



Full wwPDB EM Validation Report ⓘ

Jun 30, 2021 – 04:25 am BST

PDB ID : 7ODS
EMDB ID : EMD-12846
Title : State B of the human mitoribosomal large subunit assembly intermediate
Authors : Lenarcic, T.; Jaskolowski, M.; Leibundgut, M.; Scaiola, A.; Schoenhut, T.; Saurer, M.; Lee, R.G.; Rackham, O.; Filipovska, A.; Ban, N.
Deposited on : 2021-04-30
Resolution : 3.10 Å(reported)

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 ⓘ symbol.

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

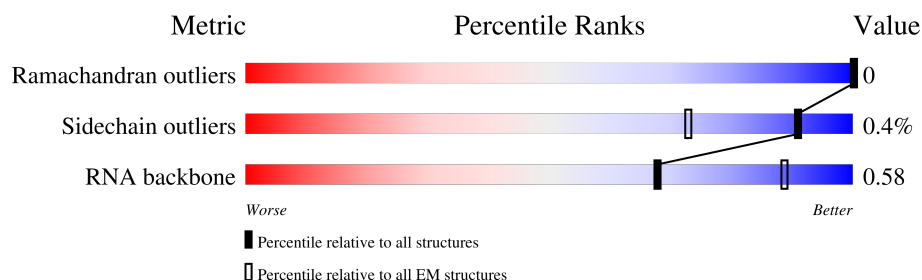
EMDB validation analysis : 0.0.0.dev84
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.22

1 Overall quality at a glance

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

The reported resolution of this entry is 3.10 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 $\leq 5\%$. 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 | u | 234 | |
| 2 | v | 70 | |
| 3 | w | 156 | |
| 4 | x | 384 | |
| 5 | y | 381 | |
| 6 | z | 246 | |
| 7 | 0 | 188 | |
| 8 | 1 | 65 | |


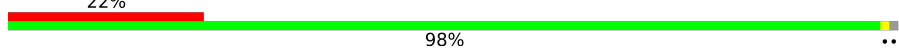
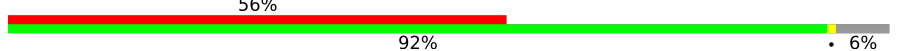

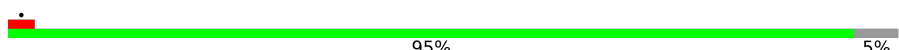
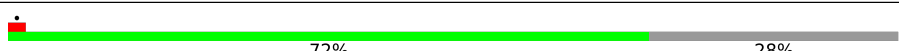
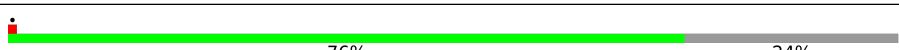

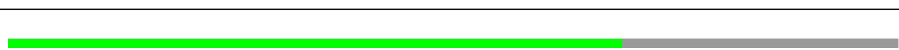




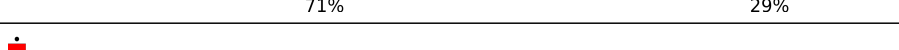
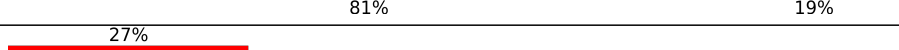
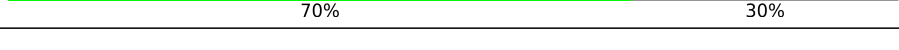





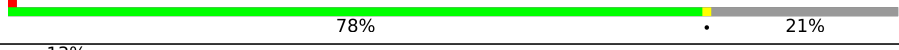
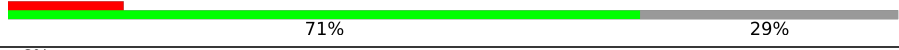


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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 9 | 2 | 92 | |
| 10 | 3 | 188 | |
| 11 | 4 | 103 | |
| 12 | 5 | 423 | |
| 13 | 6 | 380 | |
| 14 | 7 | 338 | |
| 15 | 8 | 206 | |
| 16 | 9 | 137 | |
| 17 | A | 1589 | |
| 18 | B | 72 | |
| 19 | D | 305 | |
| 20 | E | 348 | |
| 21 | F | 311 | |
| 22 | H | 267 | |
| 23 | I | 261 | |
| 24 | J | 192 | |
| 25 | K | 178 | |
| 26 | L | 145 | |
| 27 | M | 296 | |
| 28 | N | 251 | |
| 29 | O | 175 | |
| 30 | P | 180 | |
| 31 | Q | 292 | |
| 32 | R | 149 | |
| 33 | S | 205 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 34 | T | 206 |  |
| 35 | U | 153 |  |
| 36 | V | 216 |  |
| 37 | W | 148 |  |
| 38 | X | 256 |  |
| 39 | Y | 250 |  |
| 40 | Z | 161 |  |
| 41 | a | 142 |  |
| 42 | b | 215 |  |
| 43 | c | 332 |  |
| 44 | d | 306 |  |
| 45 | e | 279 |  |
| 46 | f | 212 |  |
| 47 | g | 166 |  |
| 48 | h | 158 |  |
| 49 | i | 128 |  |
| 50 | j | 123 |  |
| 51 | k | 112 |  |
| 52 | l | 138 |  |
| 53 | m | 128 |  |
| 54 | o | 102 |  |
| 55 | p | 206 |  |
| 56 | q | 222 |  |
| 57 | r | 196 |  |
| 58 | s | 439 |  |

2 Entry composition

There are 65 unique types of molecules in this entry. The entry contains 108339 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 Mitochondrial assembly of ribosomal large subunit protein 1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 1 | u | 110 | Total | C | N | O | S | 0 | 0 |
| | | | 919 | 591 | 154 | 164 | 10 | | |

- Molecule 2 is a protein called MIEF1 upstream open reading frame protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|-------|
| 2 | v | 69 | Total | C | N | O | | 0 | 0 |
| | | | 588 | 372 | 116 | 100 | | | |

- Molecule 3 is a protein called Acyl carrier protein, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|---|---------|-------|
| 3 | w | 79 | Total | C | N | O | S | 0 | 0 |
| | | | 638 | 410 | 95 | 128 | 5 | | |

- Molecule 4 is a protein called 5-methylcytosine rRNA methyltransferase NSUN4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 4 | x | 336 | Total | C | N | O | S | 0 | 0 |
| | | | 2660 | 1694 | 465 | 484 | 17 | | |

- Molecule 5 is a protein called Transcription termination factor 4, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 5 | y | 244 | Total | C | N | O | S | 0 | 0 |
| | | | 1980 | 1264 | 342 | 362 | 12 | | |

- Molecule 6 is a protein called rRNA methyltransferase 2, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 6 | z | 181 | Total | C | N | O | S | 0 | 0 |
| | | | 1366 | 869 | 238 | 253 | 6 | | |

- Molecule 7 is a protein called 39S ribosomal protein L32, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 7 | 0 | 110 | Total | C | N | O | S | 0 | 0 |
| | | | 898 | 554 | 176 | 162 | 6 | | |

- Molecule 8 is a protein called 39S ribosomal protein L33, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 8 | 1 | 55 | Total | C | N | O | S | 0 | 0 |
| | | | 455 | 290 | 87 | 76 | 2 | | |

- Molecule 9 is a protein called 39S ribosomal protein L34, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 9 | 2 | 46 | Total | C | N | O | S | 0 | 0 |
| | | | 377 | 233 | 83 | 60 | 1 | | |

- Molecule 10 is a protein called 39S ribosomal protein L35, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 10 | 3 | 95 | Total | C | N | O | S | 0 | 0 |
| | | | 832 | 539 | 162 | 128 | 3 | | |

- Molecule 11 is a protein called 39S ribosomal protein L36, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 11 | 4 | 38 | Total | C | N | O | S | 0 | 0 |
| | | | 342 | 217 | 72 | 49 | 4 | | |

- Molecule 12 is a protein called 39S ribosomal protein L37, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 12 | 5 | 394 | Total | C | N | O | S | 0 | 0 |
| | | | 3210 | 2073 | 560 | 566 | 11 | | |

- Molecule 13 is a protein called 39S ribosomal protein L38, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 13 | 6 | 354 | Total | C | N | O | S | 0 | 0 |
| | | | 2948 | 1881 | 525 | 533 | 9 | | |

- Molecule 14 is a protein called 39S ribosomal protein L39, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 14 | 7 | 294 | Total | C | N | O | S | 0 | 0 |
| | | | 2390 | 1529 | 405 | 438 | 18 | | |

- Molecule 15 is a protein called 39S ribosomal protein L40, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 15 | 8 | 102 | Total | C | N | O | S | 0 | 0 |
| | | | 860 | 543 | 152 | 163 | 2 | | |

- Molecule 16 is a protein called 39S ribosomal protein L41, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 16 | 9 | 124 | Total | C | N | O | S | 0 | 0 |
| | | | 997 | 644 | 170 | 181 | 2 | | |

- Molecule 17 is a RNA chain called 16S mitochondrial rRNA, DNA (30-MER),16S mitochondrial rRNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-------|------|------|------|---------|-------|
| 17 | A | 1445 | Total | C | N | O | P | 0 | 0 |
| | | | 30407 | 13635 | 5434 | 9893 | 1445 | | |

- Molecule 18 is a RNA chain called mitochondrial tRNA^{Val}.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 18 | B | 72 | Total | C | N | O | P | 0 | 0 |
| | | | 1522 | 683 | 269 | 498 | 72 | | |

- Molecule 19 is a protein called 39S ribosomal protein L2, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 19 | D | 240 | Total | C | N | O | S | 0 | 0 |
| | | | 1872 | 1165 | 378 | 320 | 9 | | |

- Molecule 20 is a protein called 39S ribosomal protein L3, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 20 | E | 305 | Total | C | N | O | S | 0 | 0 |
| | | | 2406 | 1545 | 418 | 432 | 11 | | |

- Molecule 21 is a protein called 39S ribosomal protein L4, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 21 | F | 252 | Total | C | N | O | S | 0 | 0 |
| | | | 2031 | 1305 | 370 | 350 | 6 | | |

- Molecule 22 is a protein called 39S ribosomal protein L9, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 22 | H | 97 | Total | C | N | O | S | 0 | 0 |
| | | | 802 | 508 | 155 | 139 | | | |

- Molecule 23 is a protein called 39S ribosomal protein L10, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 23 | I | 164 | Total | C | N | O | S | 0 | 0 |
| | | | 1331 | 858 | 241 | 222 | 10 | | |

- Molecule 24 is a protein called 39S ribosomal protein L11, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 24 | J | 175 | Total | C | N | O | S | 0 | 0 |
| | | | 1330 | 847 | 237 | 244 | 2 | | |

- Molecule 25 is a protein called 39S ribosomal protein L13, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 25 | K | 177 | Total | C | N | O | S | 0 | 0 |
| | | | 1455 | 936 | 259 | 253 | 7 | | |

- Molecule 26 is a protein called 39S ribosomal protein L14, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 26 | L | 115 | Total | C | N | O | S | 0 | 0 |
| | | | 890 | 559 | 171 | 155 | 5 | | |

- Molecule 27 is a protein called 39S ribosomal protein L15, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 27 | M | 291 | Total | C | N | O | S | 0 | 0 |
| | | | 2327 | 1483 | 430 | 408 | 6 | | |

- Molecule 28 is a protein called 39S ribosomal protein L16, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 28 | N | 209 | Total | C | N | O | S | 0 | 0 |
| | | | 1702 | 1093 | 307 | 293 | 9 | | |

- Molecule 29 is a protein called 39S ribosomal protein L17, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 29 | O | 154 | Total | C | N | O | S | 0 | 0 |
| | | | 1259 | 792 | 241 | 219 | 7 | | |

- Molecule 30 is a protein called 39S ribosomal protein L18, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 30 | P | 144 | Total | C | N | O | S | 0 | 0 |
| | | | 1173 | 733 | 224 | 211 | 5 | | |

- Molecule 31 is a protein called 39S ribosomal protein L19, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 31 | Q | 221 | Total | C | N | O | S | 0 | 0 |
| | | | 1843 | 1179 | 327 | 328 | 9 | | |

- Molecule 32 is a protein called 39S ribosomal protein L20, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 32 | R | 140 | Total | C | N | O | S | 0 | 0 |
| | | | 1154 | 732 | 231 | 187 | 4 | | |

- Molecule 33 is a protein called 39S ribosomal protein L21, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 33 | S | 161 | Total | C | N | O | S | 0 | 0 |
| | | | 1293 | 835 | 227 | 227 | 4 | | |

- Molecule 34 is a protein called 39S ribosomal protein L22, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 34 | T | 166 | Total | C | N | O | S | 0 | 0 |
| | | | 1369 | 875 | 254 | 233 | 7 | | |

- Molecule 35 is a protein called 39S ribosomal protein L23, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 35 | U | 152 | Total | C | N | O | S | 0 | 0 |
| | | | 1251 | 788 | 234 | 226 | 3 | | |

- Molecule 36 is a protein called 39S ribosomal protein L24, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 36 | V | 202 | Total | C | N | O | S | 0 | 0 |
| | | | 1653 | 1053 | 294 | 298 | 8 | | |

- Molecule 37 is a protein called 39S ribosomal protein L27, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 37 | W | 106 | Total | C | N | O | S | 0 | 0 |
| | | | 835 | 536 | 157 | 139 | 3 | | |

- Molecule 38 is a protein called 39S ribosomal protein L28, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 38 | X | 244 | Total | C | N | O | S | 0 | 0 |
| | | | 2044 | 1322 | 352 | 365 | 5 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 39 | Y | 181 | Total | C | N | O | S | 0 | 0 |
| | | | 1556 | 995 | 298 | 259 | 4 | | |

- Molecule 40 is a protein called 39S ribosomal protein L30, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 40 | Z | 122 | Total | C | N | O | S | 0 | 0 |
| | | | 996 | 636 | 186 | 171 | 3 | | |

- Molecule 41 is a protein called 39S ribosomal protein L42, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 41 | a | 100 | Total | C | N | O | S | 0 | 0 |
| | | | 840 | 529 | 152 | 154 | 5 | | |

- Molecule 42 is a protein called 39S ribosomal protein L43, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 42 | b | 149 | Total | C | N | O | S | 0 | 0 |
| | | | 1189 | 739 | 230 | 217 | 3 | | |

- Molecule 43 is a protein called 39S ribosomal protein L44, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 43 | c | 286 | Total | C | N | O | S | 0 | 0 |
| | | | 2299 | 1470 | 397 | 423 | 9 | | |

- Molecule 44 is a protein called 39S ribosomal protein L45, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 44 | d | 223 | Total | C | N | O | S | 0 | 0 |
| | | | 1824 | 1160 | 316 | 335 | 13 | | |

- Molecule 45 is a protein called 39S ribosomal protein L46, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 45 | e | 228 | Total | C | N | O | S | 0 | 0 |
| | | | 1848 | 1174 | 326 | 342 | 6 | | |

- Molecule 46 is a protein called 39S ribosomal protein L48, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 46 | f | 150 | Total | C | N | O | S | 0 | 0 |
| | | | 1196 | 764 | 197 | 231 | 4 | | |

- Molecule 47 is a protein called 39S ribosomal protein L49, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 47 | g | 134 | Total | C | N | O | S | 0 | 0 |
| | | | 1113 | 719 | 193 | 199 | 2 | | |

- Molecule 48 is a protein called 39S ribosomal protein L50, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 48 | h | 110 | Total | C | N | O | S | 0 | 0 |
| | | | 895 | 568 | 156 | 168 | 3 | | |

- Molecule 49 is a protein called 39S ribosomal protein L51, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 49 | i | 97 | Total | C | N | O | S | 0 | 0 |
| | | | 828 | 532 | 165 | 127 | 4 | | |

- Molecule 50 is a protein called 39S ribosomal protein L52, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 50 | j | 94 | Total | C | N | O | S | 0 | 0 |
| | | | 745 | 463 | 144 | 136 | 2 | | |

- Molecule 51 is a protein called 39S ribosomal protein L53, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 51 | k | 101 | Total | C | N | O | S | 0 | 0 |
| | | | 774 | 479 | 148 | 142 | 5 | | |

- Molecule 52 is a protein called 39S ribosomal protein L54, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 52 | l | 82 | Total | C | N | O | S | 0 | 0 |
| | | | 688 | 437 | 120 | 128 | 3 | | |

- Molecule 53 is a protein called 39S ribosomal protein L55, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 53 | m | 51 | Total | C | N | O | S | 0 | 0 |
| | | | 419 | 262 | 82 | 73 | 2 | | |

- Molecule 54 is a protein called Ribosomal protein 63, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 54 | o | 81 | Total | C | N | O | S | 0 | 0 |
| | | | 688 | 432 | 138 | 115 | 3 | | |

- Molecule 55 is a protein called Peptidyl-tRNA hydrolase ICT1, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 55 | p | 147 | Total | C | N | O | S | 0 | 0 |
| | | | 1205 | 748 | 228 | 225 | 4 | | |

- Molecule 56 is a protein called Growth arrest and DNA damage-inducible proteins-interacting protein 1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 56 | q | 141 | Total | C | N | O | S | 0 | 0 |
| | | | 1177 | 732 | 229 | 211 | 5 | | |

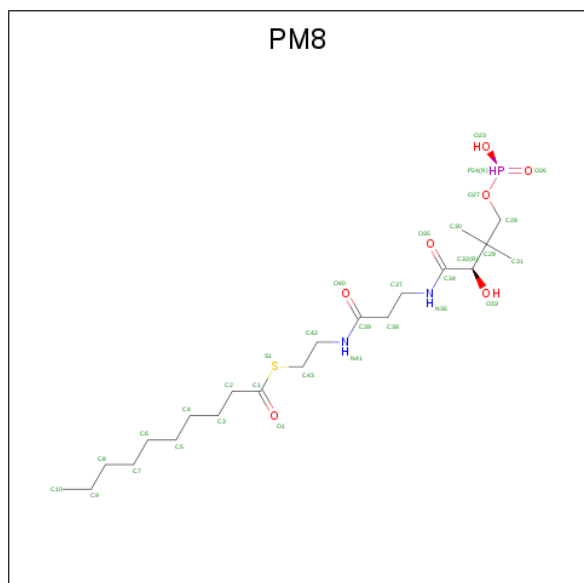
- Molecule 57 is a protein called 39S ribosomal protein S18a, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 57 | r | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 1322 | 839 | 252 | 223 | 8 | | |

- Molecule 58 is a protein called 39S ribosomal protein S30, mitochondrial.

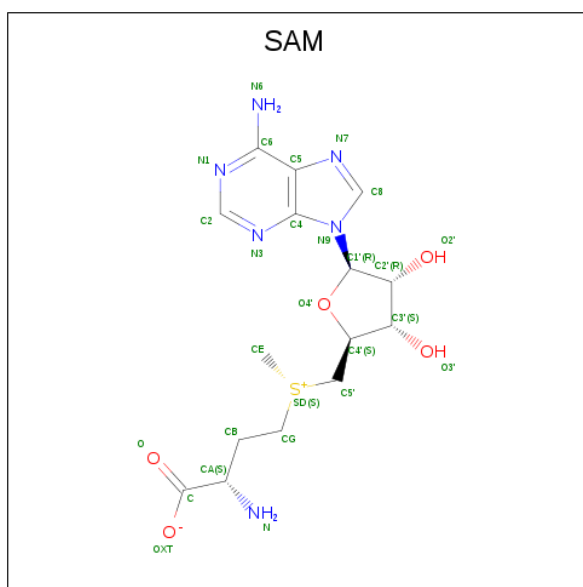
| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 58 | s | 386 | Total | C | N | O | S | 0 | 0 |
| | | | 3155 | 2023 | 559 | 559 | 14 | | |

- Molecule 59 is S-(2-{[N-(2-HYDROXY-4-{[HYDROXY(OXIDO)PHOSPHINO]OXY}-3,3-DIMETHYLBUTANOYL)-BETA-ALANYL]AMINO}ETHYL) DECANETHIOATE (three-letter code: PM8) (formula: C₂₁H₄₁N₂O₇PS).



| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 59 | w | 1 | Total | C | N | O | P | S |
| | | | 32 | 21 | 2 | 7 | 1 | 1 |
| | | | | | | | | 0 |

- Molecule 60 is S-ADENOSYLMETHIONINE (three-letter code: SAM) (formula: C₁₅H₂₂N₆O₅S).



| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 60 | x | 1 | Total | C | N | O | S | 0 |
| | | | 27 | 15 | 6 | 5 | 1 | |

- Molecule 61 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|----|---------|
| 61 | 0 | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |
| 61 | 4 | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |

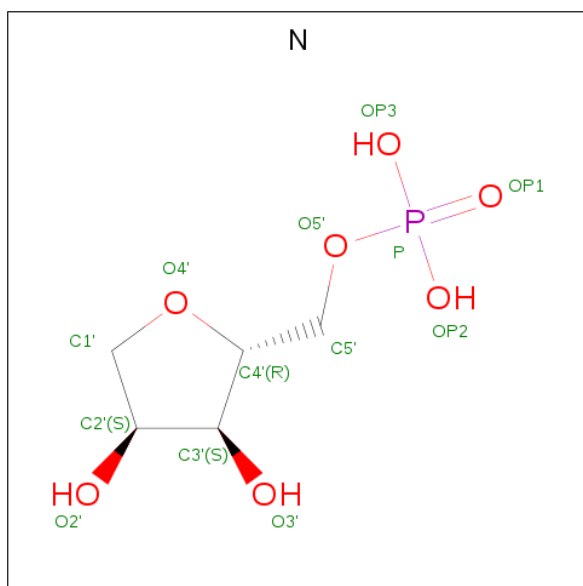
- Molecule 62 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|----|---------|
| 62 | A | 85 | Total | Mg | 0 |
| | | | 85 | 85 | |
| 62 | D | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 62 | E | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 62 | O | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |

- Molecule 63 is POTASSIUM ION (three-letter code: K) (formula: K).

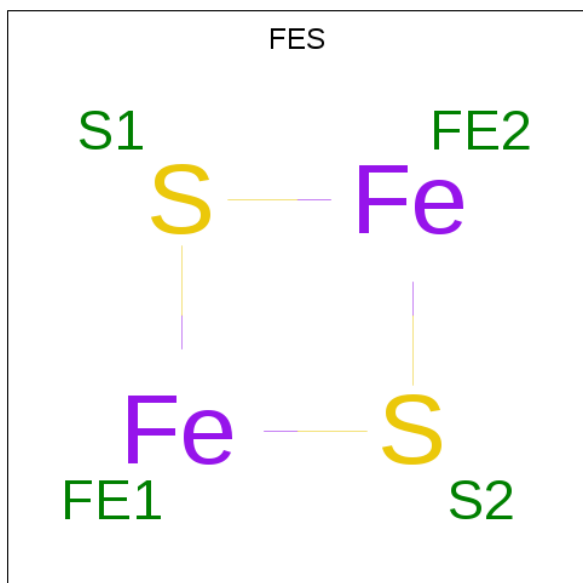
| Mol | Chain | Residues | Atoms | | | AltConf |
|-----|-------|----------|-------|---|--|---------|
| 63 | A | 8 | Total | K | | 0 |
| | | | 8 | 8 | | |

- Molecule 64 is ANY 5'-MONOPHOSPHATE NUCLEOTIDE (three-letter code: N) (formula: $C_5H_{11}O_7P$).



| Mol | Chain | Residues | Atoms | | | | AltConf |
|-----|-------|----------|-------|---|---|---|---------|
| 64 | A | 1 | Total | C | O | P | 0 |
| | | | 12 | 5 | 6 | 1 | |

- Molecule 65 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).

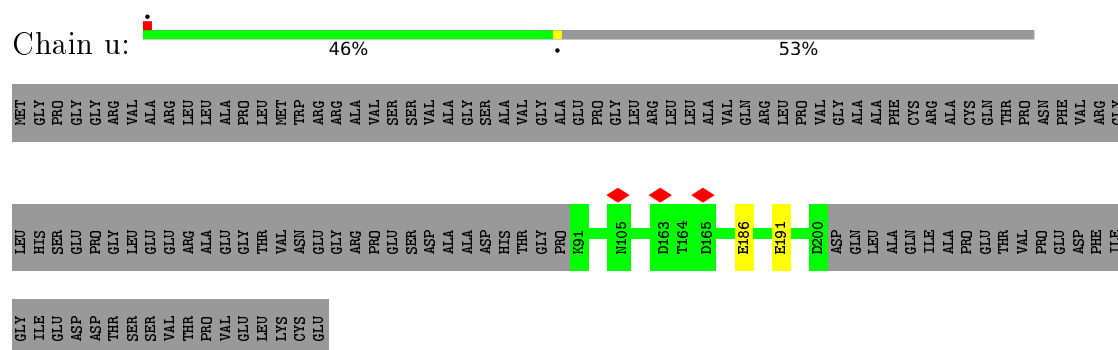


| Mol | Chain | Residues | Atoms | | | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 65 | r | 1 | Total | Fe | S | 0 |
| | | | 4 | 2 | 2 | |

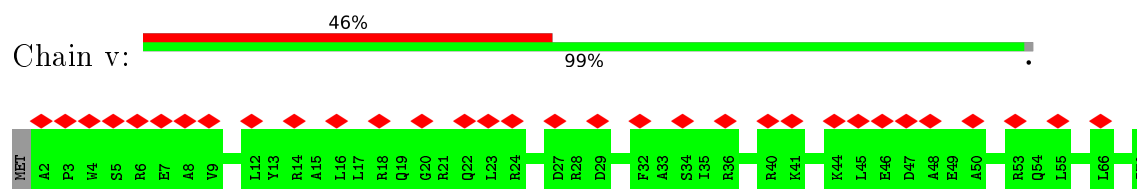
3 Residue-property plots [i](#)

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.

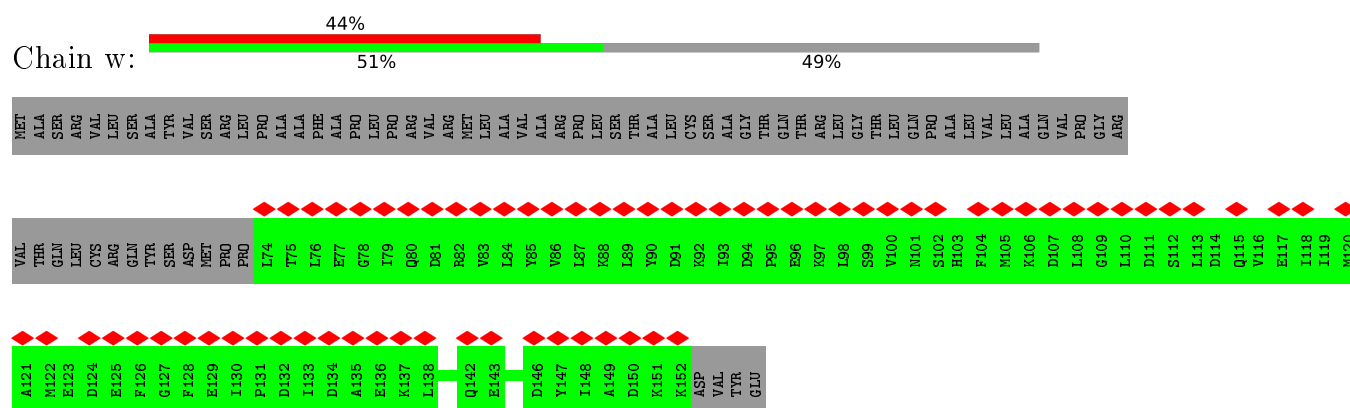
- Molecule 1: Mitochondrial assembly of ribosomal large subunit protein 1



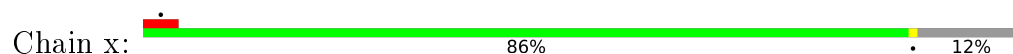
- Molecule 2: MIEF1 upstream open reading frame protein

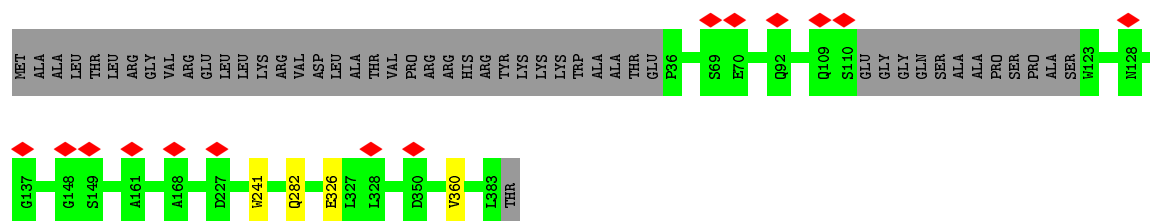


- Molecule 3: Acyl carrier protein, mitochondrial



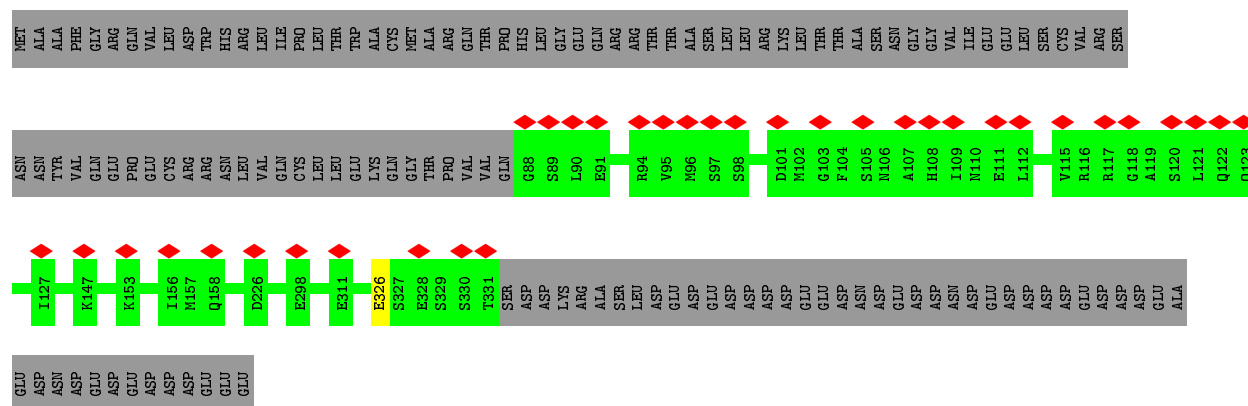
- Molecule 4: 5-methylcytosine rRNA methyltransferase NSUN4





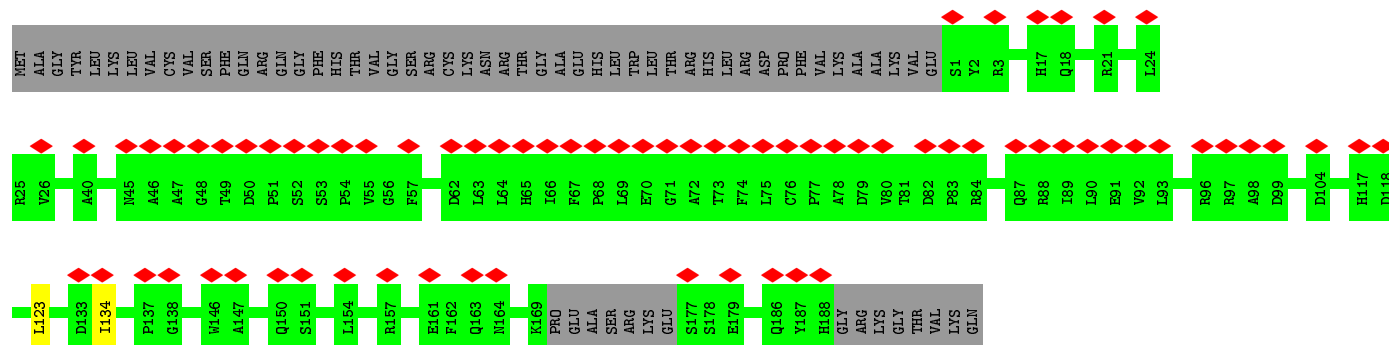
- Molecule 5: Transcription termination factor 4, mitochondrial

Chain y: 9% 64% 36%



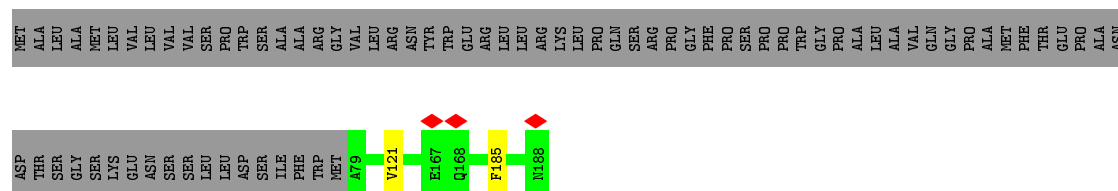
- Molecule 6: rRNA methyltransferase 2, mitochondrial

Chain z: 30% 73% 26%

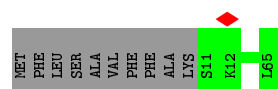


- Molecule 7: 39S ribosomal protein L32, mitochondrial

Chain 0: 57% 41%



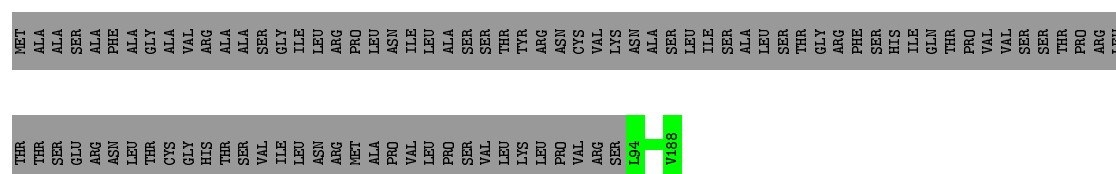
- Molecule 8: 39S ribosomal protein L33, mitochondrial



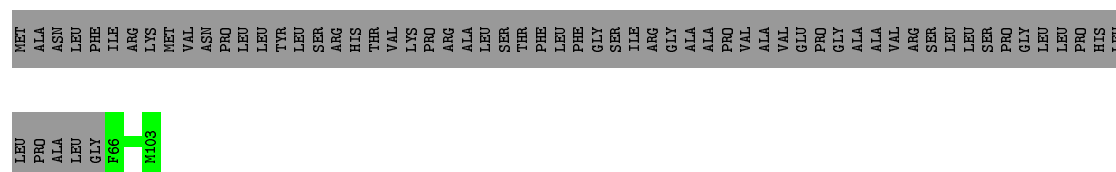
- Chain 2: 



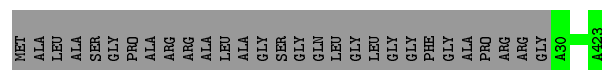
- Chain 3: 51% 49%



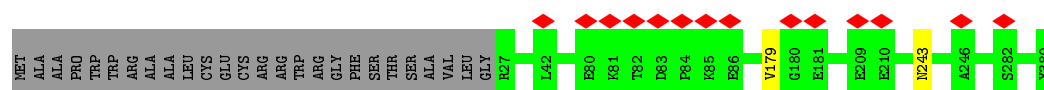
- Chain 4: 37% 63%

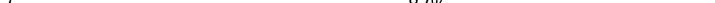


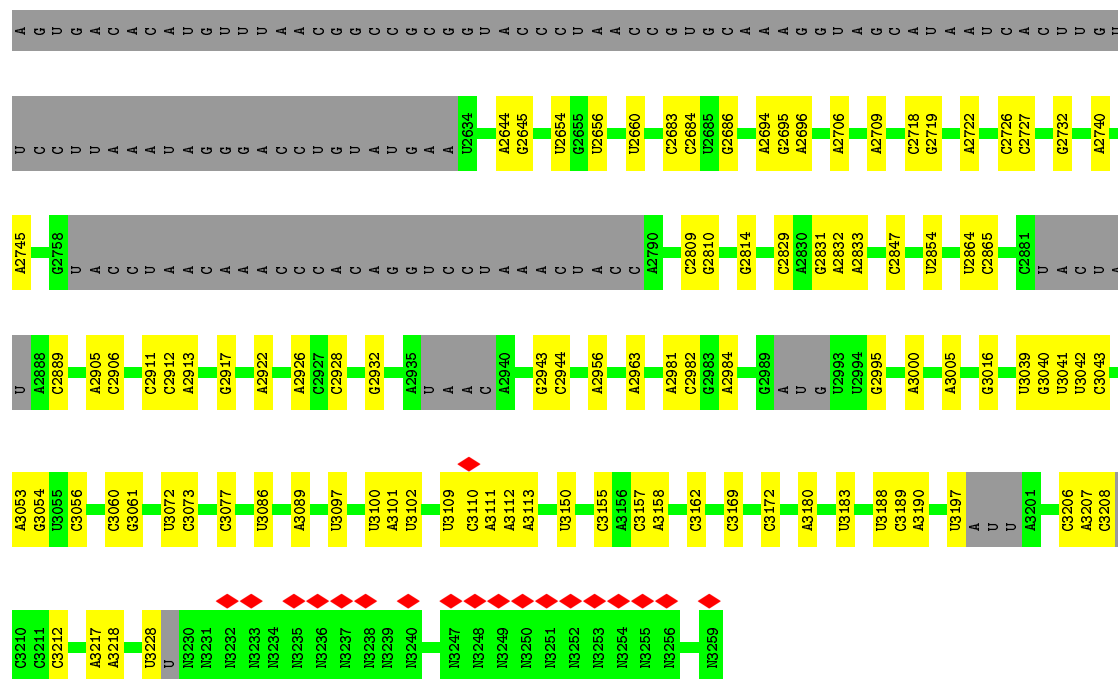
- Chain 5:  93% 7%



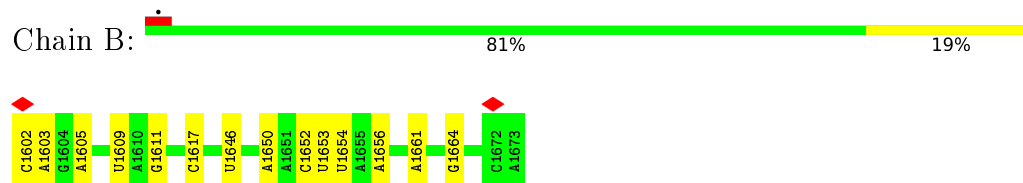
- Chain 6: 93% 7%



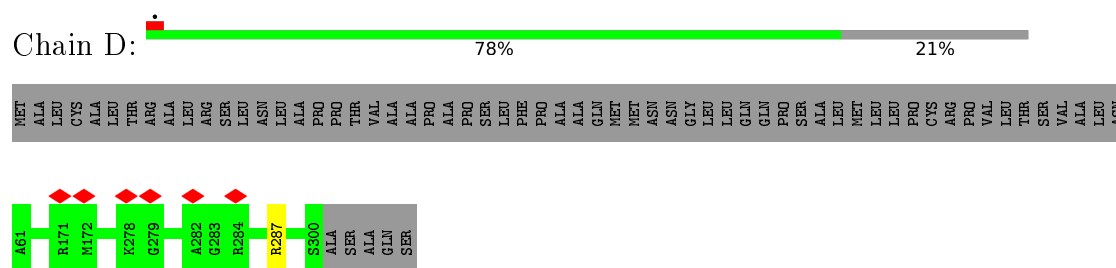
- Chain 7:  14% 87% 13%



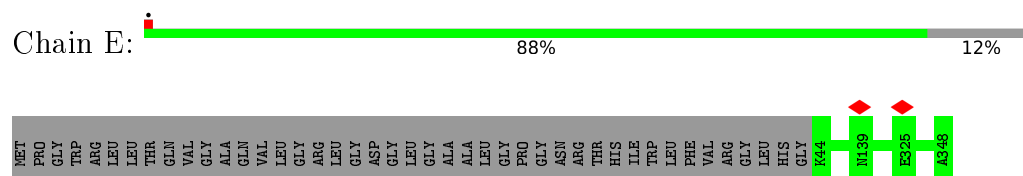
- Molecule 18: mitochondrial tRNA^{Val}



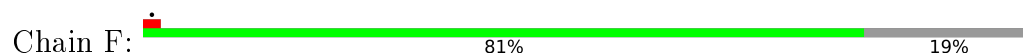
- Molecule 19: 39S ribosomal protein L2, mitochondrial



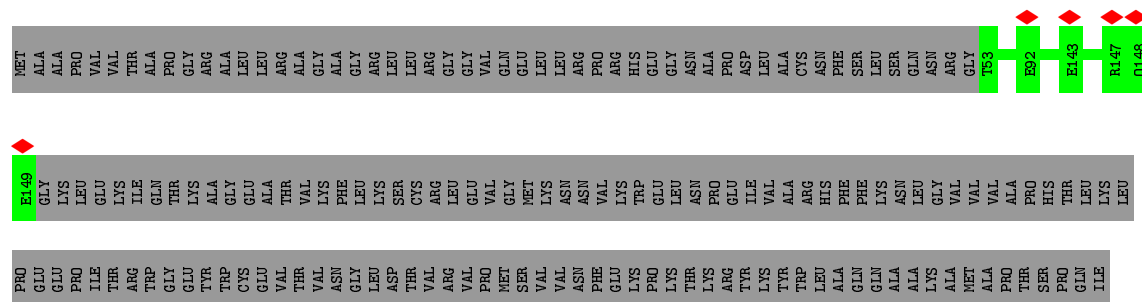
- Molecule 20: 39S ribosomal protein L3, mitochondrial



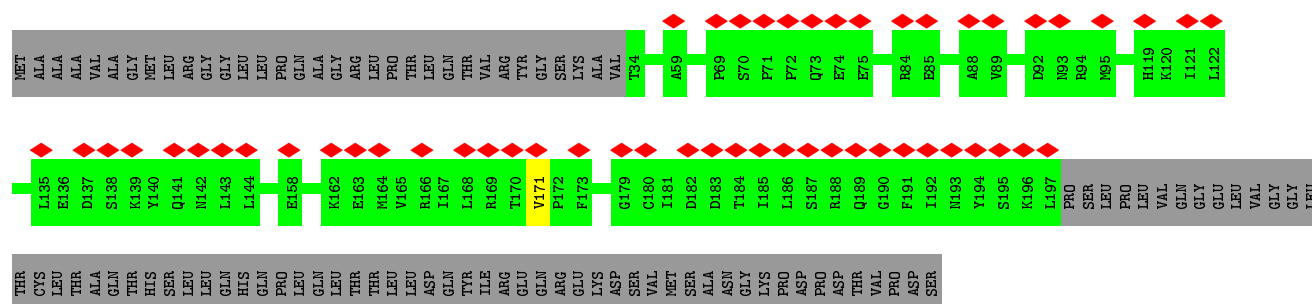
- Molecule 21: 39S ribosomal protein L4, mitochondrial



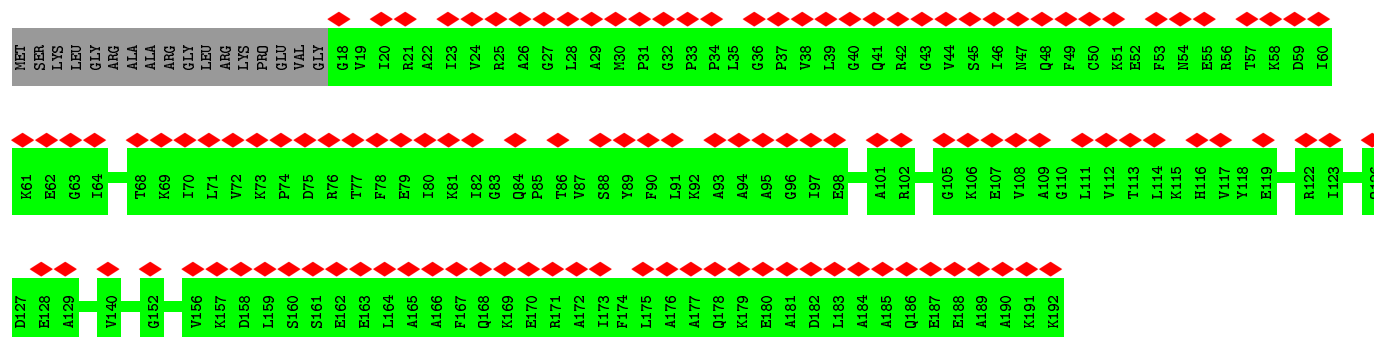
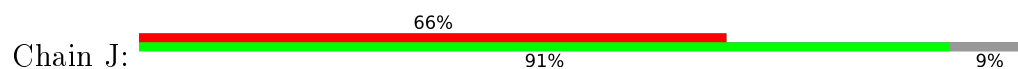
- Molecule 22: 39S ribosomal protein L9, mitochondrial



- Molecule 23: 39S ribosomal protein L10, mitochondrial



- Molecule 24: 39S ribosomal protein L11, mitochondrial





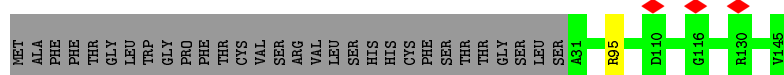
- Molecule 25: 39S ribosomal protein L13, mitochondrial

Chain K:  98%



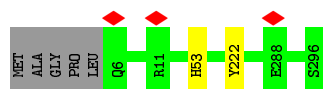
- Molecule 26: 39S ribosomal protein L14, mitochondrial

Chain L:  79%  21%


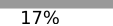


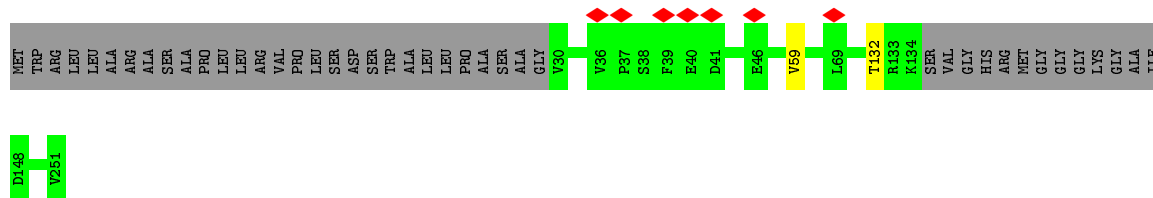
- Molecule 27: 39S ribosomal protein L15, mitochondrial

Chain M:  98%


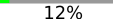


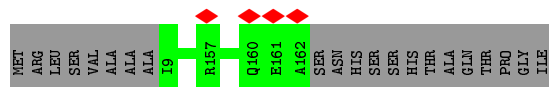
- Molecule 28: 39S ribosomal protein L16, mitochondrial

Chain N:  82%  17%





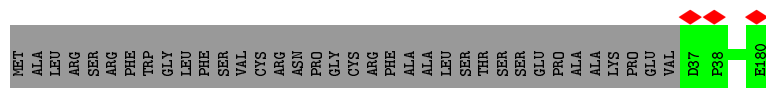
- Molecule 29: 39S ribosomal protein L17, mitochondrial

Chain O:  88%  12%





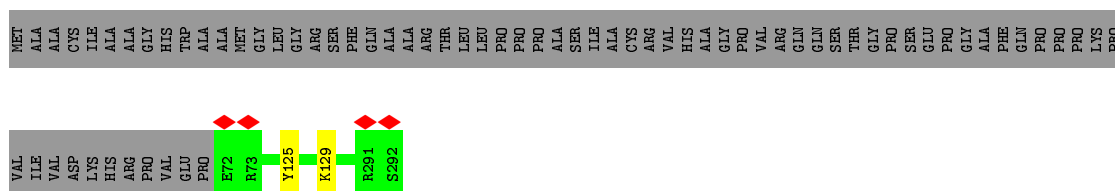
- Molecule 30: 39S ribosomal protein L18, mitochondrial

Chain P:  80%  20%

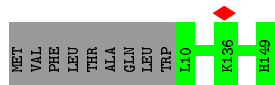


- Molecule 31: 39S ribosomal protein L19, mitochondrial

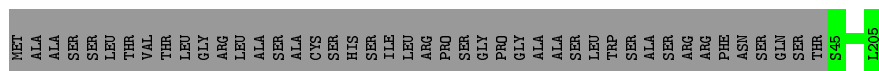
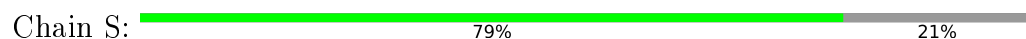
Chain Q:  75%  24%



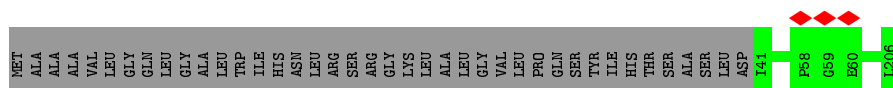
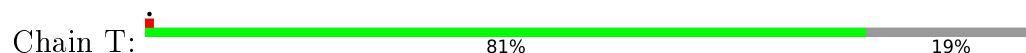
- Molecule 32: 39S ribosomal protein L20, mitochondrial



- Molecule 33: 39S ribosomal protein L21, mitochondrial



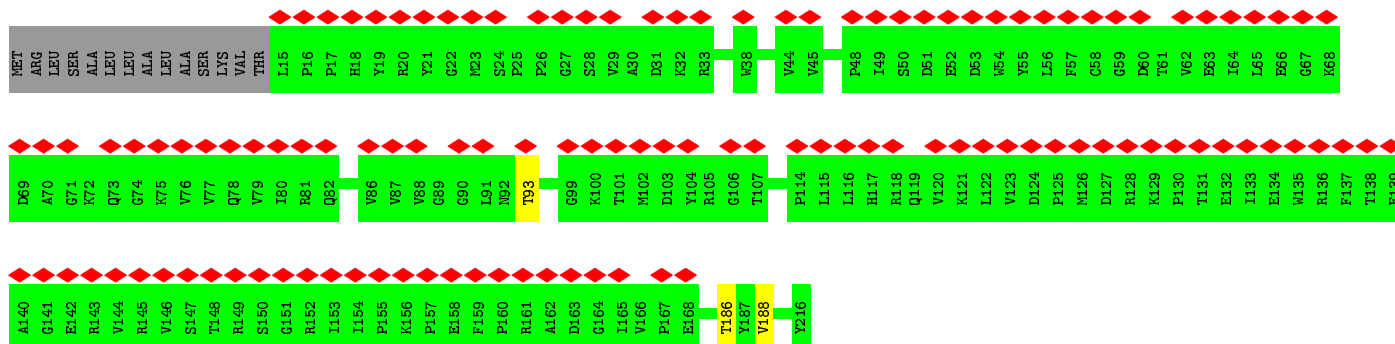
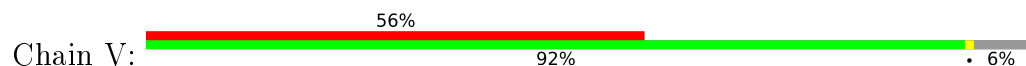
- Molecule 34: 39S ribosomal protein L22, mitochondrial



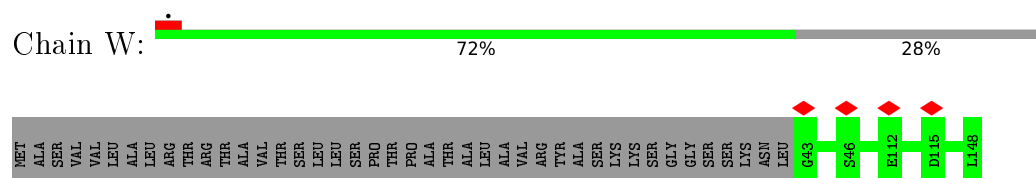
- Molecule 35: 39S ribosomal protein L23, mitochondrial



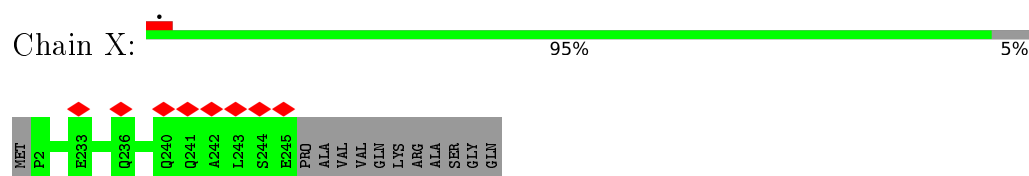
- Molecule 36: 39S ribosomal protein L24, mitochondrial



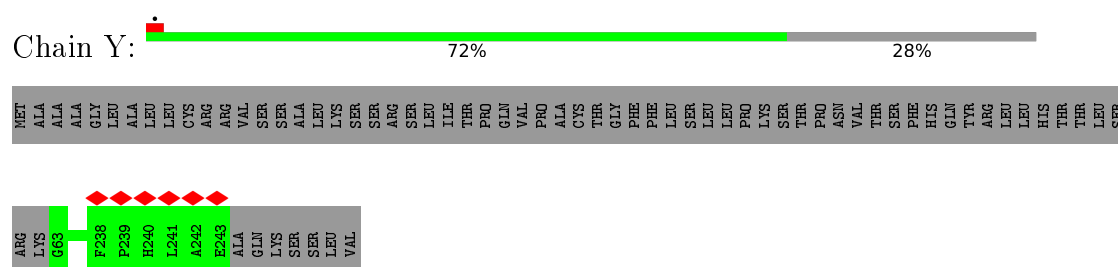
- Molecule 37: 39S ribosomal protein L27, mitochondrial



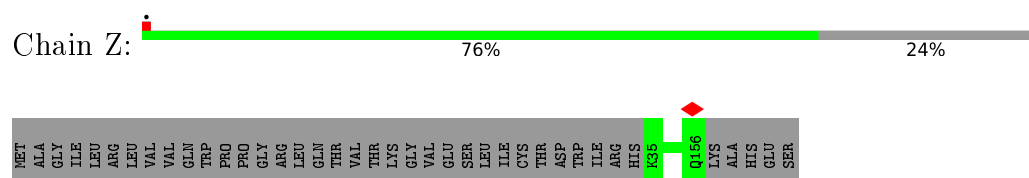
- Molecule 38: 39S ribosomal protein L28, mitochondrial



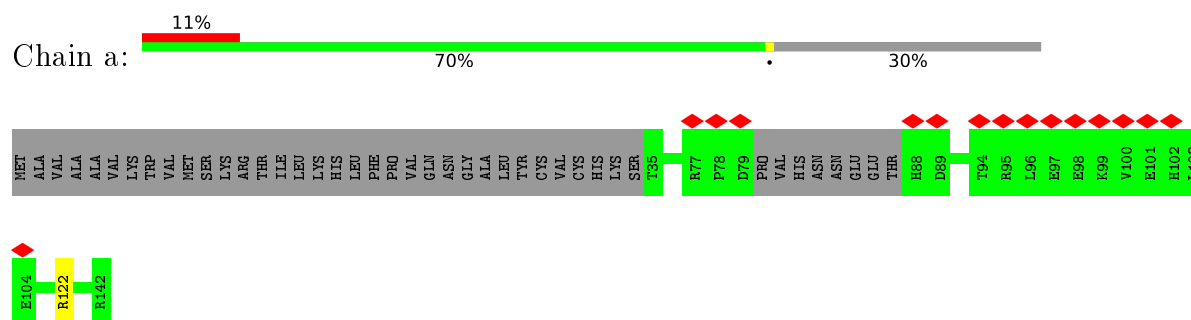
- Molecule 39: 39S ribosomal protein L47, mitochondrial



- Molecule 40: 39S ribosomal protein L30, mitochondrial



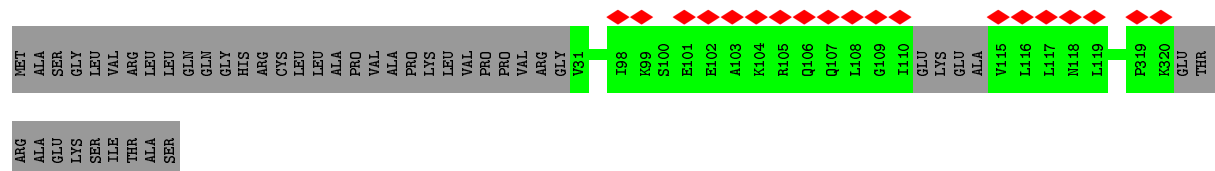
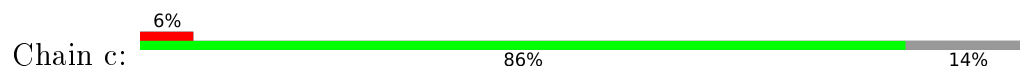
- Molecule 41: 39S ribosomal protein L42, mitochondrial



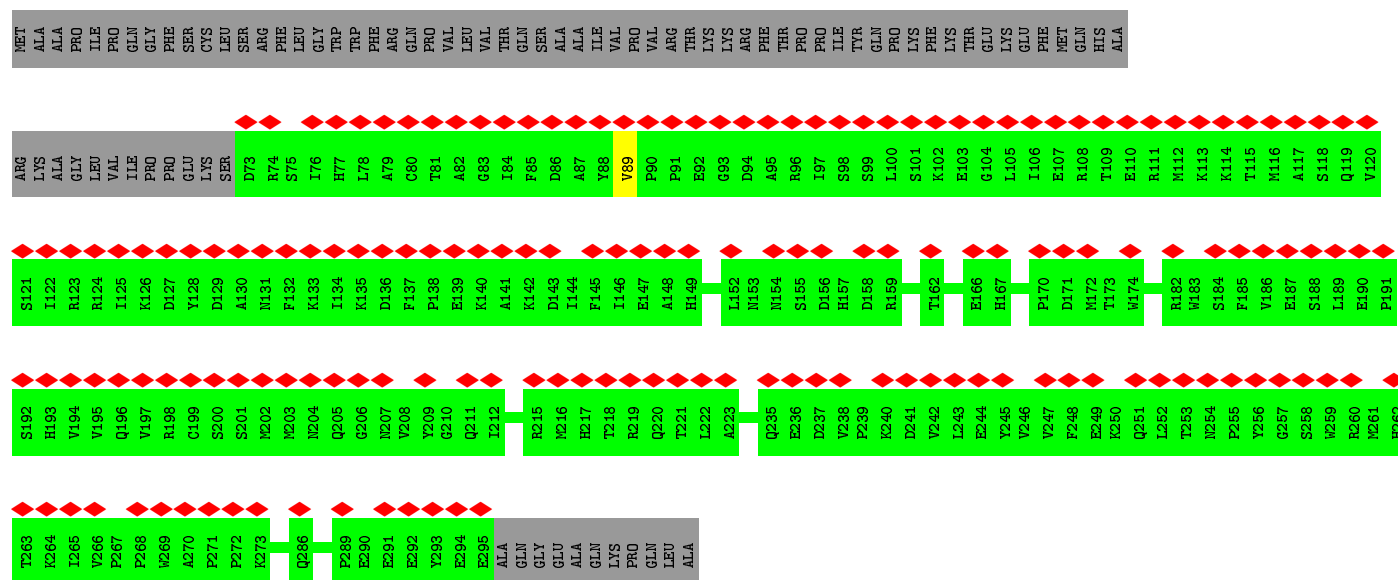
- Molecule 42: 39S ribosomal protein L43, mitochondrial



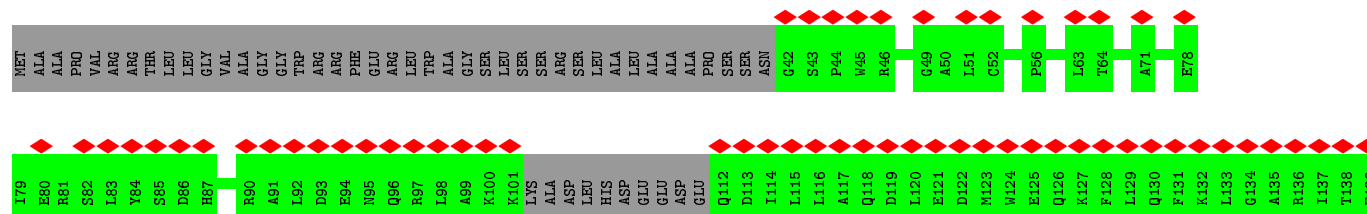
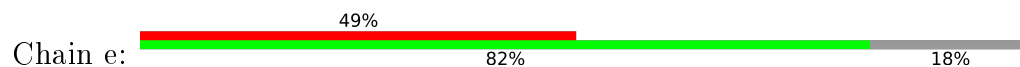
- Molecule 43: 39S ribosomal protein L44, mitochondrial

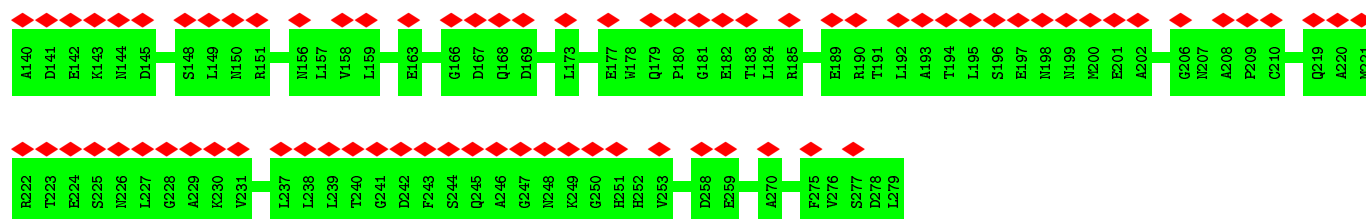


- Molecule 44: 39S ribosomal protein L45, mitochondrial

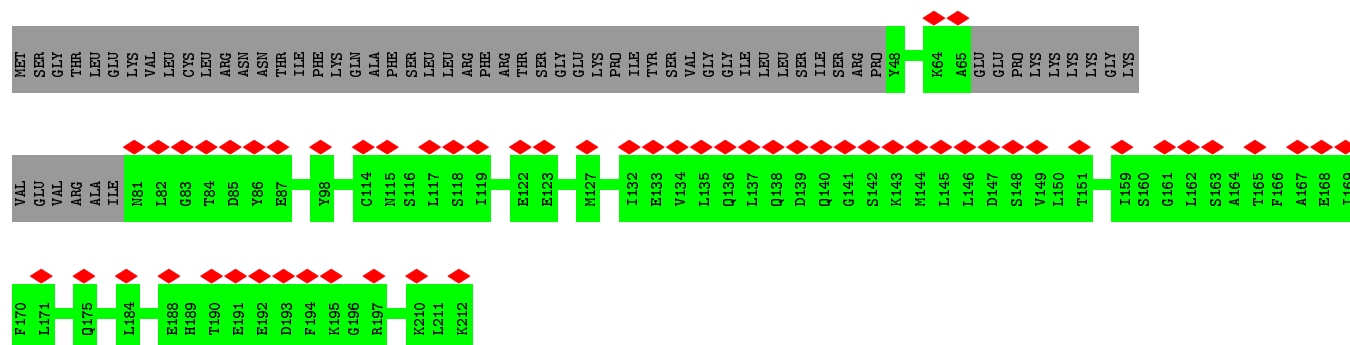


- Molecule 45: 39S ribosomal protein L46, mitochondrial

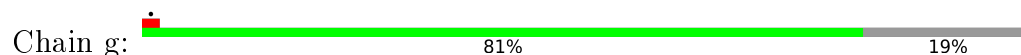




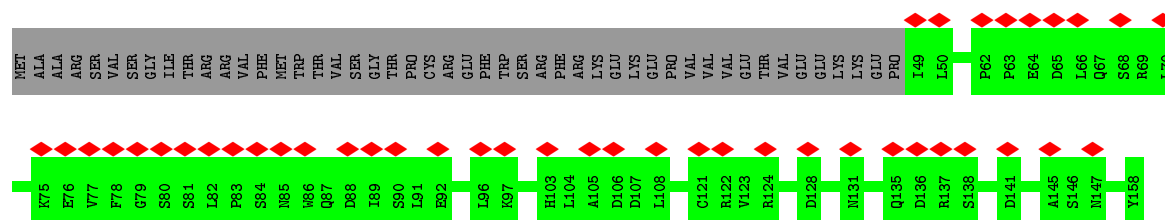
- Molecule 46: 39S ribosomal protein L48, mitochondrial



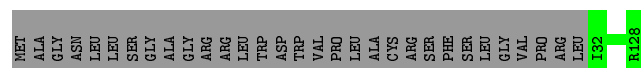
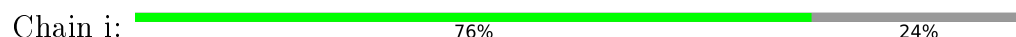
- Molecule 47: 39S ribosomal protein L49, mitochondrial




- Molecule 48: 39S ribosomal protein L50, mitochondrial

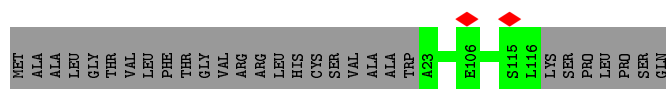


- Molecule 49: 39S ribosomal protein L51, mitochondrial

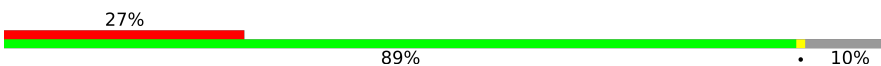


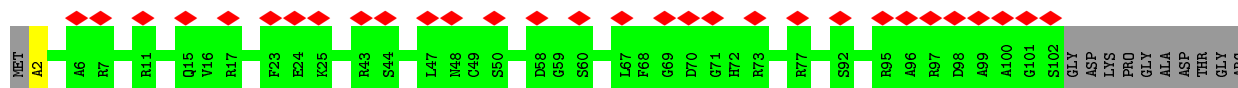
- Molecule 50: 39S ribosomal protein L52, mitochondrial

Chain j: 



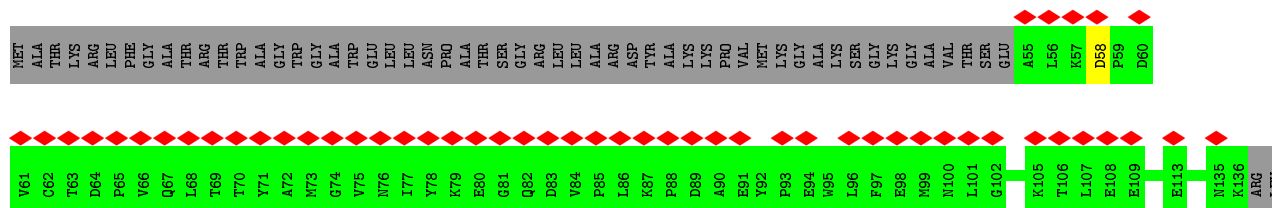
- Molecule 51: 39S ribosomal protein L53, mitochondrial

Chain k: 



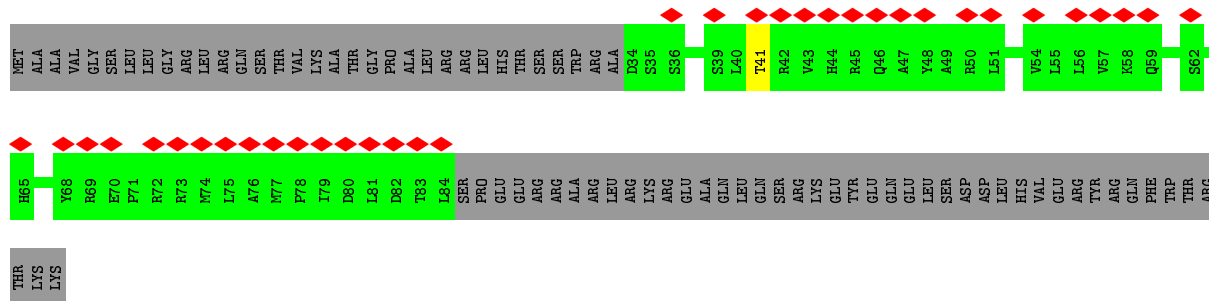
- Molecule 52: 39S ribosomal protein L54, mitochondrial

Chain l: 




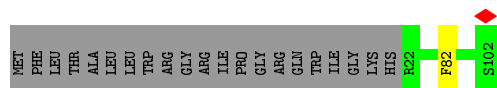
- Molecule 53: 39S ribosomal protein L55, mitochondrial

Chain m: 



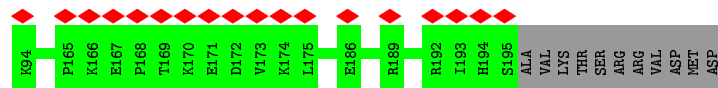
- Molecule 54: Ribosomal protein 63, mitochondrial

Chain o: 

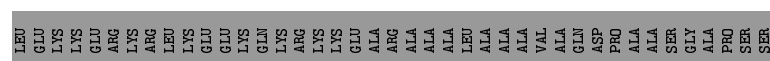


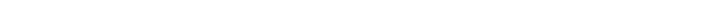
- Molecule 55: Peptidyl-tRNA hydrolase ICT1, mitochondrial

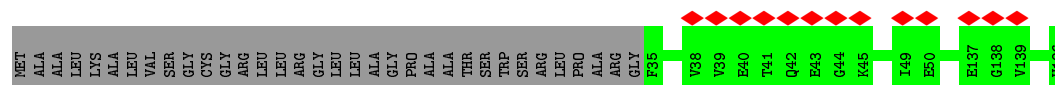
Chain p: 




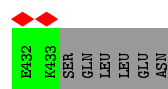
- Chain q:  6% 64% 36%



- Chain r:  7% 83% 17%



- Chain s:  88% 12%



4 Experimental information

| Property | Value | Source |
|--------------------------------------|---|-----------|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 114557 | 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 ($e^-/\text{\AA}^2$) | 60 | Depositor |
| Minimum defocus (nm) | Not provided | |
| Maximum defocus (nm) | Not provided | |
| Magnification | Not provided | |
| Image detector | FEI FALCON III (4k x 4k) | Depositor |
| Maximum map value | 5.839 | Depositor |
| Minimum map value | -1.970 | Depositor |
| Average map value | -0.002 | Depositor |
| Map value standard deviation | 0.190 | Depositor |
| Recommended contour level | 0.7 | Depositor |
| Map size (\AA) | 486.976, 486.976, 486.976 | wwPDB |
| Map dimensions | 448, 448, 448 | wwPDB |
| Map angles ($^\circ$) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (\AA) | 1.087, 1.087, 1.087 | 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, SAM, PM8, ZN, FES, THC, OMU, AYA, SAC, K

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 | u | 0.23 | 0/941 | 0.45 | 0/1270 |
| 2 | v | 0.23 | 0/597 | 0.52 | 0/796 |
| 3 | w | 0.24 | 0/647 | 0.40 | 0/871 |
| 4 | x | 0.24 | 0/2721 | 0.46 | 0/3691 |
| 5 | y | 0.23 | 0/2011 | 0.43 | 0/2702 |
| 6 | z | 0.24 | 0/1394 | 0.45 | 0/1901 |
| 7 | 0 | 0.24 | 0/913 | 0.50 | 0/1224 |
| 8 | 1 | 0.24 | 0/460 | 0.54 | 0/610 |
| 9 | 2 | 0.23 | 0/383 | 0.52 | 0/507 |
| 10 | 3 | 0.23 | 0/853 | 0.50 | 0/1136 |
| 11 | 4 | 0.24 | 0/350 | 0.54 | 0/461 |
| 12 | 5 | 0.24 | 0/3305 | 0.46 | 0/4502 |
| 13 | 6 | 0.24 | 0/3043 | 0.48 | 0/4140 |
| 14 | 7 | 0.23 | 0/2447 | 0.43 | 0/3310 |
| 15 | 8 | 0.23 | 0/880 | 0.44 | 0/1188 |
| 16 | 9 | 0.26 | 0/1025 | 0.47 | 0/1379 |
| 17 | A | 0.17 | 0/33594 | 0.69 | 5/52281 (0.0%) |
| 18 | B | 0.28 | 1/1700 (0.1%) | 0.65 | 0/2641 |
| 19 | D | 0.24 | 0/1910 | 0.53 | 0/2569 |
| 20 | E | 0.24 | 0/2475 | 0.44 | 0/3355 |
| 21 | F | 0.24 | 0/2090 | 0.48 | 0/2842 |
| 22 | H | 0.23 | 0/816 | 0.50 | 0/1097 |
| 23 | I | 0.23 | 0/1361 | 0.46 | 0/1839 |
| 24 | J | 0.24 | 0/1348 | 0.44 | 0/1813 |
| 25 | K | 0.24 | 0/1490 | 0.45 | 0/2021 |
| 26 | L | 0.24 | 0/905 | 0.51 | 0/1218 |
| 27 | M | 0.25 | 0/2381 | 0.50 | 0/3212 |
| 28 | N | 0.24 | 0/1747 | 0.48 | 0/2354 |
| 29 | O | 0.23 | 0/1283 | 0.50 | 0/1727 |
| 30 | P | 0.23 | 0/1199 | 0.51 | 0/1623 |
| 31 | Q | 0.24 | 0/1884 | 0.49 | 0/2535 |
| 32 | R | 0.24 | 0/1175 | 0.50 | 0/1572 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|-----------------|-------------|-----------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 33 | S | 0.24 | 0/1320 | 0.50 | 0/1789 |
| 34 | T | 0.25 | 0/1403 | 0.47 | 0/1886 |
| 35 | U | 0.24 | 0/1274 | 0.50 | 0/1723 |
| 36 | V | 0.23 | 0/1698 | 0.49 | 0/2302 |
| 37 | W | 0.25 | 0/857 | 0.47 | 0/1155 |
| 38 | X | 0.24 | 0/2099 | 0.45 | 0/2837 |
| 39 | Y | 0.23 | 0/1593 | 0.47 | 0/2136 |
| 40 | Z | 0.23 | 0/1021 | 0.46 | 0/1378 |
| 41 | a | 0.24 | 0/866 | 0.48 | 0/1174 |
| 42 | b | 0.24 | 0/1203 | 0.52 | 0/1627 |
| 43 | c | 0.24 | 0/2347 | 0.44 | 0/3171 |
| 44 | d | 0.23 | 0/1871 | 0.45 | 0/2533 |
| 45 | e | 0.23 | 0/1885 | 0.45 | 0/2542 |
| 46 | f | 0.24 | 0/1216 | 0.43 | 0/1638 |
| 47 | g | 0.25 | 0/1151 | 0.48 | 0/1569 |
| 48 | h | 0.23 | 0/918 | 0.44 | 0/1249 |
| 49 | i | 0.23 | 0/850 | 0.50 | 0/1135 |
| 50 | j | 0.23 | 0/760 | 0.46 | 0/1023 |
| 51 | k | 0.23 | 0/777 | 0.49 | 0/1048 |
| 52 | l | 0.23 | 0/707 | 0.44 | 0/960 |
| 53 | m | 0.22 | 0/426 | 0.56 | 0/575 |
| 54 | o | 0.24 | 0/705 | 0.49 | 0/945 |
| 55 | p | 0.23 | 0/1223 | 0.48 | 0/1641 |
| 56 | q | 0.23 | 0/1208 | 0.47 | 0/1633 |
| 57 | r | 0.24 | 0/1362 | 0.49 | 0/1846 |
| 58 | s | 0.24 | 0/3239 | 0.48 | 0/4400 |
| All | All | 0.22 | 1/113307 (0.0%) | 0.55 | 5/160302 (0.0%) |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|--------|-------------|----------|
| 18 | B | 1602 | C | OP3-P | -10.54 | 1.48 | 1.61 |

All (5) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|------|-------------|----------|
| 17 | A | 1711 | C | C2-N1-C1' | 5.70 | 125.07 | 118.80 |
| 17 | A | 2079 | C | C2-N1-C1' | 5.65 | 125.02 | 118.80 |
| 17 | A | 2499 | U | C2-N1-C1' | 5.58 | 124.40 | 117.70 |
| 17 | A | 1711 | C | N1-C2-O2 | 5.16 | 122.00 | 118.90 |
| 17 | A | 2079 | C | N1-C2-O2 | 5.16 | 122.00 | 118.90 |

There are no chirality outliers.

There are no planarity outliers.

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 | u | 108/234 (46%) | 106 (98%) | 2 (2%) | 0 | 100 | 100 |
| 2 | v | 67/70 (96%) | 67 (100%) | 0 | 0 | 100 | 100 |
| 3 | w | 77/156 (49%) | 72 (94%) | 5 (6%) | 0 | 100 | 100 |
| 4 | x | 332/384 (86%) | 329 (99%) | 3 (1%) | 0 | 100 | 100 |
| 5 | y | 242/381 (64%) | 241 (100%) | 1 (0%) | 0 | 100 | 100 |
| 6 | z | 177/246 (72%) | 176 (99%) | 1 (1%) | 0 | 100 | 100 |
| 7 | 0 | 108/188 (57%) | 107 (99%) | 1 (1%) | 0 | 100 | 100 |
| 8 | 1 | 53/65 (82%) | 53 (100%) | 0 | 0 | 100 | 100 |
| 9 | 2 | 44/92 (48%) | 43 (98%) | 1 (2%) | 0 | 100 | 100 |
| 10 | 3 | 93/188 (50%) | 92 (99%) | 1 (1%) | 0 | 100 | 100 |
| 11 | 4 | 36/103 (35%) | 36 (100%) | 0 | 0 | 100 | 100 |
| 12 | 5 | 392/423 (93%) | 384 (98%) | 8 (2%) | 0 | 100 | 100 |
| 13 | 6 | 352/380 (93%) | 345 (98%) | 7 (2%) | 0 | 100 | 100 |
| 14 | 7 | 292/338 (86%) | 286 (98%) | 6 (2%) | 0 | 100 | 100 |
| 15 | 8 | 100/206 (48%) | 100 (100%) | 0 | 0 | 100 | 100 |
| 16 | 9 | 122/137 (89%) | 121 (99%) | 1 (1%) | 0 | 100 | 100 |
| 19 | D | 238/305 (78%) | 234 (98%) | 4 (2%) | 0 | 100 | 100 |
| 20 | E | 303/348 (87%) | 296 (98%) | 7 (2%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|------------|---------|----------|-------------|-----|
| 21 | F | 250/311 (80%) | 248 (99%) | 2 (1%) | 0 | 100 | 100 |
| 22 | H | 95/267 (36%) | 95 (100%) | 0 | 0 | 100 | 100 |
| 23 | I | 162/261 (62%) | 160 (99%) | 2 (1%) | 0 | 100 | 100 |
| 24 | J | 173/192 (90%) | 173 (100%) | 0 | 0 | 100 | 100 |
| 25 | K | 175/178 (98%) | 174 (99%) | 1 (1%) | 0 | 100 | 100 |
| 26 | L | 113/145 (78%) | 113 (100%) | 0 | 0 | 100 | 100 |
| 27 | M | 289/296 (98%) | 283 (98%) | 6 (2%) | 0 | 100 | 100 |
| 28 | N | 205/251 (82%) | 204 (100%) | 1 (0%) | 0 | 100 | 100 |
| 29 | O | 152/175 (87%) | 150 (99%) | 2 (1%) | 0 | 100 | 100 |
| 30 | P | 142/180 (79%) | 139 (98%) | 3 (2%) | 0 | 100 | 100 |
| 31 | Q | 219/292 (75%) | 218 (100%) | 1 (0%) | 0 | 100 | 100 |
| 32 | R | 138/149 (93%) | 138 (100%) | 0 | 0 | 100 | 100 |
| 33 | S | 159/205 (78%) | 159 (100%) | 0 | 0 | 100 | 100 |
| 34 | T | 164/206 (80%) | 162 (99%) | 2 (1%) | 0 | 100 | 100 |
| 35 | U | 150/153 (98%) | 149 (99%) | 1 (1%) | 0 | 100 | 100 |
| 36 | V | 200/216 (93%) | 198 (99%) | 2 (1%) | 0 | 100 | 100 |
| 37 | W | 104/148 (70%) | 102 (98%) | 2 (2%) | 0 | 100 | 100 |
| 38 | X | 242/256 (94%) | 240 (99%) | 2 (1%) | 0 | 100 | 100 |
| 39 | Y | 179/250 (72%) | 178 (99%) | 1 (1%) | 0 | 100 | 100 |
| 40 | Z | 120/161 (74%) | 119 (99%) | 1 (1%) | 0 | 100 | 100 |
| 41 | a | 96/142 (68%) | 95 (99%) | 1 (1%) | 0 | 100 | 100 |
| 42 | b | 147/215 (68%) | 144 (98%) | 3 (2%) | 0 | 100 | 100 |
| 43 | c | 282/332 (85%) | 278 (99%) | 4 (1%) | 0 | 100 | 100 |
| 44 | d | 221/306 (72%) | 219 (99%) | 2 (1%) | 0 | 100 | 100 |
| 45 | e | 224/279 (80%) | 219 (98%) | 5 (2%) | 0 | 100 | 100 |
| 46 | f | 146/212 (69%) | 142 (97%) | 4 (3%) | 0 | 100 | 100 |
| 47 | g | 132/166 (80%) | 131 (99%) | 1 (1%) | 0 | 100 | 100 |
| 48 | h | 108/158 (68%) | 106 (98%) | 2 (2%) | 0 | 100 | 100 |
| 49 | i | 95/128 (74%) | 95 (100%) | 0 | 0 | 100 | 100 |
| 50 | j | 92/123 (75%) | 90 (98%) | 2 (2%) | 0 | 100 | 100 |
| 51 | k | 99/112 (88%) | 98 (99%) | 1 (1%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|------------------|------------|----------|----------|-------------|-----|
| 52 | l | 80/138 (58%) | 80 (100%) | 0 | 0 | 100 | 100 |
| 53 | m | 49/128 (38%) | 49 (100%) | 0 | 0 | 100 | 100 |
| 54 | o | 79/102 (78%) | 79 (100%) | 0 | 0 | 100 | 100 |
| 55 | p | 141/206 (68%) | 139 (99%) | 2 (1%) | 0 | 100 | 100 |
| 56 | q | 139/222 (63%) | 139 (100%) | 0 | 0 | 100 | 100 |
| 57 | r | 160/196 (82%) | 159 (99%) | 1 (1%) | 0 | 100 | 100 |
| 58 | s | 382/439 (87%) | 376 (98%) | 6 (2%) | 0 | 100 | 100 |
| All | All | 9239/12140 (76%) | 9128 (99%) | 111 (1%) | 0 | 100 | 100 |

There are no Ramachandran outliers to report.

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 | u | 104/200 (52%) | 102 (98%) | 2 (2%) | 57 | 81 |
| 2 | v | 59/60 (98%) | 59 (100%) | 0 | 100 | 100 |
| 3 | w | 73/136 (54%) | 73 (100%) | 0 | 100 | 100 |
| 4 | x | 291/328 (89%) | 287 (99%) | 4 (1%) | 67 | 86 |
| 5 | y | 226/350 (65%) | 225 (100%) | 1 (0%) | 91 | 96 |
| 6 | z | 146/209 (70%) | 144 (99%) | 2 (1%) | 67 | 86 |
| 7 | 0 | 99/164 (60%) | 97 (98%) | 2 (2%) | 55 | 80 |
| 8 | 1 | 52/60 (87%) | 52 (100%) | 0 | 100 | 100 |
| 9 | 2 | 40/72 (56%) | 40 (100%) | 0 | 100 | 100 |
| 10 | 3 | 88/166 (53%) | 88 (100%) | 0 | 100 | 100 |
| 11 | 4 | 37/89 (42%) | 37 (100%) | 0 | 100 | 100 |
| 12 | 5 | 353/368 (96%) | 353 (100%) | 0 | 100 | 100 |
| 13 | 6 | 313/332 (94%) | 311 (99%) | 2 (1%) | 86 | 94 |
| 14 | 7 | 270/303 (89%) | 269 (100%) | 1 (0%) | 91 | 96 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|---------------|------------|----------|-------------|-----|
| 15 | 8 | 93/190 (49%) | 93 (100%) | 0 | 100 | 100 |
| 16 | 9 | 104/112 (93%) | 104 (100%) | 0 | 100 | 100 |
| 19 | D | 194/245 (79%) | 193 (100%) | 1 (0%) | 88 | 94 |
| 20 | E | 260/290 (90%) | 260 (100%) | 0 | 100 | 100 |
| 21 | F | 219/262 (84%) | 219 (100%) | 0 | 100 | 100 |
| 22 | H | 88/228 (39%) | 88 (100%) | 0 | 100 | 100 |
| 23 | I | 152/232 (66%) | 151 (99%) | 1 (1%) | 84 | 93 |
| 24 | J | 138/150 (92%) | 138 (100%) | 0 | 100 | 100 |
| 25 | K | 154/155 (99%) | 153 (99%) | 1 (1%) | 86 | 94 |
| 26 | L | 98/124 (79%) | 97 (99%) | 1 (1%) | 76 | 90 |
| 27 | M | 246/249 (99%) | 244 (99%) | 2 (1%) | 81 | 92 |
| 28 | N | 182/211 (86%) | 180 (99%) | 2 (1%) | 73 | 89 |
| 29 | O | 134/150 (89%) | 134 (100%) | 0 | 100 | 100 |
| 30 | P | 126/155 (81%) | 126 (100%) | 0 | 100 | 100 |
| 31 | Q | 203/256 (79%) | 201 (99%) | 2 (1%) | 76 | 90 |
| 32 | R | 118/126 (94%) | 118 (100%) | 0 | 100 | 100 |
| 33 | S | 146/180 (81%) | 146 (100%) | 0 | 100 | 100 |
| 34 | T | 146/176 (83%) | 146 (100%) | 0 | 100 | 100 |
| 35 | U | 134/135 (99%) | 133 (99%) | 1 (1%) | 84 | 93 |
| 36 | V | 180/191 (94%) | 177 (98%) | 3 (2%) | 60 | 83 |
| 37 | W | 86/119 (72%) | 86 (100%) | 0 | 100 | 100 |
| 38 | X | 220/229 (96%) | 220 (100%) | 0 | 100 | 100 |
| 39 | Y | 163/223 (73%) | 163 (100%) | 0 | 100 | 100 |
| 40 | Z | 113/147 (77%) | 113 (100%) | 0 | 100 | 100 |
| 41 | a | 96/133 (72%) | 95 (99%) | 1 (1%) | 76 | 90 |
| 42 | b | 130/185 (70%) | 130 (100%) | 0 | 100 | 100 |
| 43 | c | 251/288 (87%) | 251 (100%) | 0 | 100 | 100 |
| 44 | d | 204/274 (74%) | 203 (100%) | 1 (0%) | 88 | 94 |
| 45 | e | 198/236 (84%) | 198 (100%) | 0 | 100 | 100 |
| 46 | f | 133/188 (71%) | 133 (100%) | 0 | 100 | 100 |
| 47 | g | 124/148 (84%) | 124 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|------------------|-------------|----------|-------------|-----|
| 48 | h | 104/148 (70%) | 104 (100%) | 0 | 100 | 100 |
| 49 | i | 86/110 (78%) | 86 (100%) | 0 | 100 | 100 |
| 50 | j | 74/97 (76%) | 74 (100%) | 0 | 100 | 100 |
| 51 | k | 83/90 (92%) | 83 (100%) | 0 | 100 | 100 |
| 52 | l | 76/116 (66%) | 75 (99%) | 1 (1%) | 69 | 87 |
| 53 | m | 46/113 (41%) | 45 (98%) | 1 (2%) | 52 | 78 |
| 54 | o | 70/87 (80%) | 69 (99%) | 1 (1%) | 67 | 86 |
| 55 | p | 135/181 (75%) | 135 (100%) | 0 | 100 | 100 |
| 56 | q | 119/178 (67%) | 119 (100%) | 0 | 100 | 100 |
| 57 | r | 147/169 (87%) | 147 (100%) | 0 | 100 | 100 |
| 58 | s | 340/381 (89%) | 340 (100%) | 0 | 100 | 100 |
| All | All | 8264/10494 (79%) | 8231 (100%) | 33 (0%) | 91 | 96 |

All (33) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | u | 186 | GLU |
| 1 | u | 191 | GLU |
| 4 | x | 241 | TRP |
| 4 | x | 282 | GLN |
| 4 | x | 326 | GLU |
| 4 | x | 360 | VAL |
| 5 | y | 326 | GLU |
| 6 | z | 123 | LEU |
| 6 | z | 134 | ILE |
| 7 | 0 | 121 | VAL |
| 7 | 0 | 185 | PHE |
| 13 | 6 | 179 | VAL |
| 13 | 6 | 243 | ASN |
| 14 | 7 | 70 | VAL |
| 19 | D | 287 | ARG |
| 23 | I | 171 | VAL |
| 25 | K | 67 | PHE |
| 26 | L | 95 | ARG |
| 27 | M | 53 | HIS |
| 27 | M | 222 | TYR |
| 28 | N | 59 | VAL |
| 28 | N | 132 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 31 | Q | 125 | TYR |
| 31 | Q | 129 | LYS |
| 35 | U | 19 | VAL |
| 36 | V | 93 | THR |
| 36 | V | 186 | THR |
| 36 | V | 188 | VAL |
| 41 | a | 122 | ARG |
| 44 | d | 89 | VAL |
| 52 | l | 58 | ASP |
| 53 | m | 41 | THR |
| 54 | o | 82 | PHE |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | v | 19 | GLN |
| 4 | x | 85 | HIS |
| 4 | x | 109 | GLN |
| 4 | x | 172 | GLN |
| 4 | x | 214 | GLN |
| 4 | x | 230 | GLN |
| 4 | x | 304 | HIS |
| 4 | x | 316 | GLN |
| 4 | x | 322 | GLN |
| 5 | y | 122 | GLN |
| 5 | y | 123 | GLN |
| 5 | y | 192 | GLN |
| 5 | y | 195 | ASN |
| 5 | y | 210 | GLN |
| 5 | y | 235 | GLN |
| 5 | y | 255 | GLN |
| 5 | y | 284 | GLN |
| 6 | z | 136 | GLN |
| 6 | z | 150 | GLN |
| 6 | z | 163 | GLN |
| 6 | z | 186 | GLN |
| 8 | 1 | 31 | ASN |
| 10 | 3 | 154 | GLN |
| 12 | 5 | 96 | HIS |
| 12 | 5 | 191 | GLN |
| 13 | 6 | 320 | GLN |
| 13 | 6 | 354 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 14 | 7 | 198 | ASN |
| 14 | 7 | 290 | GLN |
| 21 | F | 103 | GLN |
| 21 | F | 241 | ASN |
| 23 | I | 43 | GLN |
| 23 | I | 150 | HIS |
| 26 | L | 52 | HIS |
| 33 | S | 118 | ASN |
| 35 | U | 27 | GLN |
| 35 | U | 136 | GLN |
| 36 | V | 73 | GLN |
| 40 | Z | 64 | HIS |
| 41 | a | 46 | ASN |
| 42 | b | 66 | ASN |
| 44 | d | 235 | GLN |
| 45 | e | 67 | GLN |
| 45 | e | 75 | GLN |
| 45 | e | 219 | GLN |
| 46 | f | 138 | GLN |
| 46 | f | 189 | HIS |
| 47 | g | 93 | ASN |
| 48 | h | 118 | HIS |
| 52 | l | 82 | GLN |
| 52 | l | 135 | ASN |
| 54 | o | 85 | HIS |
| 54 | o | 91 | GLN |
| 54 | o | 94 | HIS |
| 55 | p | 194 | HIS |
| 58 | s | 239 | ASN |
| 58 | s | 358 | GLN |

5.3.3 RNA ⓘ

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 17 | A | 1406/1589 (88%) | 262 (18%) | 8 (0%) |
| 18 | B | 71/72 (98%) | 13 (18%) | 0 |
| All | All | 1477/1661 (88%) | 275 (18%) | 8 (0%) |

All (275) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 17 | A | 1689 | C |
| 17 | A | 1694 | U |
| 17 | A | 1699 | C |
| 17 | A | 1700 | U |
| 17 | A | 1704 | U |
| 17 | A | 1707 | C |
| 17 | A | 1708 | A |
| 17 | A | 1711 | C |
| 17 | A | 1713 | A |
| 17 | A | 1724 | A |
| 17 | A | 1727 | A |
| 17 | A | 1728 | U |
| 17 | A | 1748 | G |
| 17 | A | 1750 | G |
| 17 | A | 1751 | A |
| 17 | A | 1761 | A |
| 17 | A | 1765 | C |
| 17 | A | 1767 | G |
| 17 | A | 1770 | G |
| 17 | A | 1780 | U |
| 17 | A | 1805 | A |
| 17 | A | 1807 | U |
| 17 | A | 1808 | A |
| 17 | A | 1809 | U |
| 17 | A | 1810 | A |
| 17 | A | 1817 | C |
| 17 | A | 1821 | A |
| 17 | A | 1827 | C |
| 17 | A | 1828 | A |
| 17 | A | 1829 | A |
| 17 | A | 1832 | A |
| 17 | A | 1836 | A |
| 17 | A | 1844 | A |
| 17 | A | 1853 | A |
| 17 | A | 1854 | U |
| 17 | A | 1855 | A |
| 17 | A | 1868 | G |
| 17 | A | 1869 | A |
| 17 | A | 1872 | U |
| 17 | A | 1882 | A |
| 17 | A | 1883 | G |
| 17 | A | 1887 | A |
| 17 | A | 1892 | A |

Continued on next page...

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 17 | A | 1893 | A |
| 17 | A | 1902 | C |
| 17 | A | 1903 | C |
| 17 | A | 1918 | G |
| 17 | A | 1937 | A |
| 17 | A | 1940 | A |
| 17 | A | 1962 | A |
| 17 | A | 1968 | G |
| 17 | A | 1974 | A |
| 17 | A | 1985 | G |
| 17 | A | 1986 | A |
| 17 | A | 1994 | A |
| 17 | A | 2002 | G |
| 17 | A | 2015 | G |
| 17 | A | 2021 | U |
| 17 | A | 2022 | G |
| 17 | A | 2029 | A |
| 17 | A | 2030 | U |
| 17 | A | 2031 | A |
| 17 | A | 2036 | C |
| 17 | A | 2037 | U |
| 17 | A | 2039 | A |
| 17 | A | 2060 | A |
| 17 | A | 2065 | A |
| 17 | A | 2068 | C |
| 17 | A | 2069 | U |
| 17 | A | 2074 | A |
| 17 | A | 2079 | C |
| 17 | A | 2083 | U |
| 17 | A | 2092 | C |
| 17 | A | 2098 | G |
| 17 | A | 2109 | A |
| 17 | A | 2110 | A |
| 17 | A | 2125 | C |
| 17 | A | 2132 | A |
| 17 | A | 2147 | G |
| 17 | A | 2154 | A |
| 17 | A | 2159 | U |
| 17 | A | 2163 | A |
| 17 | A | 2167 | A |
| 17 | A | 2168 | U |
| 17 | A | 2169 | A |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 17 | A | 2171 | U |
| 17 | A | 2172 | A |
| 17 | A | 2173 | G |
| 17 | A | 2181 | A |
| 17 | A | 2182 | G |
| 17 | A | 2183 | C |
| 17 | A | 2184 | A |
| 17 | A | 2187 | C |
| 17 | A | 2189 | C |
| 17 | A | 2190 | C |
| 17 | A | 2195 | A |
| 17 | A | 2197 | G |
| 17 | A | 2198 | A |
| 17 | A | 2199 | A |
| 17 | A | 2200 | A |
| 17 | A | 2202 | C |
| 17 | A | 2203 | G |
| 17 | A | 2210 | C |
| 17 | A | 2211 | U |
| 17 | A | 2216 | A |
| 17 | A | 2233 | U |
| 17 | A | 2237 | A |
| 17 | A | 2239 | A |
| 17 | A | 2241 | A |
| 17 | A | 2245 | A |
| 17 | A | 2246 | A |
| 17 | A | 2260 | A |
| 17 | A | 2262 | C |
| 17 | A | 2263 | C |
| 17 | A | 2283 | C |
| 17 | A | 2284 | C |
| 17 | A | 2293 | A |
| 17 | A | 2297 | A |
| 17 | A | 2300 | G |
| 17 | A | 2322 | C |
| 17 | A | 2324 | U |
| 17 | A | 2332 | C |
| 17 | A | 2345 | G |
| 17 | A | 2350 | A |
| 17 | A | 2351 | U |
| 17 | A | 2352 | U |
| 17 | A | 2353 | A |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 17 | A | 2354 | A |
| 17 | A | 2355 | A |
| 17 | A | 2356 | A |
| 17 | A | 2359 | C |
| 17 | A | 2360 | U |
| 17 | A | 2361 | G |
| 17 | A | 2362 | A |
| 17 | A | 2363 | A |
| 17 | A | 2374 | A |
| 17 | A | 2390 | A |
| 17 | A | 2393 | C |
| 17 | A | 2396 | C |
| 17 | A | 2401 | A |
| 17 | A | 2405 | C |
| 17 | A | 2406 | A |
| 17 | A | 2407 | U |
| 17 | A | 2415 | C |
| 17 | A | 2432 | A |
| 17 | A | 2444 | A |
| 17 | A | 2446 | A |
| 17 | A | 2451 | A |
| 17 | A | 2452 | A |
| 17 | A | 2458 | A |
| 17 | A | 2464 | G |
| 17 | A | 2478 | G |
| 17 | A | 2480 | A |
| 17 | A | 2493 | C |
| 17 | A | 2500 | A |
| 17 | A | 2502 | C |
| 17 | A | 2507 | A |
| 17 | A | 2511 | C |
| 17 | A | 2520 | C |
| 17 | A | 2521 | A |
| 17 | A | 2522 | U |
| 17 | A | 2527 | A |
| 17 | A | 2530 | A |
| 17 | A | 2531 | U |
| 17 | A | 2540 | C |
| 17 | A | 2644 | A |
| 17 | A | 2645 | G |
| 17 | A | 2654 | U |
| 17 | A | 2656 | U |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 17 | A | 2660 | U |
| 17 | A | 2683 | C |
| 17 | A | 2684 | C |
| 17 | A | 2686 | G |
| 17 | A | 2694 | A |
| 17 | A | 2695 | G |
| 17 | A | 2696 | A |
| 17 | A | 2706 | A |
| 17 | A | 2709 | A |
| 17 | A | 2718 | C |
| 17 | A | 2719 | G |
| 17 | A | 2722 | A |
| 17 | A | 2726 | C |
| 17 | A | 2727 | C |
| 17 | A | 2732 | G |
| 17 | A | 2740 | A |
| 17 | A | 2745 | A |
| 17 | A | 2809 | C |
| 17 | A | 2810 | G |
| 17 | A | 2814 | G |
| 17 | A | 2829 | C |
| 17 | A | 2831 | G |
| 17 | A | 2832 | A |
| 17 | A | 2833 | A |
| 17 | A | 2847 | C |
| 17 | A | 2854 | U |
| 17 | A | 2864 | U |
| 17 | A | 2865 | C |
| 17 | A | 2889 | C |
| 17 | A | 2906 | C |
| 17 | A | 2911 | C |
| 17 | A | 2912 | C |
| 17 | A | 2913 | A |
| 17 | A | 2917 | G |
| 17 | A | 2922 | A |
| 17 | A | 2926 | A |
| 17 | A | 2928 | C |
| 17 | A | 2932 | G |
| 17 | A | 2943 | G |
| 17 | A | 2944 | C |
| 17 | A | 2956 | A |
| 17 | A | 2963 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 17 | A | 2981 | A |
| 17 | A | 2982 | C |
| 17 | A | 2984 | A |
| 17 | A | 2995 | G |
| 17 | A | 3000 | A |
| 17 | A | 3005 | A |
| 17 | A | 3016 | G |
| 17 | A | 3039 | OMU |
| 17 | A | 3040 | G |
| 17 | A | 3041 | U |
| 17 | A | 3042 | U |
| 17 | A | 3043 | C |
| 17 | A | 3053 | A |
| 17 | A | 3054 | G |
| 17 | A | 3056 | C |
| 17 | A | 3060 | C |
| 17 | A | 3061 | G |
| 17 | A | 3072 | U |
| 17 | A | 3073 | C |
| 17 | A | 3077 | C |
| 17 | A | 3086 | U |
| 17 | A | 3089 | A |
| 17 | A | 3097 | U |
| 17 | A | 3100 | U |
| 17 | A | 3101 | A |
| 17 | A | 3102 | U |
| 17 | A | 3109 | U |
| 17 | A | 3110 | C |
| 17 | A | 3111 | A |
| 17 | A | 3112 | A |
| 17 | A | 3113 | A |
| 17 | A | 3150 | U |
| 17 | A | 3155 | C |
| 17 | A | 3157 | C |
| 17 | A | 3158 | A |
| 17 | A | 3162 | C |
| 17 | A | 3169 | C |
| 17 | A | 3172 | C |
| 17 | A | 3180 | A |
| 17 | A | 3183 | U |
| 17 | A | 3188 | U |
| 17 | A | 3189 | C |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 17 | A | 3190 | A |
| 17 | A | 3197 | U |
| 17 | A | 3206 | C |
| 17 | A | 3207 | A |
| 17 | A | 3208 | C |
| 17 | A | 3212 | C |
| 17 | A | 3217 | A |
| 17 | A | 3218 | A |
| 17 | A | 3228 | U |
| 18 | B | 1603 | A |
| 18 | B | 1605 | A |
| 18 | B | 1609 | U |
| 18 | B | 1611 | G |
| 18 | B | 1617 | C |
| 18 | B | 1646 | U |
| 18 | B | 1650 | A |
| 18 | B | 1652 | C |
| 18 | B | 1653 | U |
| 18 | B | 1654 | U |
| 18 | B | 1656 | A |
| 18 | B | 1661 | A |
| 18 | B | 1664 | G |

All (8) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 17 | A | 1766 | U |
| 17 | A | 2030 | U |
| 17 | A | 2186 | C |
| 17 | A | 2245 | A |
| 17 | A | 2457 | A |
| 17 | A | 2530 | A |
| 17 | A | 2905 | A |
| 17 | A | 3040 | G |

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 35 | AYA | U | 2 | 35 | 6,7,8 | 1.27 | 1 (16%) | 5,8,10 | 1.24 | 1 (20%) |
| 17 | OMU | A | 3039 | 17 | 14,22,23 | 0.78 | 0 | 14,31,34 | 0.79 | 0 |
| 25 | SAC | K | 2 | 25 | 7,8,9 | 1.03 | 0 | 8,9,11 | 0.83 | 1 (12%) |
| 51 | AYA | k | 2 | 51 | 6,7,8 | 1.26 | 1 (16%) | 5,8,10 | 1.31 | 1 (20%) |
| 42 | THC | b | 2 | 42 | 8,9,10 | 1.06 | 1 (12%) | 9,11,13 | 0.66 | 0 |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|-----------|---------|
| 35 | AYA | U | 2 | 35 | - | 1/4/6/8 | - |
| 17 | OMU | A | 3039 | 17 | - | 4/7/27/28 | 0/2/2/2 |
| 25 | SAC | K | 2 | 25 | - | 2/7/8/10 | - |
| 51 | AYA | k | 2 | 51 | - | 0/4/6/8 | - |
| 42 | THC | b | 2 | 42 | - | 0/8/10/12 | - |

All (3) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 35 | U | 2 | AYA | CA-N | -2.43 | 1.44 | 1.46 |
| 51 | k | 2 | AYA | CA-N | -2.37 | 1.44 | 1.46 |
| 42 | b | 2 | THC | CA-N | -2.07 | 1.43 | 1.46 |

All (3) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 51 | k | 2 | AYA | CB-CA-N | 2.72 | 112.63 | 109.61 |
| 35 | U | 2 | AYA | CB-CA-N | 2.62 | 112.52 | 109.61 |
| 25 | K | 2 | SAC | OG-CB-CA | -2.01 | 105.83 | 110.97 |

There are no chirality outliers.

All (7) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 25 | K | 2 | SAC | N-CA-CB-OG |
| 25 | K | 2 | SAC | C-CA-CB-OG |
| 17 | A | 3039 | OMU | O4'-C4'-C5'-O5' |
| 17 | A | 3039 | OMU | C3'-C4'-C5'-O5' |
| 17 | A | 3039 | OMU | C4'-C5'-O5'-P |
| 35 | U | 2 | AYA | C-CA-N-CT |
| 17 | A | 3039 | OMU | C3'-C2'-O2'-CM2 |

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 102 ligands modelled in this entry, 98 are monoatomic - leaving 4 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 | $\# Z > 2$ |
| 59 | PM8 | w | 200 | 3 | 25,31,31 | 0.22 | 0 | 30,38,38 | 0.41 | 0 |
| 64 | N | A | 3394 | 17 | 9,12,13 | 0.66 | 0 | 10,16,19 | 0.65 | 0 |
| 65 | FES | r | 201 | 57,23 | 0,4,4 | 0.00 | - | - | | |
| 60 | SAM | x | 401 | - | 21,29,29 | 1.20 | 2 (9%) | 18,42,42 | 1.55 | 2 (11%) |

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 |
|-----|------|-------|-----|------|---------|-------------|-------|
| 59 | PM8 | w | 200 | 3 | - | 13/36/38/38 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|-------|---------|-----------|---------|
| 64 | N | A | 3394 | 17 | - | 0/3/18/19 | 0/1/1/1 |
| 65 | FES | r | 201 | 57,23 | - | - | 0/1/1/1 |
| 60 | SAM | x | 401 | - | - | 4/8/33/33 | 0/3/3/3 |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 60 | x | 401 | SAM | C2-N3 | 3.99 | 1.38 | 1.32 |
| 60 | x | 401 | SAM | C2-N1 | 2.44 | 1.38 | 1.33 |

All (2) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 60 | x | 401 | SAM | N3-C2-N1 | -5.38 | 120.26 | 128.68 |
| 60 | x | 401 | SAM | C3'-C2'-C1' | 2.56 | 104.83 | 100.98 |

There are no chirality outliers.

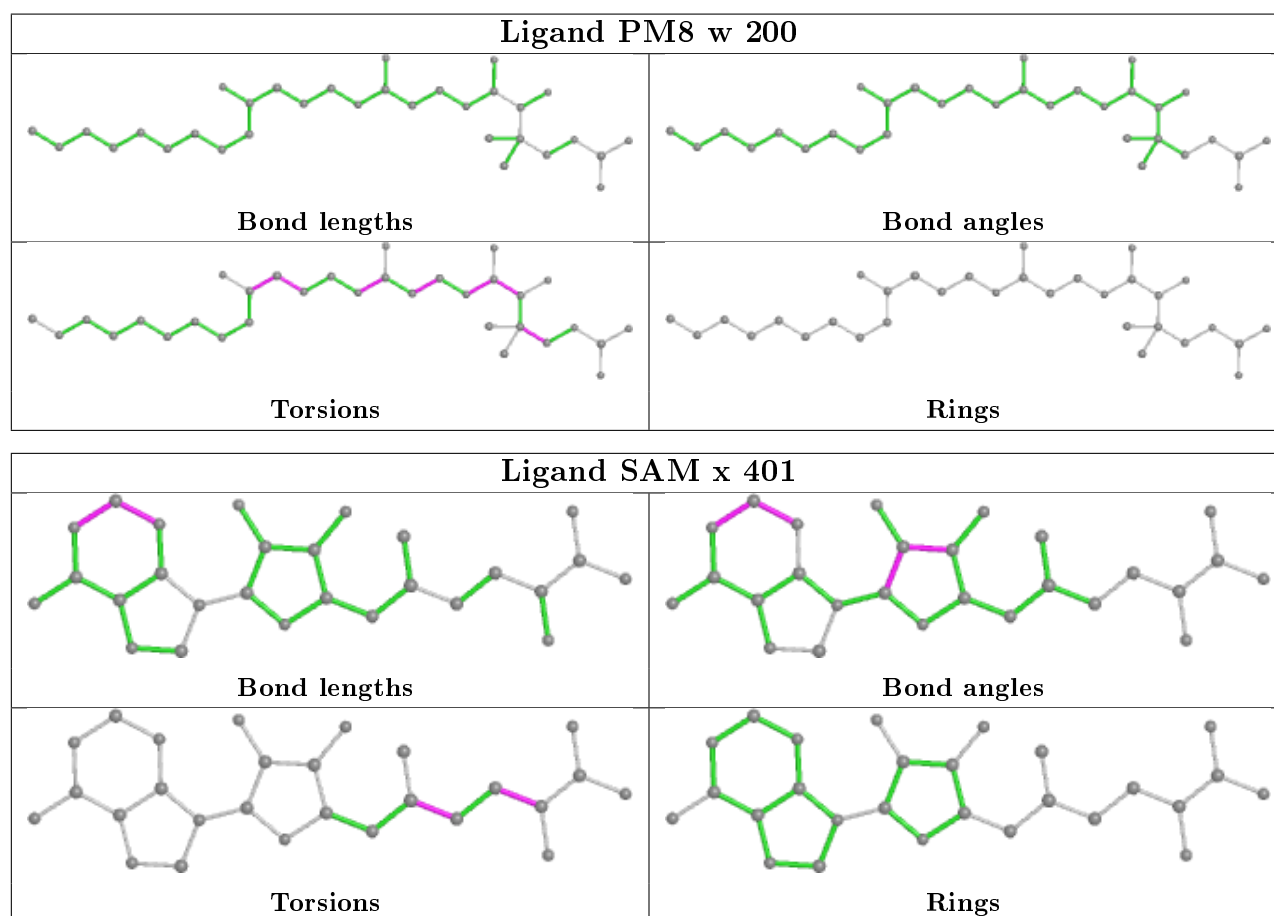
All (17) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 59 | w | 200 | PM8 | O27-C28-C29-C32 |
| 59 | w | 200 | PM8 | C32-C34-N36-C37 |
| 59 | w | 200 | PM8 | O1-C1-S1-C43 |
| 59 | w | 200 | PM8 | C2-C1-S1-C43 |
| 60 | x | 401 | SAM | N-CA-CB-CG |
| 60 | x | 401 | SAM | C-CA-CB-CG |
| 60 | x | 401 | SAM | CB-CG-SD-CE |
| 60 | x | 401 | SAM | CB-CG-SD-C5' |
| 59 | w | 200 | PM8 | C38-C39-N41-C42 |
| 59 | w | 200 | PM8 | O35-C34-N36-C37 |
| 59 | w | 200 | PM8 | O40-C39-N41-C42 |
| 59 | w | 200 | PM8 | O27-C28-C29-C30 |
| 59 | w | 200 | PM8 | O27-C28-C29-C31 |
| 59 | w | 200 | PM8 | O33-C32-C34-O35 |
| 59 | w | 200 | PM8 | O33-C32-C34-N36 |
| 59 | w | 200 | PM8 | C42-C43-S1-C1 |
| 59 | w | 200 | PM8 | N36-C37-C38-C39 |

There are no ring outliers.

No monomer is involved in short contacts.

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 17 | A | 2 |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1 | A | 3250:N | O3' | 3251:N | P | 17.38 |
| 1 | A | 3235:N | O3' | 3236:N | P | 13.89 |

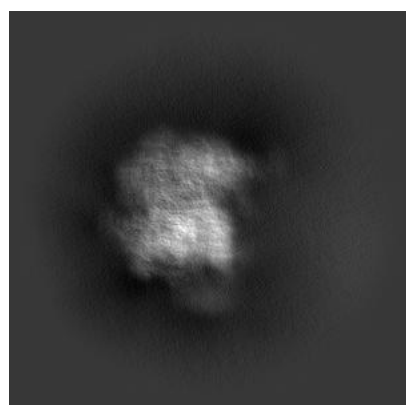
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12846. These allow visual inspection of the internal detail of the map and identification of artifacts.

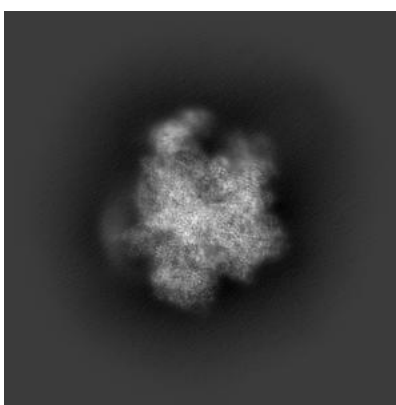
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

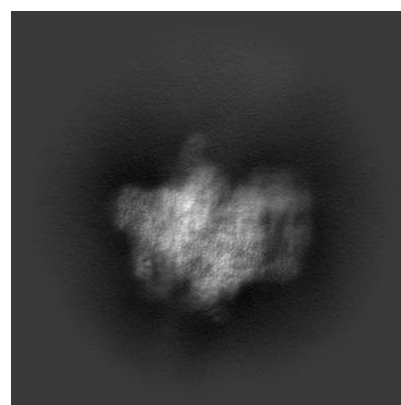
6.1.1 Primary map



X



Y

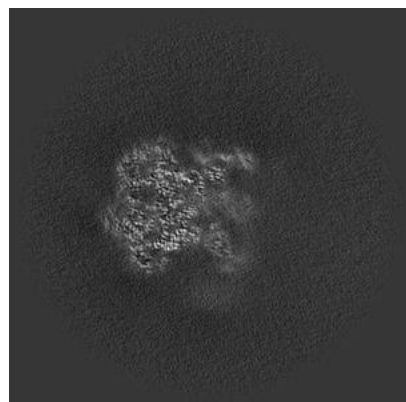


Z

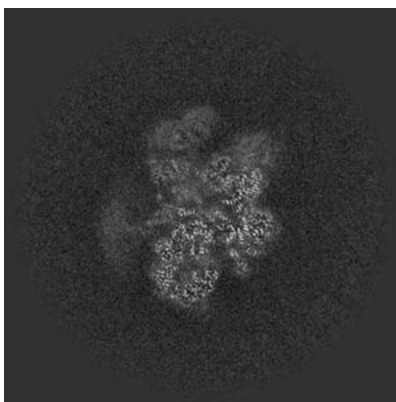
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

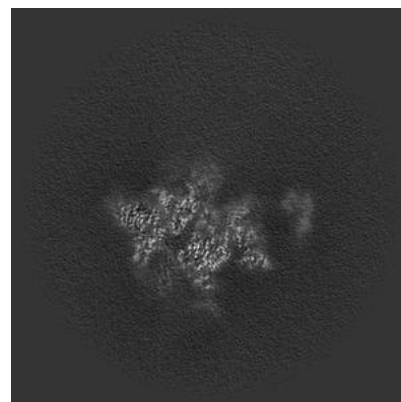
6.2.1 Primary map



X Index: 224



Y Index: 224

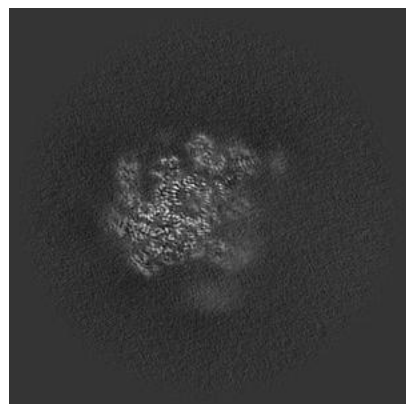


Z Index: 224

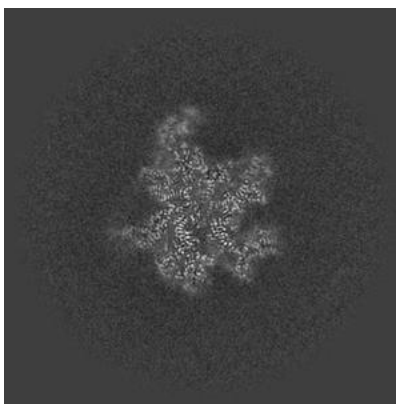
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

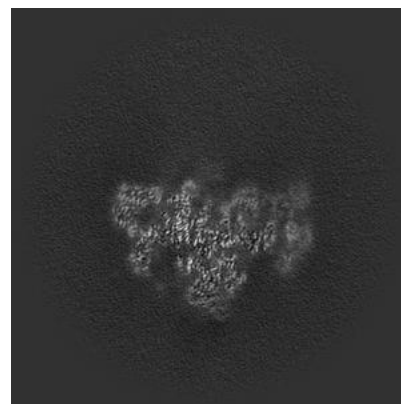
6.3.1 Primary map



X Index: 215



Y Index: 193



Z Index: 203

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 0.7. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

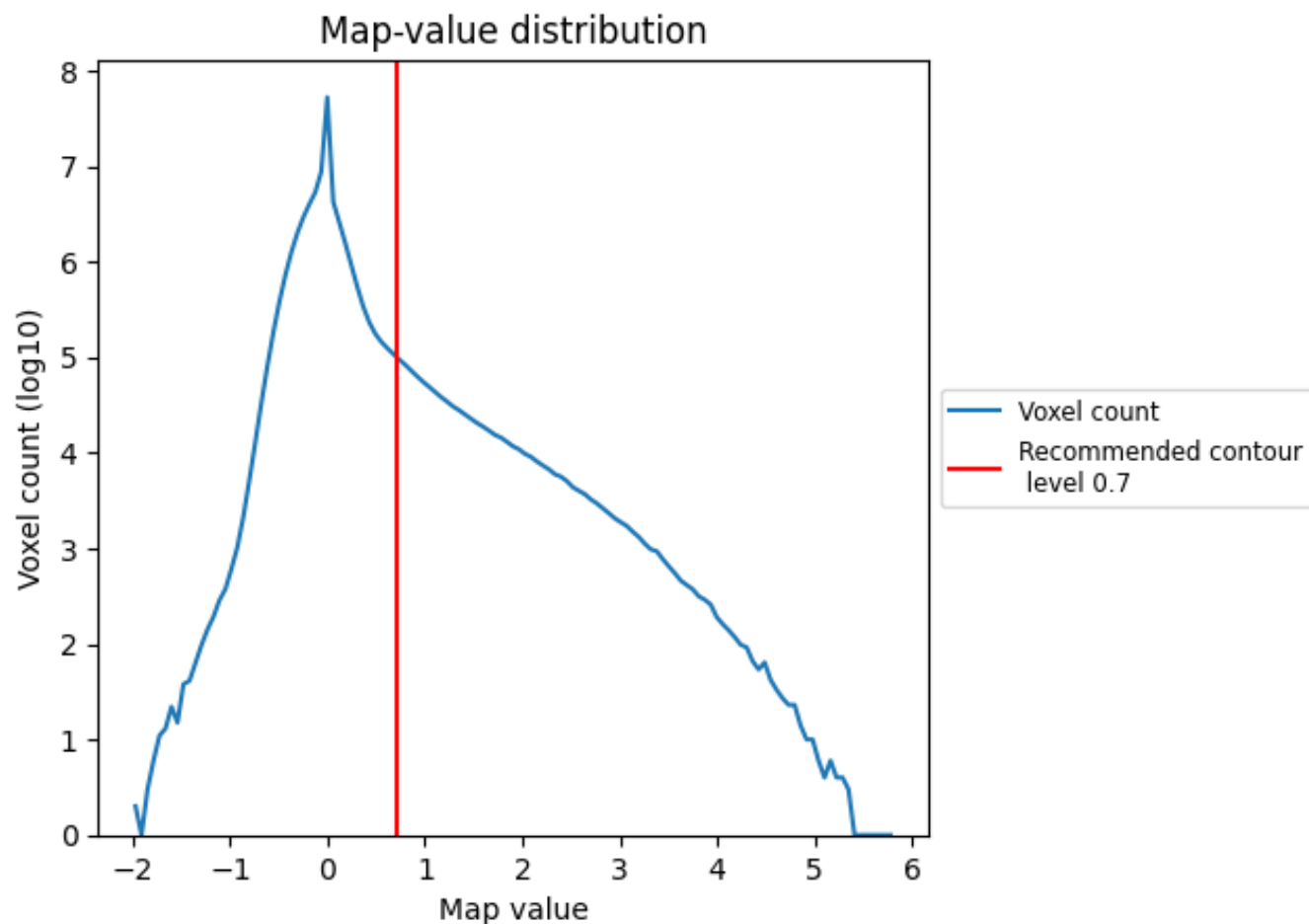
6.5 Mask visualisation

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

7 Map analysis [i](#)

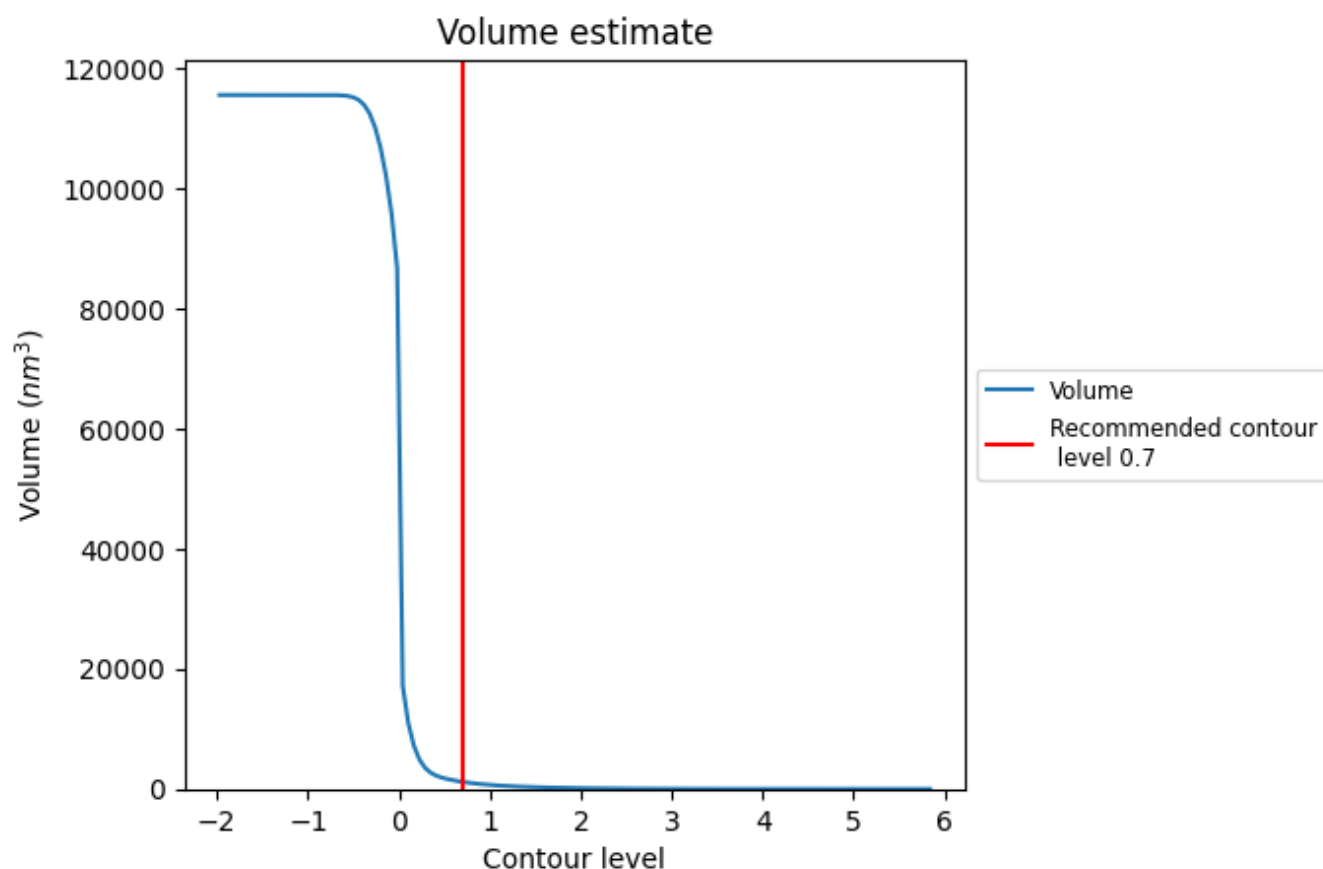
This section contains the results of statistical analysis of the map.

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.

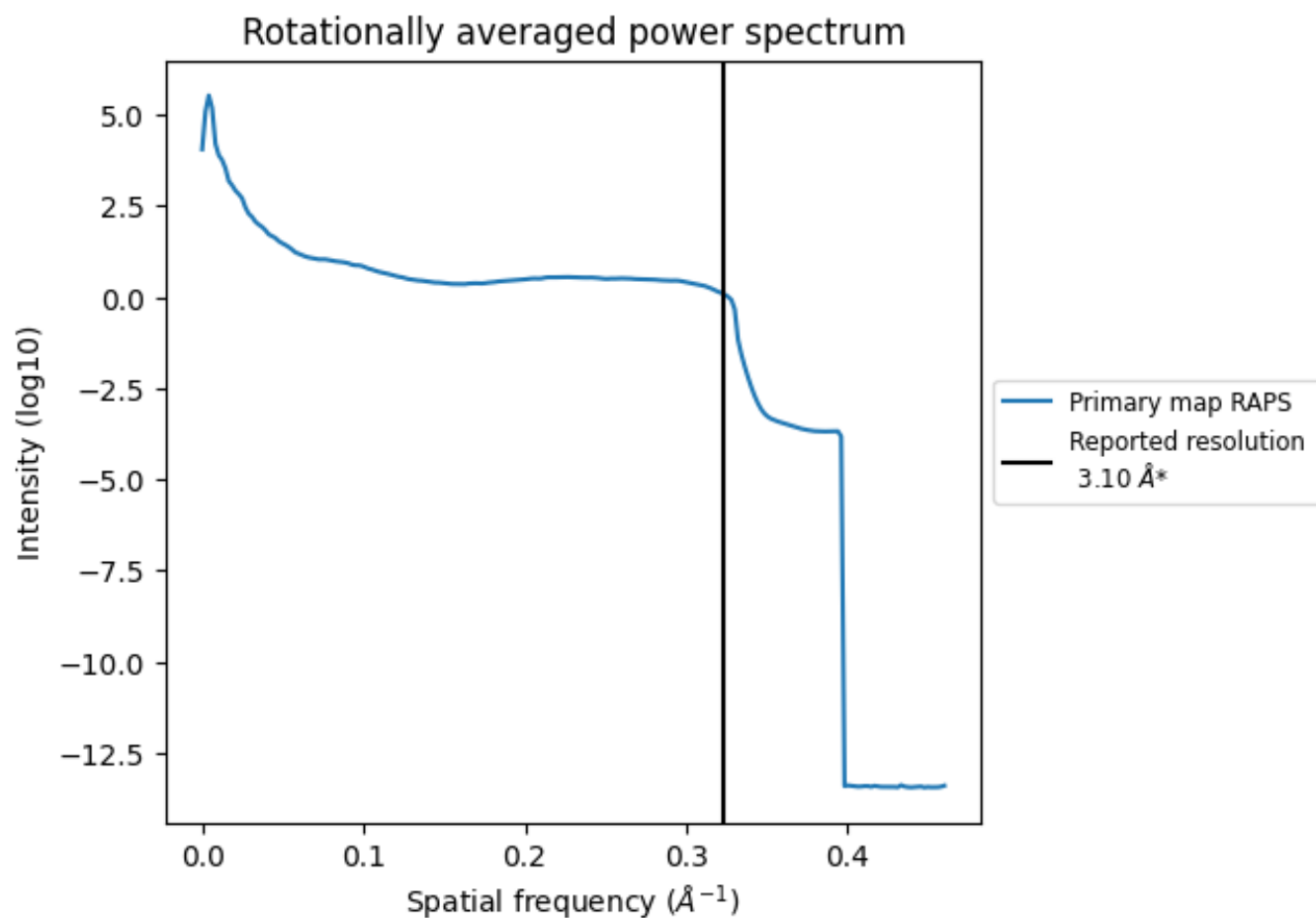
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1183 nm³; this corresponds to an approximate mass of 1069 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 0.323 Å⁻¹

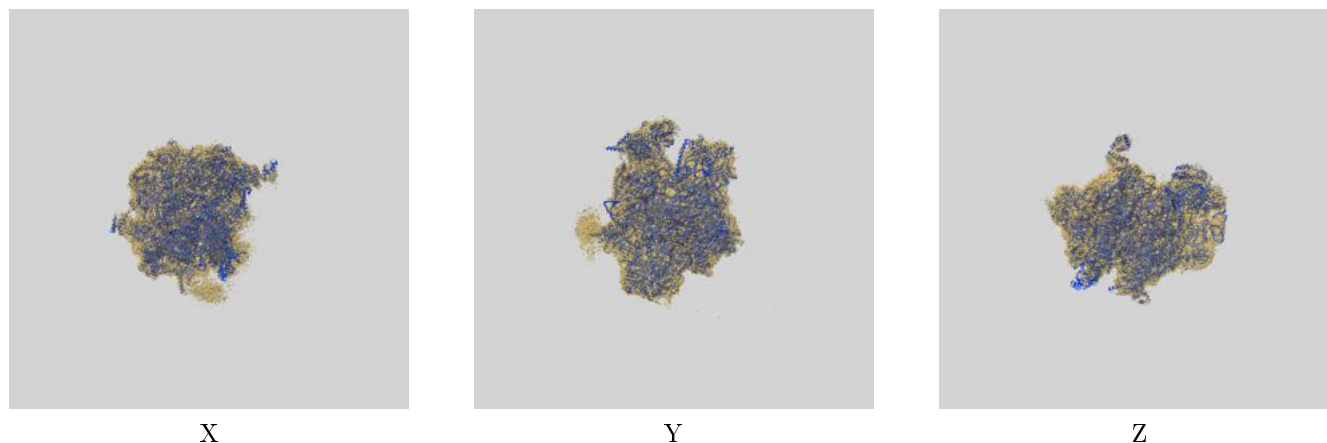
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

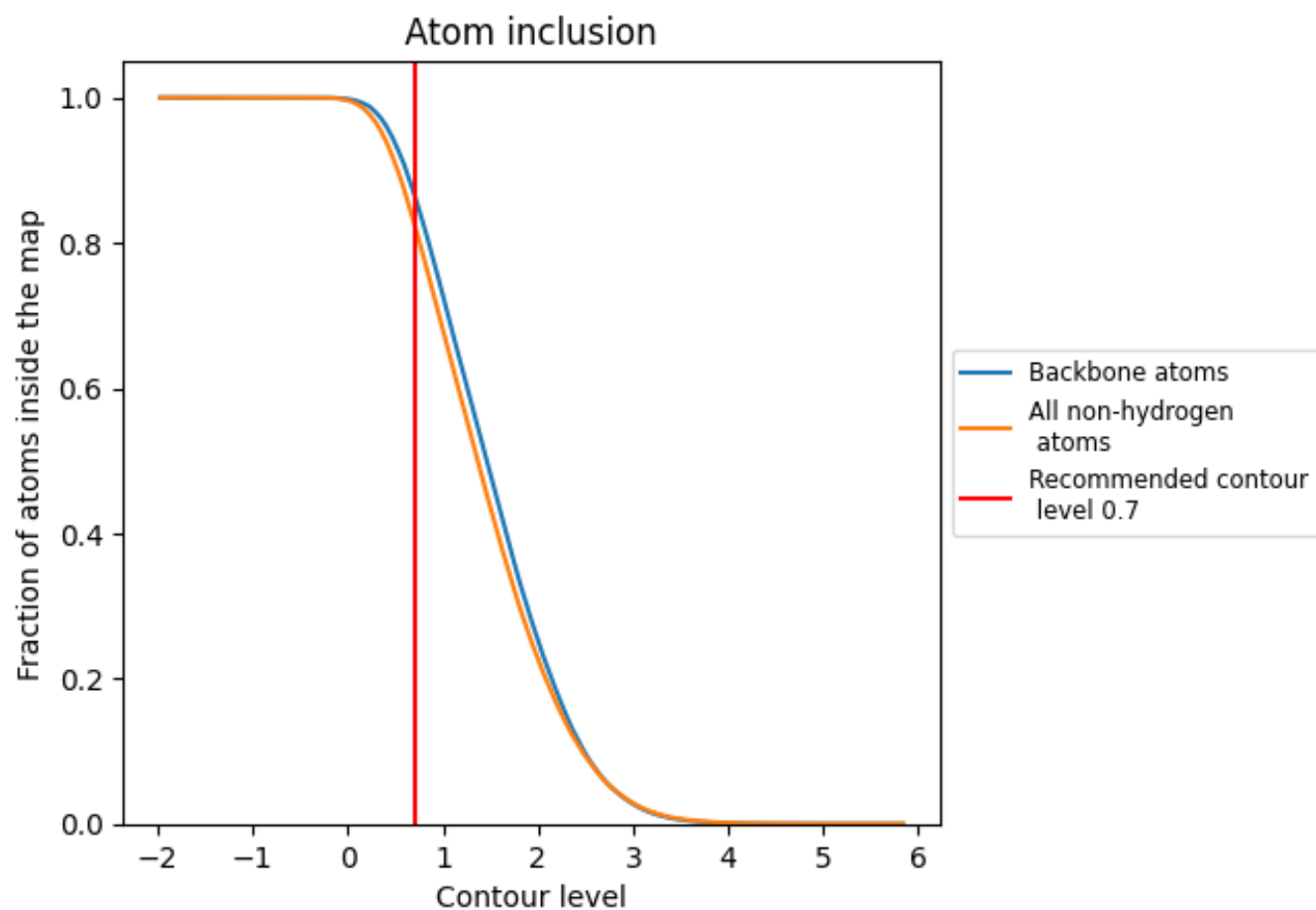
This section contains information regarding the fit between EMDB map EMD-12846 and PDB model 7ODS. Per-residue inclusion information can be found in section 3 on page 17.

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.7 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 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 83% of all non-hydrogen atoms, are inside the map.