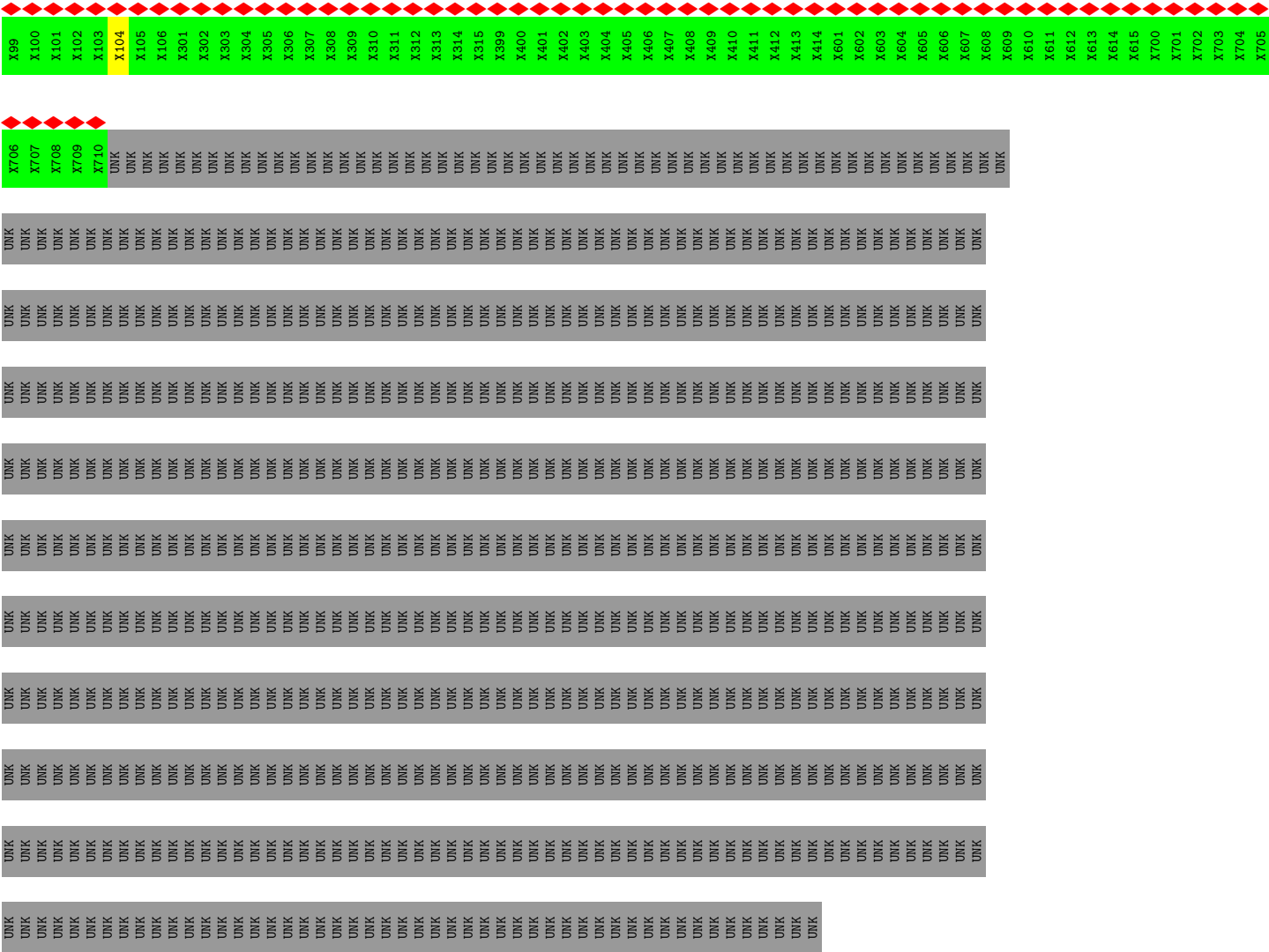


- Molecule 52: 39S ribosomal protein S30, mitochondrial





• Molecule 53: P-site finger



• Molecule 54: 39S ribosomal protein L12, mitochondrial

4 Experimental information

| Property | Value | Source |
|--------------------------------------|---|-----------|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 347872 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope | FEI TALOS ARCTICA | Depositor |
| Voltage (kV) | 200 | Depositor |
| Electron dose ($e^-/\text{\AA}^2$) | 21 | Depositor |
| Minimum defocus (nm) | 500 | Depositor |
| Maximum defocus (nm) | 2000 | Depositor |
| Magnification | Not provided | |
| Image detector | GATAN K3 (6k x 4k) | Depositor |
| Maximum map value | 4.661 | Depositor |
| Minimum map value | -2.742 | Depositor |
| Average map value | -0.001 | Depositor |
| Map value standard deviation | 0.096 | Depositor |
| Recommended contour level | 0.38 | Depositor |
| Map size (Å) | 484.4, 484.4, 484.4 | wwPDB |
| Map dimensions | 560, 560, 560 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 0.865, 0.865, 0.865 | Depositor |

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN, ZLD

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 | 0.19 | 0/895 | 0.41 | 0/1201 |
| 2 | 1 | 0.16 | 0/438 | 0.42 | 0/583 |
| 3 | 2 | 0.18 | 0/382 | 0.29 | 0/507 |
| 4 | 3 | 0.18 | 0/852 | 0.32 | 0/1136 |
| 5 | 4 | 0.14 | 0/350 | 0.36 | 0/461 |
| 6 | 5 | 0.21 | 0/3300 | 0.40 | 0/4495 |
| 7 | 6 | 0.20 | 0/3043 | 0.51 | 3/4140 (0.1%) |
| 8 | 7 | 0.14 | 0/2467 | 0.36 | 0/3337 |
| 9 | 8 | 0.15 | 0/855 | 0.36 | 0/1152 |
| 10 | 9 | 0.19 | 0/1025 | 0.42 | 1/1379 (0.1%) |
| 11 | A | 0.33 | 9/36246 (0.0%) | 0.33 | 4/56422 (0.0%) |
| 12 | B | 0.10 | 0/1328 | 0.25 | 0/2056 |
| 13 | D | 0.16 | 0/1904 | 0.37 | 0/2561 |
| 14 | E | 0.15 | 0/2479 | 0.37 | 0/3360 |
| 15 | F | 0.18 | 0/2071 | 0.42 | 0/2817 |
| 16 | H | 0.17 | 0/820 | 0.46 | 0/1102 |
| 17 | I | 0.48 | 2/1467 (0.1%) | 0.78 | 4/1984 (0.2%) |
| 18 | J | 0.87 | 6/1348 (0.4%) | 1.35 | 11/1813 (0.6%) |
| 19 | K | 0.19 | 0/1495 | 0.41 | 0/2029 |
| 20 | L | 0.17 | 0/904 | 0.45 | 2/1218 (0.2%) |
| 21 | M | 0.19 | 0/2359 | 0.44 | 0/3185 |
| 22 | N | 0.17 | 0/1833 | 0.39 | 0/2468 |
| 23 | O | 0.18 | 0/1269 | 0.38 | 0/1708 |
| 24 | P | 0.19 | 0/1191 | 0.47 | 0/1611 |
| 25 | Q | 0.15 | 0/1875 | 0.34 | 0/2523 |
| 26 | R | 0.21 | 0/1174 | 0.43 | 0/1572 |
| 27 | S | 0.19 | 0/1276 | 0.39 | 0/1729 |
| 28 | T | 0.20 | 0/1402 | 0.39 | 1/1886 (0.1%) |
| 29 | U | 0.18 | 0/1252 | 0.38 | 0/1697 |
| 30 | V | 0.14 | 0/1727 | 0.40 | 0/2341 |
| 31 | W | 0.18 | 0/893 | 0.40 | 0/1204 |
| 32 | X | 0.21 | 0/2090 | 0.41 | 0/2825 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|------------------|-------------|------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 33 | Y | 0.16 | 0/1552 | 0.34 | 0/2079 |
| 34 | Z | 0.18 | 0/1003 | 0.37 | 0/1354 |
| 35 | a | 0.16 | 0/923 | 0.34 | 0/1254 |
| 36 | b | 0.17 | 0/1202 | 0.36 | 0/1626 |
| 37 | c | 0.16 | 0/2371 | 0.32 | 0/3205 |
| 38 | d | 0.72 | 3/2132 (0.1%) | 0.78 | 5/2887 (0.2%) |
| 39 | e | 0.59 | 3/1797 (0.2%) | 0.95 | 6/2422 (0.2%) |
| 40 | f | 0.19 | 0/1144 | 0.54 | 2/1551 (0.1%) |
| 41 | g | 0.18 | 0/1132 | 0.43 | 0/1543 |
| 42 | h | 0.16 | 0/917 | 0.43 | 0/1249 |
| 43 | i | 0.21 | 0/849 | 0.41 | 0/1135 |
| 44 | j | 0.16 | 0/755 | 0.38 | 0/1016 |
| 45 | k | 0.44 | 2/754 (0.3%) | 0.88 | 4/1017 (0.4%) |
| 46 | l | 0.68 | 1/636 (0.2%) | 1.04 | 4/860 (0.5%) |
| 47 | m | 0.15 | 0/379 | 0.40 | 0/510 |
| 48 | o | 0.17 | 0/818 | 0.43 | 0/1097 |
| 49 | p | 0.18 | 0/1246 | 0.49 | 1/1675 (0.1%) |
| 50 | q | 0.35 | 1/1325 (0.1%) | 0.55 | 1/1799 (0.1%) |
| 51 | r | 0.17 | 0/1362 | 0.39 | 0/1846 |
| 52 | s | 0.17 | 0/3262 | 0.39 | 2/4435 (0.0%) |
| 54 | TA | 1.34 | 3/349 (0.9%) | 2.02 | 5/475 (1.1%) |
| 54 | TB | 0.12 | 0/212 | 0.36 | 0/286 |
| 54 | TC | 0.09 | 0/351 | 0.24 | 0/488 |
| All | All | 0.31 | 30/108481 (0.0%) | 0.46 | 56/154311 (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 |
|-----|-------|---------------------|---------------------|
| 13 | D | 0 | 1 |
| 14 | E | 0 | 1 |
| 19 | K | 0 | 1 |
| 24 | P | 0 | 1 |
| 33 | Y | 0 | 1 |
| 34 | Z | 0 | 1 |
| 42 | h | 0 | 2 |
| 49 | p | 0 | 1 |
| 50 | q | 0 | 1 |
| All | All | 0 | 10 |

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

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|--------|-------------|----------|
| 38 | d | 268 | PRO | CG-CD | -30.05 | 0.48 | 1.50 |
| 11 | A | 2576 | A | C6-N1 | 23.35 | 1.82 | 1.35 |
| 18 | J | 136 | PRO | CG-CD | -22.68 | 0.73 | 1.50 |
| 11 | A | 2576 | A | N1-C2 | 22.25 | 1.78 | 1.34 |
| 54 | TA | 52 | PRO | CG-CD | -21.99 | 0.76 | 1.50 |

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

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|--------|-------------|----------|
| 54 | TA | 52 | PRO | N-CD-CG | -32.86 | 53.91 | 103.20 |
| 38 | d | 268 | PRO | N-CD-CG | -28.97 | 59.74 | 103.20 |
| 39 | e | 62 | PRO | N-CD-CG | -28.41 | 60.59 | 103.20 |
| 18 | J | 136 | PRO | N-CD-CG | -25.46 | 65.00 | 103.20 |
| 39 | e | 62 | PRO | CA-CB-CG | -21.30 | 64.02 | 104.50 |

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 13 | D | 206 | TYR | Peptide |
| 14 | E | 316 | PHE | Peptide |
| 19 | K | 3 | SER | Peptide |
| 24 | P | 68 | TRP | Peptide |
| 33 | Y | 202 | LEU | Peptide |

5.2 Too-close contacts [i](#)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | 0 | 880 | 0 | 902 | 27 | 0 |
| 2 | 1 | 433 | 0 | 475 | 17 | 0 |
| 3 | 2 | 376 | 0 | 406 | 5 | 0 |
| 4 | 3 | 831 | 0 | 883 | 16 | 0 |
| 5 | 4 | 342 | 0 | 361 | 12 | 0 |
| 6 | 5 | 3205 | 0 | 3201 | 81 | 0 |
| 7 | 6 | 2948 | 0 | 2841 | 122 | 0 |
| 8 | 7 | 2410 | 0 | 2415 | 63 | 0 |
| 9 | 8 | 836 | 0 | 844 | 37 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 10 | 9 | 997 | 0 | 987 | 34 | 0 |
| 11 | A | 32395 | 0 | 16450 | 495 | 0 |
| 12 | B | 1191 | 0 | 607 | 41 | 0 |
| 13 | D | 1866 | 0 | 1927 | 60 | 0 |
| 14 | E | 2410 | 0 | 2418 | 47 | 0 |
| 15 | F | 2013 | 0 | 2044 | 57 | 0 |
| 16 | H | 806 | 0 | 849 | 27 | 0 |
| 17 | I | 1435 | 0 | 1521 | 58 | 0 |
| 18 | J | 1330 | 0 | 1407 | 62 | 0 |
| 19 | K | 1451 | 0 | 1448 | 40 | 0 |
| 20 | L | 889 | 0 | 941 | 23 | 0 |
| 21 | M | 2305 | 0 | 2378 | 67 | 0 |
| 22 | N | 1786 | 0 | 1817 | 41 | 0 |
| 23 | O | 1245 | 0 | 1283 | 35 | 0 |
| 24 | P | 1165 | 0 | 1162 | 54 | 0 |
| 25 | Q | 1834 | 0 | 1872 | 34 | 0 |
| 26 | R | 1153 | 0 | 1214 | 30 | 0 |
| 27 | S | 1251 | 0 | 1322 | 28 | 0 |
| 28 | T | 1368 | 0 | 1410 | 19 | 0 |
| 29 | U | 1222 | 0 | 1187 | 31 | 0 |
| 30 | V | 1682 | 0 | 1692 | 61 | 0 |
| 31 | W | 871 | 0 | 898 | 21 | 0 |
| 32 | X | 2035 | 0 | 2054 | 43 | 0 |
| 33 | Y | 1517 | 0 | 1561 | 42 | 0 |
| 34 | Z | 978 | 0 | 1030 | 24 | 0 |
| 35 | a | 896 | 0 | 847 | 19 | 0 |
| 36 | b | 1178 | 0 | 1180 | 35 | 0 |
| 37 | c | 2322 | 0 | 2338 | 55 | 0 |
| 38 | d | 2075 | 0 | 2037 | 49 | 0 |
| 39 | e | 1762 | 0 | 1767 | 94 | 0 |
| 40 | f | 1126 | 0 | 1106 | 51 | 0 |
| 41 | g | 1096 | 0 | 1081 | 35 | 0 |
| 42 | h | 894 | 0 | 881 | 34 | 0 |
| 43 | i | 827 | 0 | 857 | 18 | 0 |
| 44 | j | 740 | 0 | 741 | 20 | 0 |
| 45 | k | 743 | 0 | 758 | 33 | 0 |
| 46 | l | 619 | 0 | 611 | 29 | 0 |
| 47 | m | 372 | 0 | 387 | 31 | 0 |
| 48 | o | 797 | 0 | 804 | 15 | 0 |
| 49 | p | 1227 | 0 | 1239 | 51 | 0 |
| 50 | q | 1294 | 0 | 1178 | 58 | 0 |
| 51 | r | 1322 | 0 | 1349 | 45 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 52 | s | 3178 | 0 | 3124 | 73 | 0 |
| 53 | u | 325 | 0 | 77 | 1 | 0 |
| 54 | TA | 345 | 0 | 364 | 10 | 0 |
| 54 | TB | 213 | 0 | 234 | 8 | 0 |
| 54 | TC | 352 | 0 | 169 | 0 | 0 |
| 55 | 0 | 1 | 0 | 0 | 0 | 0 |
| 55 | 4 | 1 | 0 | 0 | 0 | 0 |
| 55 | r | 1 | 0 | 0 | 0 | 0 |
| 56 | A | 100 | 0 | 0 | 0 | 0 |
| 56 | D | 1 | 0 | 0 | 0 | 0 |
| 56 | g | 1 | 0 | 0 | 0 | 0 |
| 57 | A | 24 | 0 | 20 | 3 | 0 |
| 58 | 0 | 16 | 0 | 0 | 1 | 0 |
| 58 | 1 | 8 | 0 | 0 | 0 | 0 |
| 58 | 2 | 10 | 0 | 0 | 0 | 0 |
| 58 | 3 | 15 | 0 | 0 | 1 | 0 |
| 58 | 4 | 7 | 0 | 0 | 0 | 0 |
| 58 | 5 | 63 | 0 | 0 | 1 | 0 |
| 58 | 6 | 99 | 0 | 0 | 2 | 0 |
| 58 | 7 | 96 | 0 | 0 | 7 | 0 |
| 58 | 8 | 44 | 0 | 0 | 3 | 0 |
| 58 | 9 | 23 | 0 | 0 | 0 | 0 |
| 58 | A | 1975 | 0 | 0 | 11 | 0 |
| 58 | B | 99 | 0 | 0 | 3 | 0 |
| 58 | D | 31 | 0 | 0 | 1 | 0 |
| 58 | E | 51 | 0 | 0 | 0 | 0 |
| 58 | F | 24 | 0 | 0 | 2 | 0 |
| 58 | H | 29 | 0 | 0 | 1 | 0 |
| 58 | I | 62 | 0 | 0 | 6 | 0 |
| 58 | J | 107 | 0 | 0 | 5 | 0 |
| 58 | K | 28 | 0 | 0 | 0 | 0 |
| 58 | L | 14 | 0 | 0 | 1 | 0 |
| 58 | M | 39 | 0 | 0 | 0 | 0 |
| 58 | N | 49 | 0 | 0 | 0 | 0 |
| 58 | O | 26 | 0 | 0 | 0 | 0 |
| 58 | P | 34 | 0 | 0 | 2 | 0 |
| 58 | Q | 50 | 0 | 0 | 1 | 0 |
| 58 | R | 20 | 0 | 0 | 3 | 0 |
| 58 | S | 27 | 0 | 0 | 0 | 0 |
| 58 | T | 29 | 0 | 0 | 0 | 0 |
| 58 | TA | 43 | 0 | 0 | 0 | 0 |
| 58 | TB | 22 | 0 | 0 | 3 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 58 | TC | 37 | 0 | 0 | 0 | 0 |
| 58 | U | 35 | 0 | 0 | 1 | 0 |
| 58 | V | 37 | 0 | 0 | 2 | 0 |
| 58 | W | 19 | 0 | 0 | 0 | 0 |
| 58 | X | 30 | 0 | 0 | 2 | 0 |
| 58 | Y | 22 | 0 | 0 | 1 | 0 |
| 58 | Z | 27 | 0 | 0 | 2 | 0 |
| 58 | a | 18 | 0 | 0 | 1 | 0 |
| 58 | b | 34 | 0 | 0 | 1 | 0 |
| 58 | c | 21 | 0 | 0 | 0 | 0 |
| 58 | d | 10 | 0 | 0 | 0 | 0 |
| 58 | e | 196 | 0 | 0 | 11 | 0 |
| 58 | f | 59 | 0 | 0 | 4 | 0 |
| 58 | g | 27 | 0 | 0 | 1 | 0 |
| 58 | h | 36 | 0 | 0 | 2 | 0 |
| 58 | i | 28 | 0 | 0 | 0 | 0 |
| 58 | j | 24 | 0 | 0 | 1 | 0 |
| 58 | k | 32 | 0 | 0 | 2 | 0 |
| 58 | l | 50 | 0 | 0 | 2 | 0 |
| 58 | m | 33 | 0 | 0 | 3 | 0 |
| 58 | o | 18 | 0 | 0 | 0 | 0 |
| 58 | p | 57 | 0 | 0 | 2 | 0 |
| 58 | q | 6 | 0 | 0 | 0 | 0 |
| 58 | r | 44 | 0 | 0 | 1 | 0 |
| 58 | s | 57 | 0 | 0 | 1 | 0 |
| 58 | u | 32 | 0 | 0 | 0 | 0 |
| All | All | 107417 | 0 | 86956 | 2218 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

The worst 5 of 2218 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|----------------|--------------------------|-------------------|
| 11:A:2576:A:C5 | 11:A:2576:A:C6 | 1.77 | 1.65 |
| 11:A:2576:A:C4 | 11:A:2576:A:N3 | 1.78 | 1.52 |
| 11:A:2576:A:N3 | 11:A:2576:A:C2 | 1.75 | 1.51 |
| 11:A:2576:A:C2 | 11:A:2576:A:N1 | 1.78 | 1.48 |
| 11:A:2576:A:C6 | 11:A:2576:A:N1 | 1.82 | 1.47 |

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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 | 106/188 (56%) | 94 (89%) | 12 (11%) | 0 | 100 | 100 |
| 2 | 1 | 50/65 (77%) | 47 (94%) | 3 (6%) | 0 | 100 | 100 |
| 3 | 2 | 44/92 (48%) | 43 (98%) | 1 (2%) | 0 | 100 | 100 |
| 4 | 3 | 93/188 (50%) | 92 (99%) | 1 (1%) | 0 | 100 | 100 |
| 5 | 4 | 36/103 (35%) | 35 (97%) | 1 (3%) | 0 | 100 | 100 |
| 6 | 5 | 391/423 (92%) | 373 (95%) | 16 (4%) | 2 (0%) | 25 | 45 |
| 7 | 6 | 352/380 (93%) | 324 (92%) | 28 (8%) | 0 | 100 | 100 |
| 8 | 7 | 295/338 (87%) | 279 (95%) | 15 (5%) | 1 (0%) | 37 | 57 |
| 9 | 8 | 97/206 (47%) | 91 (94%) | 6 (6%) | 0 | 100 | 100 |
| 10 | 9 | 122/137 (89%) | 116 (95%) | 6 (5%) | 0 | 100 | 100 |
| 13 | D | 237/305 (78%) | 225 (95%) | 11 (5%) | 1 (0%) | 30 | 50 |
| 14 | E | 304/348 (87%) | 283 (93%) | 20 (7%) | 1 (0%) | 37 | 57 |
| 15 | F | 248/311 (80%) | 228 (92%) | 20 (8%) | 0 | 100 | 100 |
| 16 | H | 96/267 (36%) | 87 (91%) | 9 (9%) | 0 | 100 | 100 |
| 17 | I | 177/261 (68%) | 164 (93%) | 13 (7%) | 0 | 100 | 100 |
| 18 | J | 173/192 (90%) | 162 (94%) | 10 (6%) | 1 (1%) | 22 | 40 |
| 19 | K | 175/178 (98%) | 157 (90%) | 17 (10%) | 1 (1%) | 22 | 40 |
| 20 | L | 113/145 (78%) | 103 (91%) | 10 (9%) | 0 | 100 | 100 |
| 21 | M | 285/296 (96%) | 254 (89%) | 30 (10%) | 1 (0%) | 30 | 50 |
| 22 | N | 220/251 (88%) | 217 (99%) | 3 (1%) | 0 | 100 | 100 |
| 23 | O | 150/175 (86%) | 132 (88%) | 18 (12%) | 0 | 100 | 100 |
| 24 | P | 141/179 (79%) | 130 (92%) | 10 (7%) | 1 (1%) | 19 | 36 |
| 25 | Q | 218/292 (75%) | 211 (97%) | 7 (3%) | 0 | 100 | 100 |
| 26 | R | 138/149 (93%) | 128 (93%) | 10 (7%) | 0 | 100 | 100 |
| 27 | S | 154/205 (75%) | 147 (96%) | 7 (4%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|------------------|------------|----------|----------|-------------|-----|
| 28 | T | 164/212 (77%) | 157 (96%) | 7 (4%) | 0 | 100 | 100 |
| 29 | U | 150/153 (98%) | 144 (96%) | 6 (4%) | 0 | 100 | 100 |
| 30 | V | 204/216 (94%) | 200 (98%) | 4 (2%) | 0 | 100 | 100 |
| 31 | W | 109/148 (74%) | 103 (94%) | 6 (6%) | 0 | 100 | 100 |
| 32 | X | 241/256 (94%) | 226 (94%) | 15 (6%) | 0 | 100 | 100 |
| 33 | Y | 174/250 (70%) | 164 (94%) | 10 (6%) | 0 | 100 | 100 |
| 34 | Z | 118/161 (73%) | 109 (92%) | 9 (8%) | 0 | 100 | 100 |
| 35 | a | 106/142 (75%) | 103 (97%) | 3 (3%) | 0 | 100 | 100 |
| 36 | b | 146/155 (94%) | 139 (95%) | 7 (5%) | 0 | 100 | 100 |
| 37 | c | 287/332 (86%) | 265 (92%) | 22 (8%) | 0 | 100 | 100 |
| 38 | d | 255/306 (83%) | 241 (94%) | 14 (6%) | 0 | 100 | 100 |
| 39 | e | 211/279 (76%) | 194 (92%) | 17 (8%) | 0 | 100 | 100 |
| 40 | f | 144/194 (74%) | 136 (94%) | 8 (6%) | 0 | 100 | 100 |
| 41 | g | 130/166 (78%) | 121 (93%) | 9 (7%) | 0 | 100 | 100 |
| 42 | h | 108/158 (68%) | 99 (92%) | 9 (8%) | 0 | 100 | 100 |
| 43 | i | 95/128 (74%) | 91 (96%) | 4 (4%) | 0 | 100 | 100 |
| 44 | j | 91/123 (74%) | 87 (96%) | 4 (4%) | 0 | 100 | 100 |
| 45 | k | 94/112 (84%) | 90 (96%) | 4 (4%) | 0 | 100 | 100 |
| 46 | l | 70/138 (51%) | 62 (89%) | 8 (11%) | 0 | 100 | 100 |
| 47 | m | 43/128 (34%) | 39 (91%) | 4 (9%) | 0 | 100 | 100 |
| 48 | o | 92/102 (90%) | 86 (94%) | 6 (6%) | 0 | 100 | 100 |
| 49 | p | 148/206 (72%) | 134 (90%) | 14 (10%) | 0 | 100 | 100 |
| 50 | q | 166/222 (75%) | 154 (93%) | 6 (4%) | 6 (4%) | 3 | 3 |
| 51 | r | 160/196 (82%) | 150 (94%) | 10 (6%) | 0 | 100 | 100 |
| 52 | s | 391/439 (89%) | 364 (93%) | 27 (7%) | 0 | 100 | 100 |
| 54 | TA | 43/198 (22%) | 39 (91%) | 4 (9%) | 0 | 100 | 100 |
| 54 | TB | 25/198 (13%) | 24 (96%) | 1 (4%) | 0 | 100 | 100 |
| 54 | TC | 69/198 (35%) | 64 (93%) | 5 (7%) | 0 | 100 | 100 |
| All | All | 8449/11190 (76%) | 7907 (94%) | 527 (6%) | 15 (0%) | 45 | 65 |

5 of 15 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6 | 5 | 70 | LEU |
| 24 | P | 69 | ARG |
| 50 | q | 43 | GLU |
| 50 | q | 132 | ILE |
| 19 | K | 160 | GLN |

5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|-------------|-----|
| 1 | 0 | 97/164 (59%) | 95 (98%) | 2 (2%) | 48 | 72 |
| 2 | 1 | 49/60 (82%) | 49 (100%) | 0 | 100 | 100 |
| 3 | 2 | 40/72 (56%) | 40 (100%) | 0 | 100 | 100 |
| 4 | 3 | 88/166 (53%) | 85 (97%) | 3 (3%) | 32 | 56 |
| 5 | 4 | 37/89 (42%) | 36 (97%) | 1 (3%) | 40 | 65 |
| 6 | 5 | 353/368 (96%) | 333 (94%) | 20 (6%) | 17 | 35 |
| 7 | 6 | 313/332 (94%) | 299 (96%) | 14 (4%) | 23 | 45 |
| 8 | 7 | 272/303 (90%) | 264 (97%) | 8 (3%) | 37 | 62 |
| 9 | 8 | 91/190 (48%) | 89 (98%) | 2 (2%) | 47 | 70 |
| 10 | 9 | 104/112 (93%) | 100 (96%) | 4 (4%) | 28 | 52 |
| 13 | D | 193/245 (79%) | 184 (95%) | 9 (5%) | 22 | 43 |
| 14 | E | 260/290 (90%) | 251 (96%) | 9 (4%) | 31 | 55 |
| 15 | F | 217/262 (83%) | 213 (98%) | 4 (2%) | 54 | 76 |
| 16 | H | 88/228 (39%) | 84 (96%) | 4 (4%) | 23 | 45 |
| 17 | I | 164/232 (71%) | 158 (96%) | 6 (4%) | 29 | 53 |
| 18 | J | 138/150 (92%) | 132 (96%) | 6 (4%) | 25 | 47 |
| 19 | K | 155/156 (99%) | 151 (97%) | 4 (3%) | 41 | 66 |
| 20 | L | 98/124 (79%) | 95 (97%) | 3 (3%) | 35 | 60 |
| 21 | M | 245/249 (98%) | 241 (98%) | 4 (2%) | 58 | 78 |
| 22 | N | 189/211 (90%) | 184 (97%) | 5 (3%) | 41 | 66 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|---------------|------------|----------|-------------|-----|
| 23 | O | 133/150 (89%) | 131 (98%) | 2 (2%) | 60 | 80 |
| 24 | P | 125/154 (81%) | 121 (97%) | 4 (3%) | 34 | 59 |
| 25 | Q | 202/256 (79%) | 201 (100%) | 1 (0%) | 86 | 95 |
| 26 | R | 118/126 (94%) | 116 (98%) | 2 (2%) | 56 | 77 |
| 27 | S | 141/180 (78%) | 136 (96%) | 5 (4%) | 31 | 55 |
| 28 | T | 146/182 (80%) | 138 (94%) | 8 (6%) | 18 | 37 |
| 29 | U | 125/135 (93%) | 123 (98%) | 2 (2%) | 58 | 78 |
| 30 | V | 184/191 (96%) | 179 (97%) | 5 (3%) | 40 | 65 |
| 31 | W | 91/119 (76%) | 86 (94%) | 5 (6%) | 18 | 37 |
| 32 | X | 219/229 (96%) | 210 (96%) | 9 (4%) | 26 | 49 |
| 33 | Y | 159/223 (71%) | 155 (98%) | 4 (2%) | 42 | 67 |
| 34 | Z | 111/147 (76%) | 108 (97%) | 3 (3%) | 40 | 65 |
| 35 | a | 101/133 (76%) | 97 (96%) | 4 (4%) | 27 | 50 |
| 36 | b | 130/135 (96%) | 127 (98%) | 3 (2%) | 45 | 69 |
| 37 | c | 253/288 (88%) | 244 (96%) | 9 (4%) | 30 | 54 |
| 38 | d | 224/274 (82%) | 214 (96%) | 10 (4%) | 23 | 45 |
| 39 | e | 188/236 (80%) | 183 (97%) | 5 (3%) | 40 | 65 |
| 40 | f | 122/173 (70%) | 117 (96%) | 5 (4%) | 26 | 49 |
| 41 | g | 122/148 (82%) | 118 (97%) | 4 (3%) | 33 | 57 |
| 42 | h | 104/148 (70%) | 96 (92%) | 8 (8%) | 10 | 21 |
| 43 | i | 86/110 (78%) | 84 (98%) | 2 (2%) | 45 | 69 |
| 44 | j | 74/97 (76%) | 72 (97%) | 2 (3%) | 40 | 65 |
| 45 | k | 81/90 (90%) | 74 (91%) | 7 (9%) | 8 | 17 |
| 46 | l | 67/116 (58%) | 67 (100%) | 0 | 100 | 100 |
| 47 | m | 40/113 (35%) | 39 (98%) | 1 (2%) | 42 | 67 |
| 48 | o | 80/87 (92%) | 79 (99%) | 1 (1%) | 65 | 83 |
| 49 | p | 134/181 (74%) | 127 (95%) | 7 (5%) | 19 | 39 |
| 50 | q | 114/178 (64%) | 107 (94%) | 7 (6%) | 15 | 32 |
| 51 | r | 147/169 (87%) | 143 (97%) | 4 (3%) | 40 | 65 |
| 52 | s | 336/381 (88%) | 324 (96%) | 12 (4%) | 30 | 54 |
| 54 | TA | 39/158 (25%) | 38 (97%) | 1 (3%) | 41 | 66 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|-----|-------|-----------------|------------|----------|-------------|
| 54 | TB | 26/158 (16%) | 25 (96%) | 1 (4%) | 28 52 |
| All | All | 7413/9468 (78%) | 7162 (97%) | 251 (3%) | 34 56 |

5 of 251 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 26 | R | 95 | VAL |
| 49 | p | 96 | ASN |
| 32 | X | 60 | GLU |
| 49 | p | 42 | ILE |
| 51 | r | 159 | VAL |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 71 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 39 | e | 248 | ASN |
| 44 | j | 89 | GLN |
| 50 | q | 157 | GLN |
| 17 | I | 100 | GLN |
| 17 | I | 43 | GLN |

5.3.3 RNA ⓘ

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 11 | A | 1523/1559 (97%) | 360 (23%) | 24 (1%) |
| 12 | B | 51/72 (70%) | 12 (23%) | 1 (1%) |
| All | All | 1574/1631 (96%) | 372 (23%) | 25 (1%) |

5 of 372 RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 11 | A | 1678 | C |
| 11 | A | 1679 | U |
| 11 | A | 1681 | G |
| 11 | A | 1689 | C |
| 11 | A | 1690 | C |

5 of 25 RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 11 | A | 2559 | U |
| 11 | A | 2905 | A |
| 12 | B | 1607 | U |
| 11 | A | 2628 | U |
| 11 | A | 2989 | 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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 106 ligands modelled in this entry, 105 are monoatomic - leaving 1 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
| | | | | | Counts | RMSZ | $\# Z > 2$ | Counts | RMSZ | $\# Z > 2$ |
| 57 | ZLD | A | 3400 | 56 | 26,26,26 | 0.88 | 1 (3%) | 36,36,36 | 1.21 | 2 (5%) |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|------------|---------|
| 57 | ZLD | A | 3400 | 56 | - | 2/13/33/33 | 0/3/3/3 |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 57 | A | 3400 | ZLD | C7-N4 | -2.31 | 1.34 | 1.36 |

All (2) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 57 | A | 3400 | ZLD | C6-C8-C9 | 4.30 | 118.25 | 113.38 |
| 57 | A | 3400 | ZLD | O10-C7-O15 | -2.63 | 119.32 | 122.40 |

There are no chirality outliers.

All (2) torsion outliers are listed below:

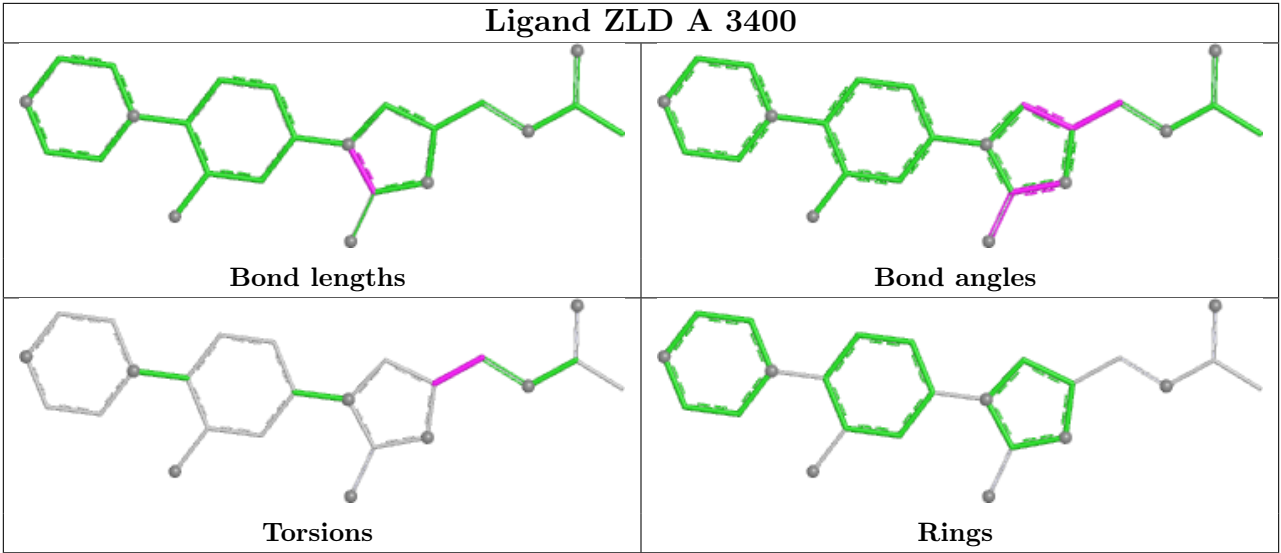
| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|---------------|
| 57 | A | 3400 | ZLD | C6-C8-C9-N11 |
| 57 | A | 3400 | ZLD | O10-C8-C9-N11 |

There are no ring outliers.

1 monomer is involved in 3 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 57 | A | 3400 | ZLD | 3 | 0 |

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



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 53 | u | 4 |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1 | u | 414:UNK | C | 601:UNK | N | 50.73 |
| 1 | u | 106:UNK | C | 301:UNK | N | 32.84 |
| 1 | u | 315:UNK | C | 399:UNK | N | 24.40 |
| 1 | u | 615:UNK | C | 700:UNK | N | 14.68 |

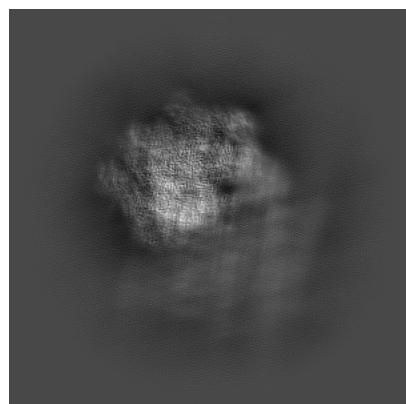
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-45757. These allow visual inspection of the internal detail of the map and identification of artifacts.

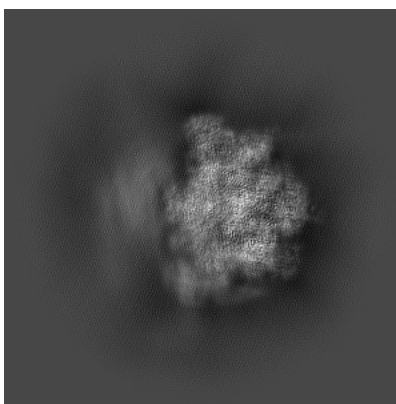
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

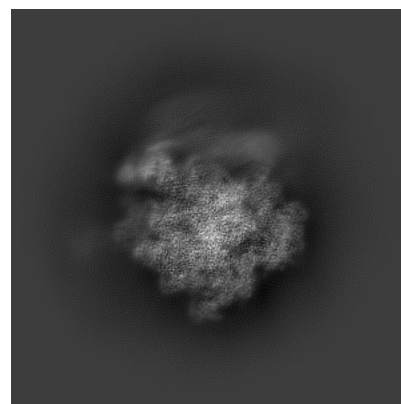
6.1.1 Primary map



X

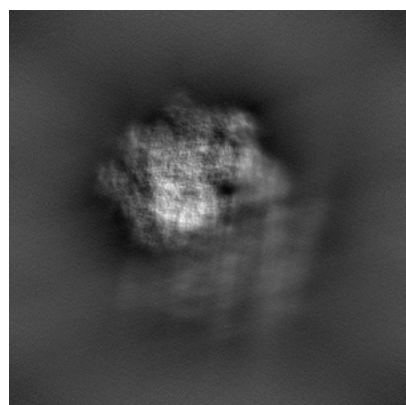


Y

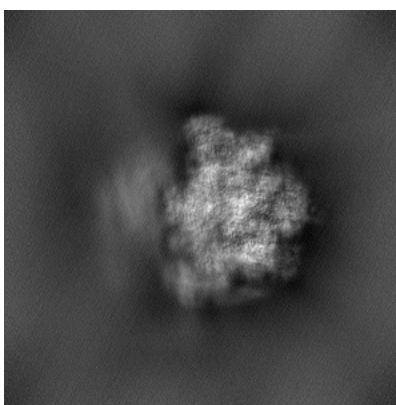


Z

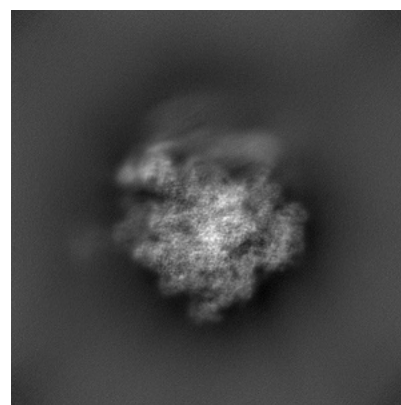
6.1.2 Raw map



X



Y

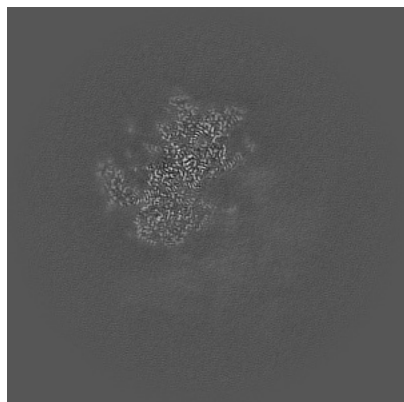


Z

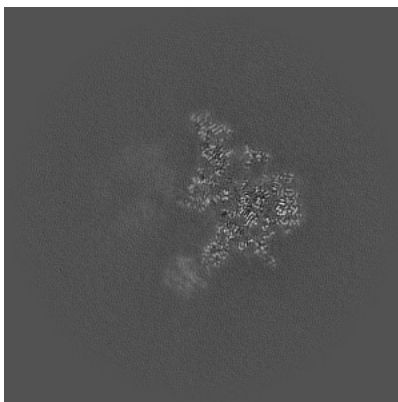
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

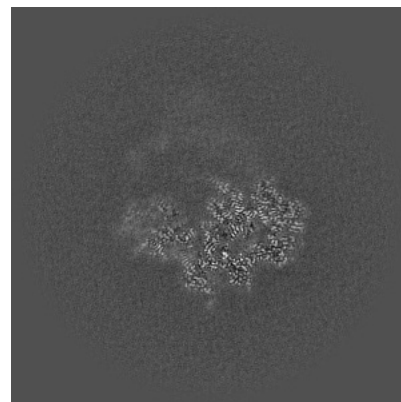
6.2.1 Primary map



X Index: 280

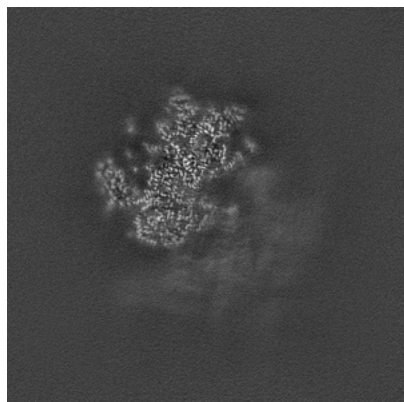


Y Index: 280

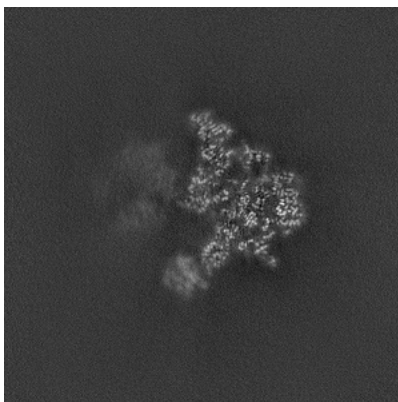


Z Index: 280

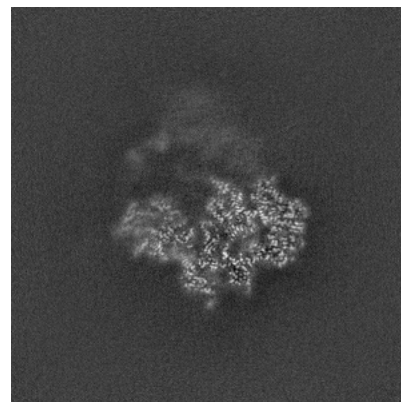
6.2.2 Raw map



X Index: 280



Y Index: 280

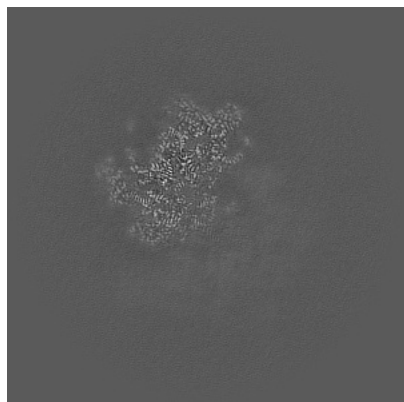


Z Index: 280

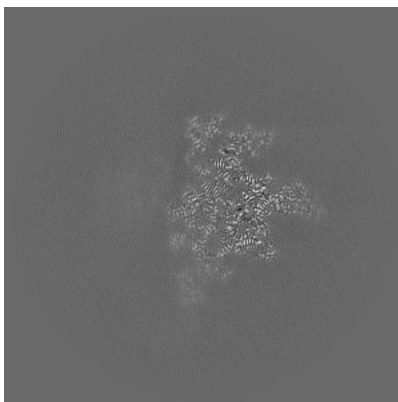
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

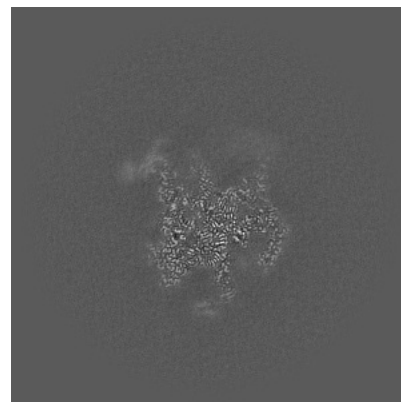
6.3.1 Primary map



X Index: 286

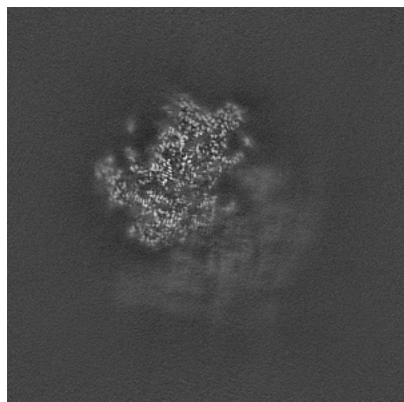


Y Index: 239

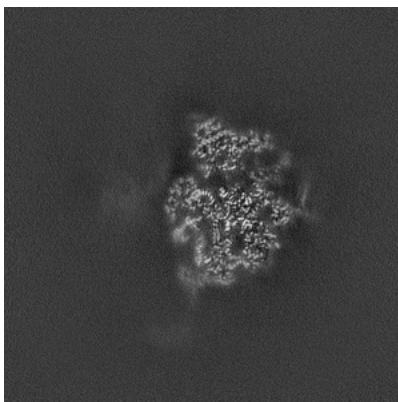


Z Index: 338

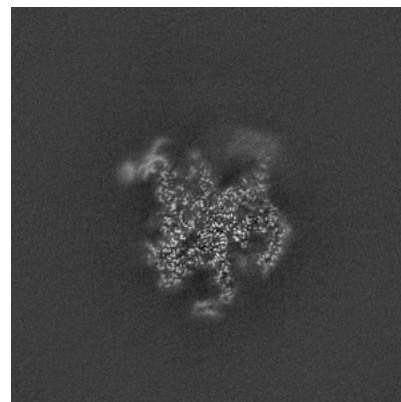
6.3.2 Raw map



X Index: 286



Y Index: 220

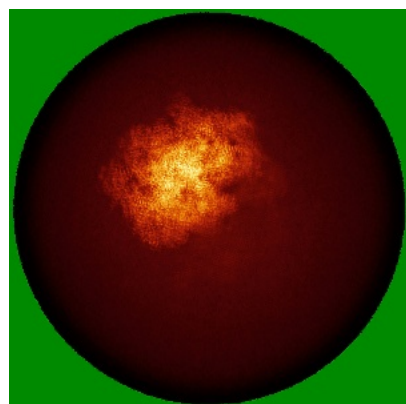


Z Index: 338

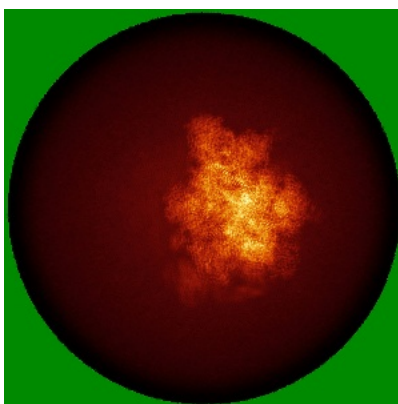
The images above show the largest variance slices of the map in three orthogonal directions.

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

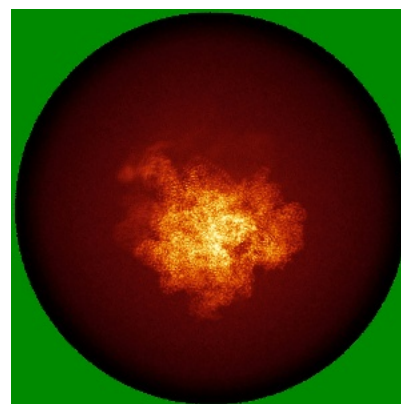
6.4.1 Primary map



X

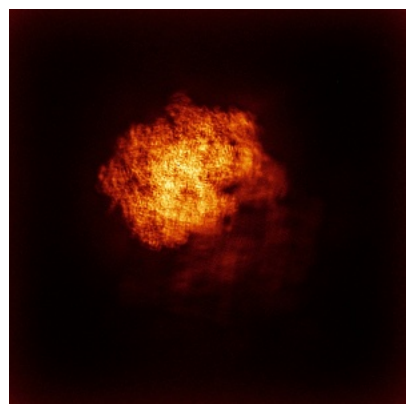


Y

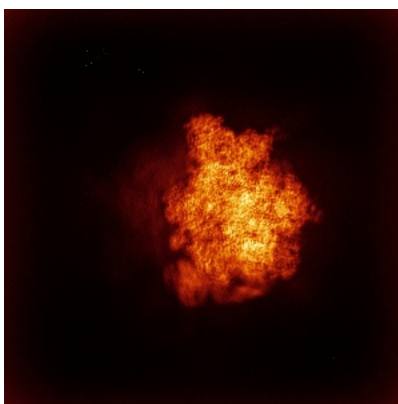


Z

6.4.2 Raw map



X



Y

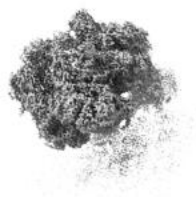


Z

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

6.5 Orthogonal surface views [i](#)

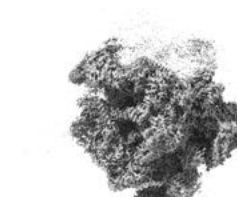
6.5.1 Primary map



X



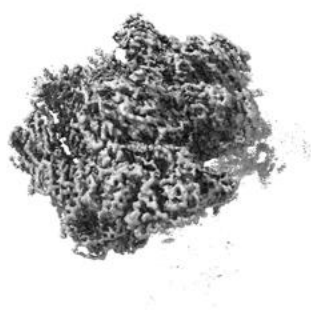
Y



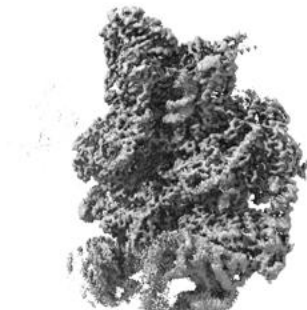
Z

The images above show the 3D surface view of the map at the recommended contour level 0.38. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y



Z

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

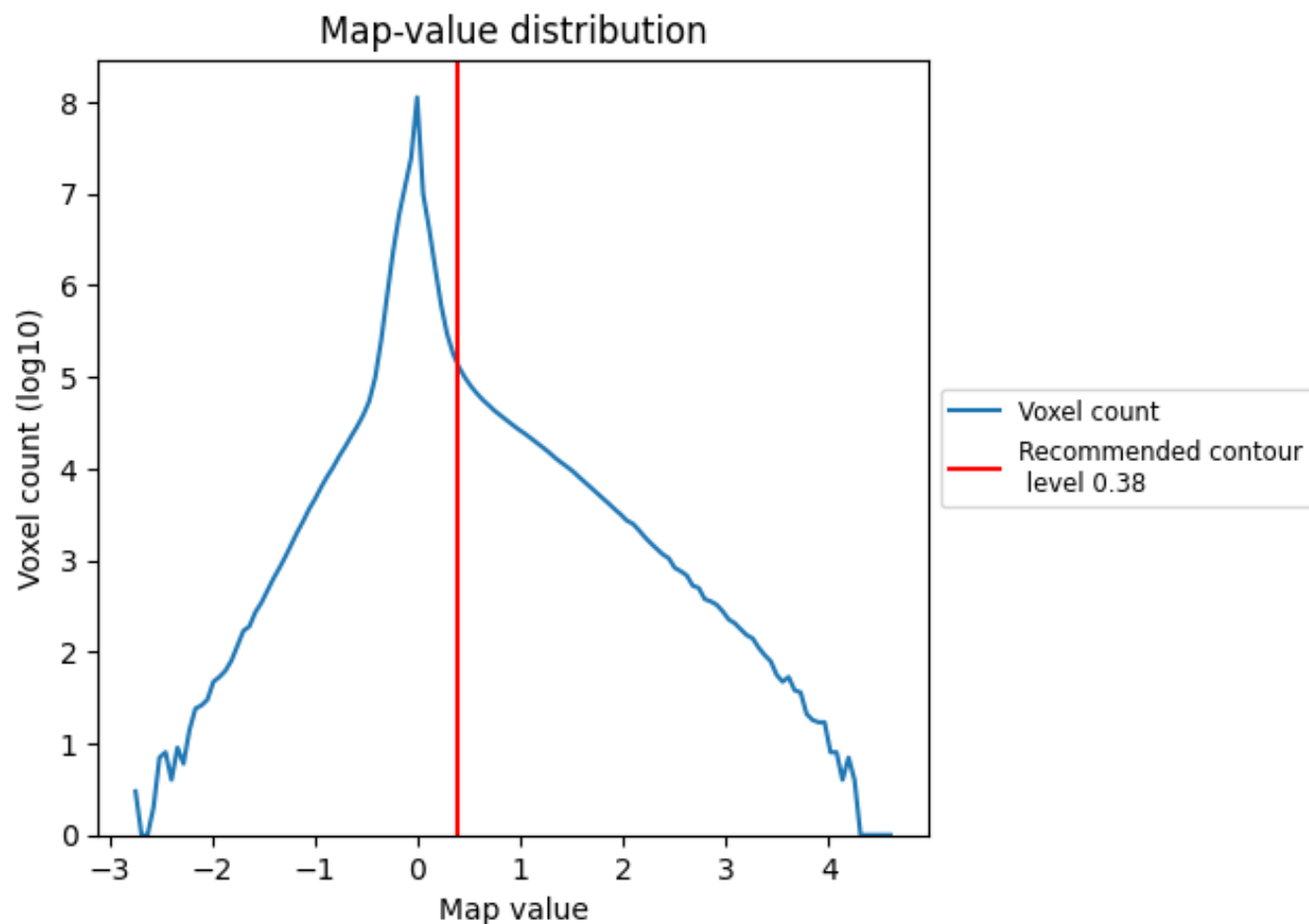
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

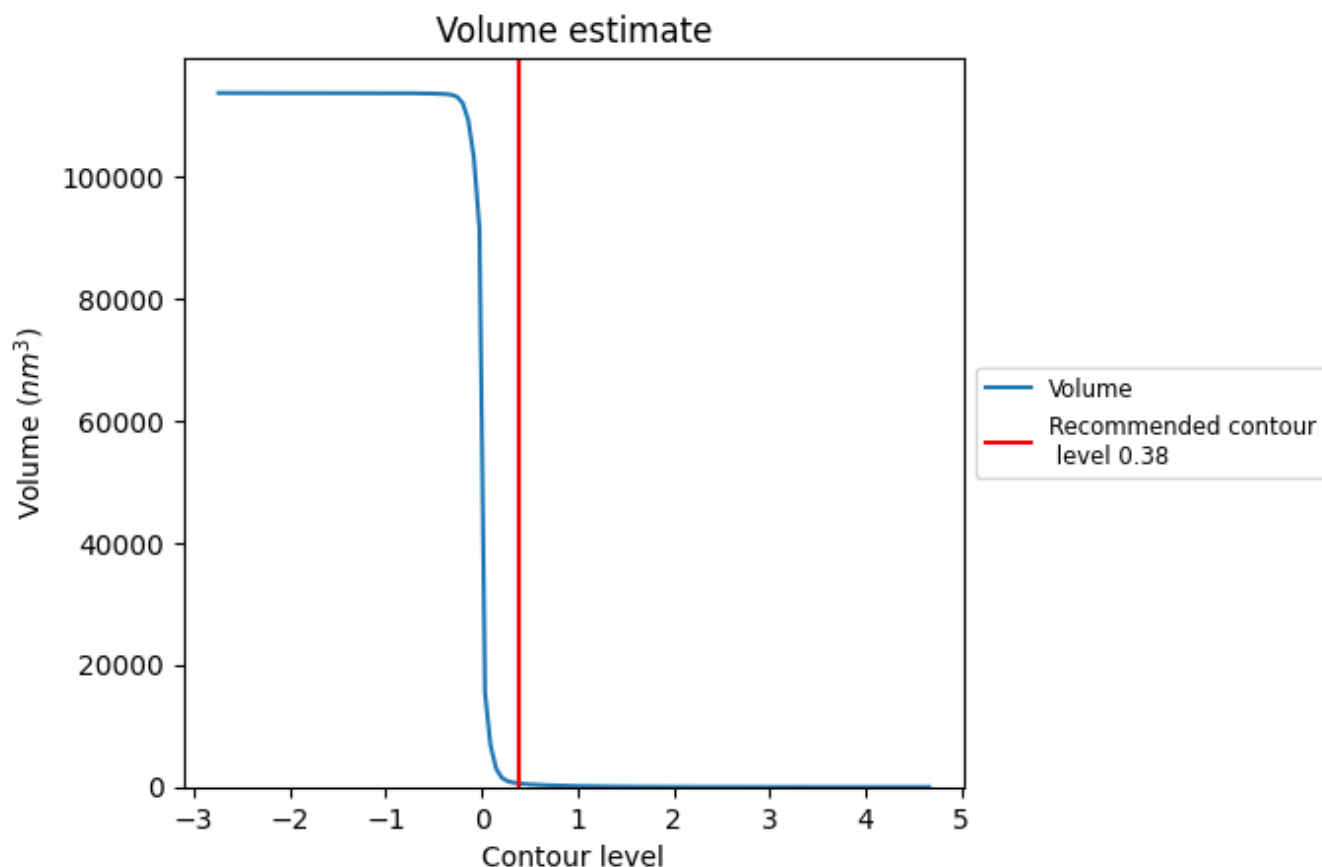
This section contains the results of statistical analysis of the map.

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.

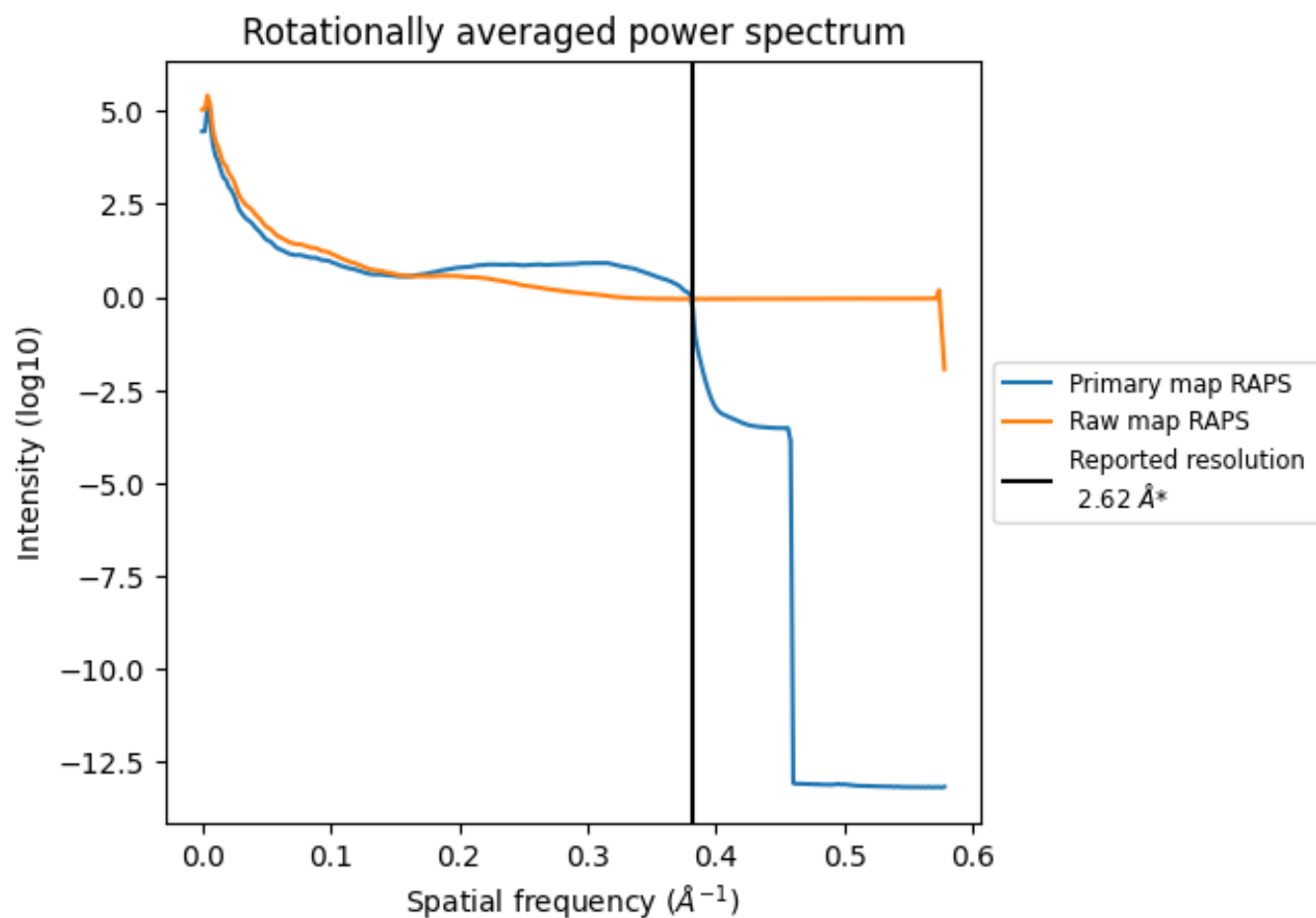
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 592 nm³; this corresponds to an approximate mass of 535 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

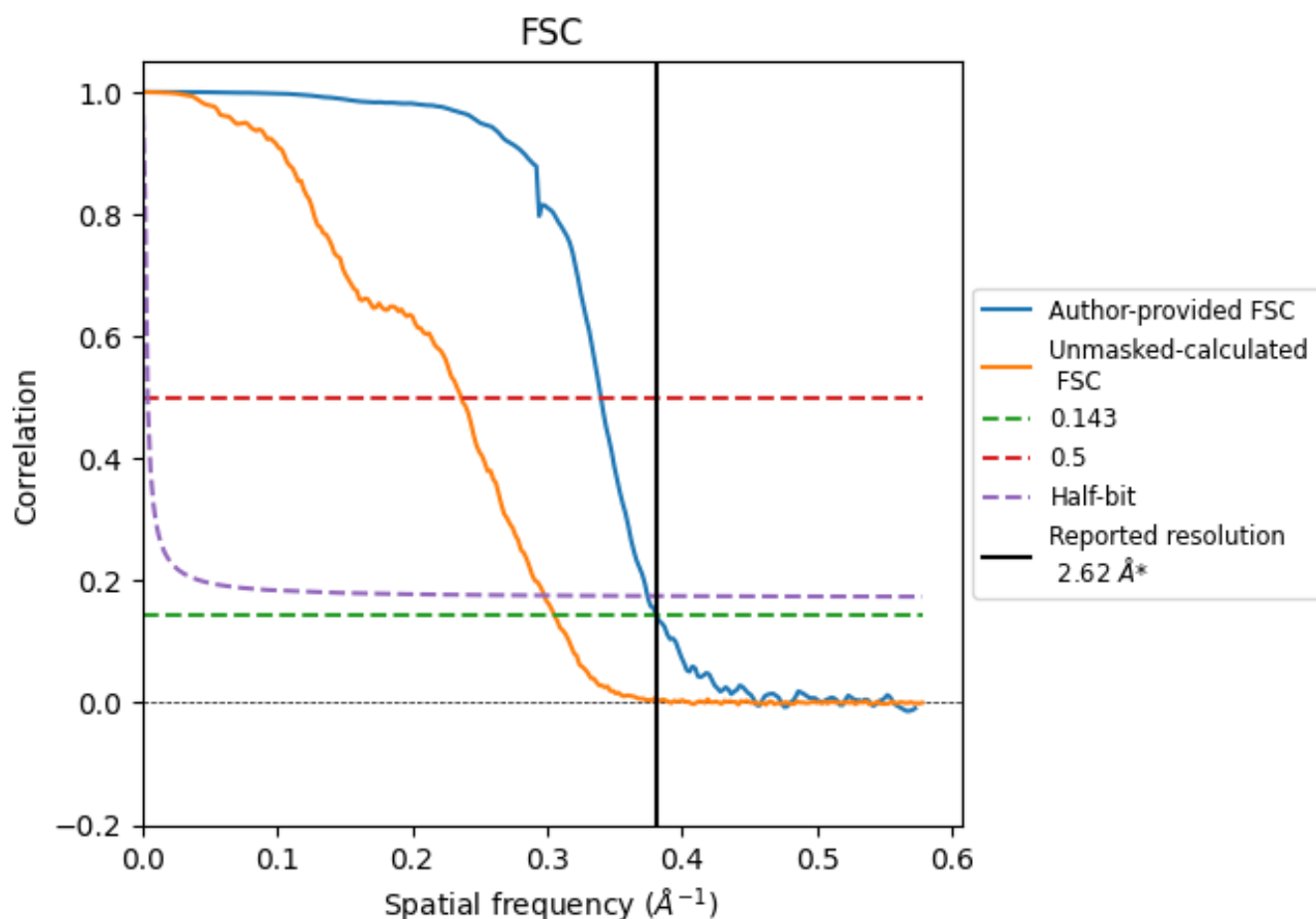


*Reported resolution corresponds to spatial frequency of 0.382 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.382 \AA^{-1}

8.2 Resolution estimates [i](#)

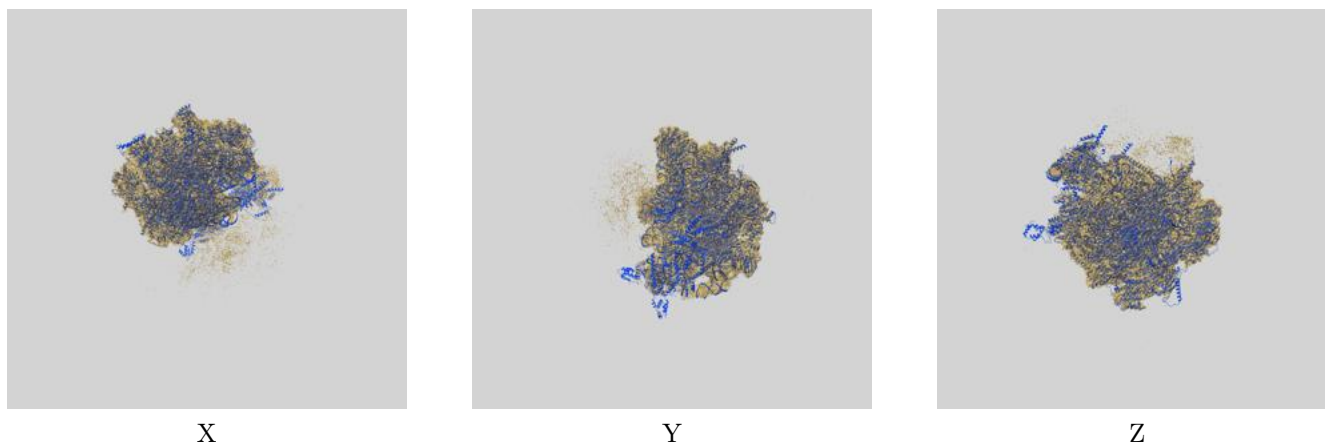
| Resolution estimate (Å) | Estimation criterion (FSC cut-off) | | |
|---------------------------|------------------------------------|------|----------|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | 2.62 | - | - |
| Author-provided FSC curve | 2.62 | 2.94 | 2.67 |
| Unmasked-calculated* | 3.27 | 4.23 | 3.36 |

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.27 differs from the reported value 2.62 by more than 10 %

9 Map-model fit [i](#)

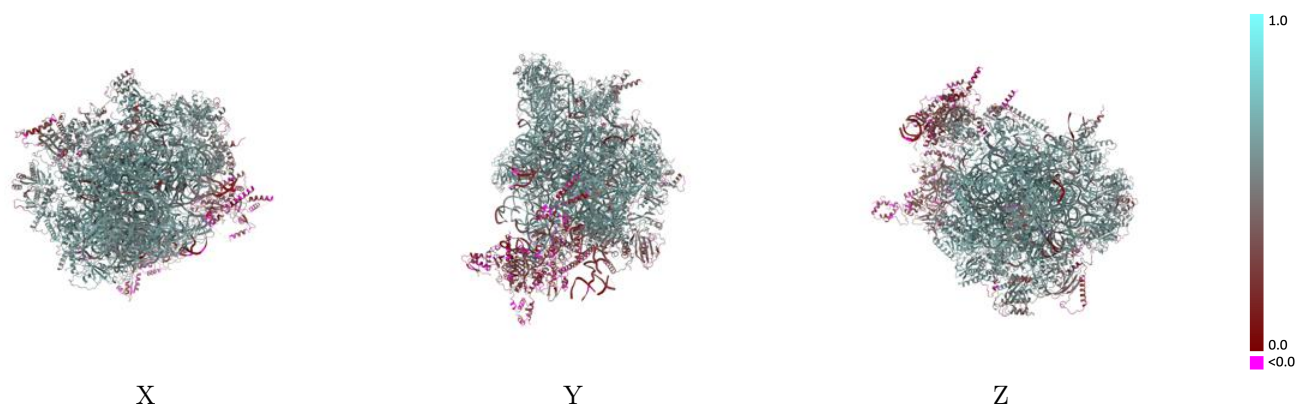
This section contains information regarding the fit between EMDB map EMD-45757 and PDB model 9CN3. Per-residue inclusion information can be found in section [3](#) on page [17](#).

9.1 Map-model overlay [i](#)



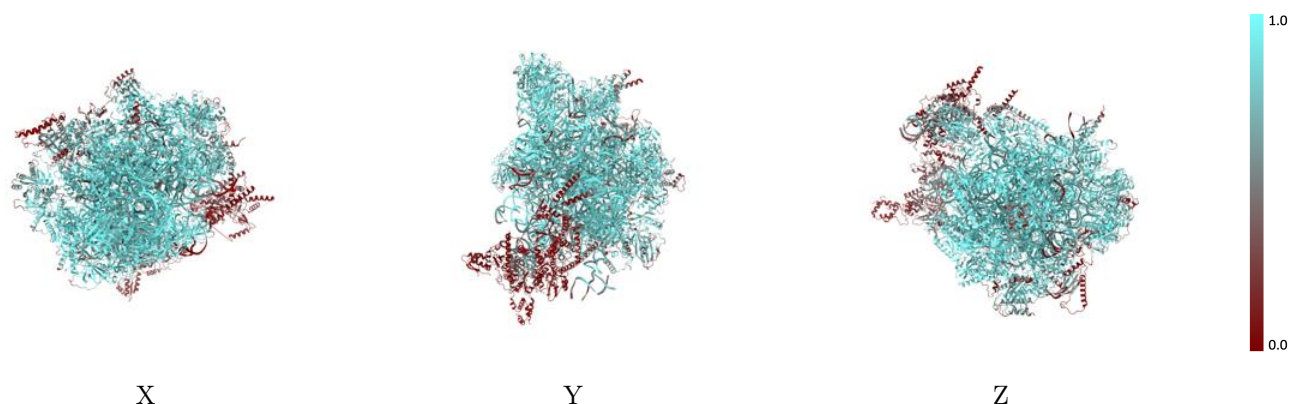
The images above show the 3D surface view of the map at the recommended contour level 0.38 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



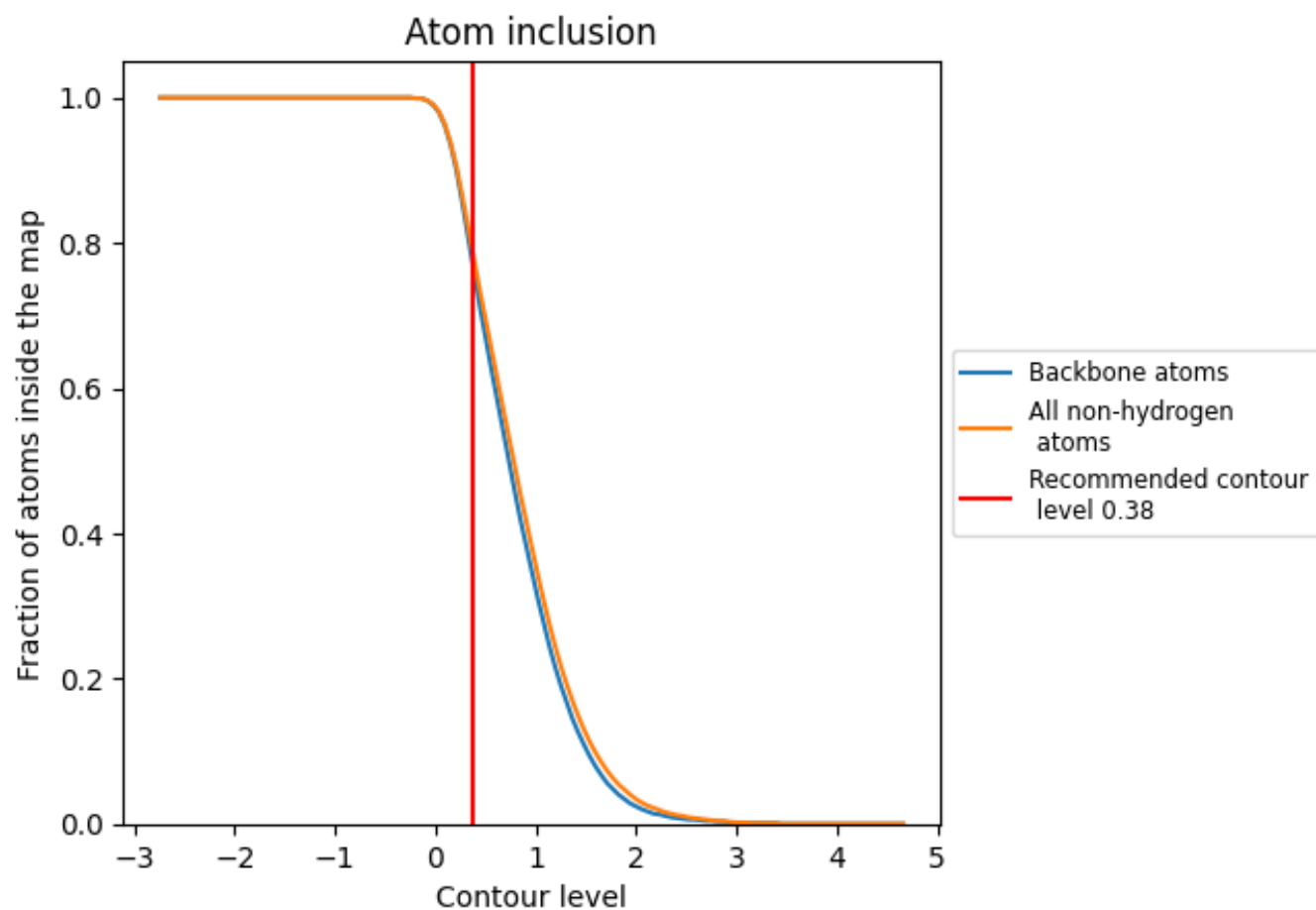
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.38).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 78% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ













































The table lists the average atom inclusion at the recommended contour level (0.38) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|-------|--|--|
| All |  0.7800 |  0.5250 |
| 0 |  0.8840 |  0.5860 |
| 1 |  0.8090 |  0.5550 |
| 2 |  0.9830 |  0.6510 |
| 3 |  0.9640 |  0.6510 |
| 4 |  0.9390 |  0.6080 |
| 5 |  0.8520 |  0.5610 |
| 6 |  0.7050 |  0.4490 |
| 7 |  0.7500 |  0.5070 |
| 8 |  0.1510 |  0.1860 |
| 9 |  0.7750 |  0.5410 |
| A |  0.8900 |  0.5670 |
| B |  0.6800 |  0.2220 |
| D |  0.8750 |  0.5870 |
| E |  0.8990 |  0.5950 |
| F |  0.9020 |  0.6000 |
| H |  0.7490 |  0.5100 |
| I |  0.3410 |  0.2930 |
| J |  0.1060 |  0.1880 |
| K |  0.9370 |  0.6170 |
| L |  0.8700 |  0.5820 |
| M |  0.8900 |  0.5990 |
| N |  0.8590 |  0.5830 |
| O |  0.9270 |  0.6070 |
| P |  0.8180 |  0.5070 |
| Q |  0.8540 |  0.5870 |
| R |  0.9320 |  0.6180 |
| S |  0.9500 |  0.6200 |
| T |  0.9220 |  0.6250 |
| TA |  0.0000 |  0.1000 |
| TB |  0.0000 |  0.0950 |
| TC |  0.0000 |  0.0990 |
| U |  0.7970 |  0.5530 |
| V |  0.5390 |  0.4850 |
| W |  0.9150 |  0.6090 |



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| Chain | Atom inclusion | Q-score |
|-------|--|--|
| X |  0.8270 |  0.5680 |
| Y |  0.9100 |  0.5990 |
| Z |  0.9450 |  0.6270 |
| a |  0.7170 |  0.5100 |
| b |  0.9470 |  0.6200 |
| c |  0.8330 |  0.5610 |
| d |  0.4200 |  0.4060 |
| e |  0.0830 |  0.1650 |
| f |  0.2070 |  0.2670 |
| g |  0.9000 |  0.5900 |
| h |  0.5180 |  0.4440 |
| i |  0.9430 |  0.6320 |
| j |  0.8100 |  0.5520 |
| k |  0.3390 |  0.2760 |
| l |  0.2530 |  0.3000 |
| m |  0.1440 |  0.1790 |
| o |  0.9230 |  0.6150 |
| p |  0.5740 |  0.4420 |
| q |  0.5340 |  0.4170 |
| r |  0.8410 |  0.5380 |
| s |  0.8790 |  0.5800 |
| u |  0.0090 |  0.0780 |