



wwPDB EM Validation Summary Report ⓘ

Oct 20, 2024 – 02:26 AM EDT

PDB ID : 6VMI
EMDB ID : EMD-21242
Title : Structure of the human mitochondrial ribosome-EF-G1 complex (ClassIII)
Authors : Sharma, M.R.; Koripella, R.K.; Agrawal, R.K.
Deposited on : 2020-01-28
Resolution : 2.96 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:

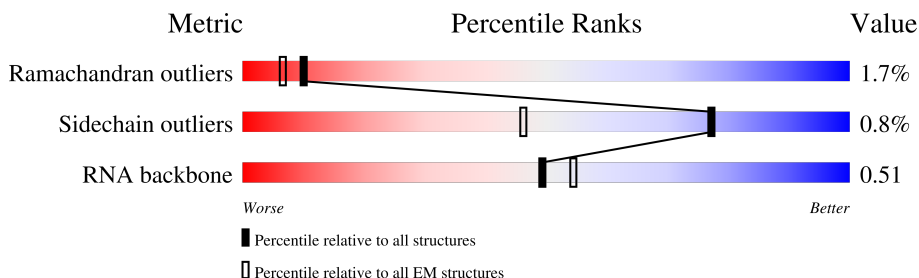
EMDB validation analysis : 0.0.1.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

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 2.96 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.






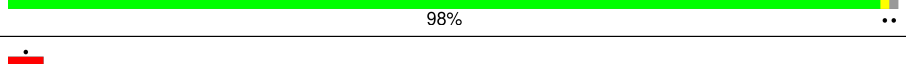
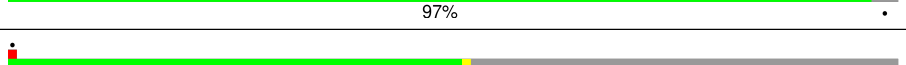

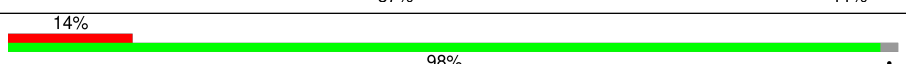
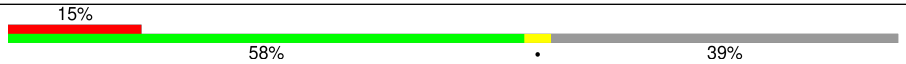


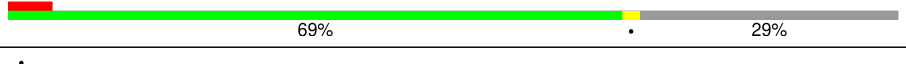
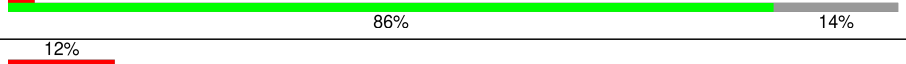

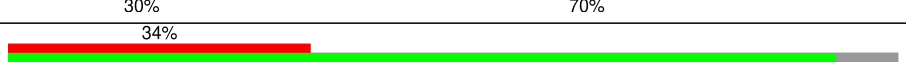
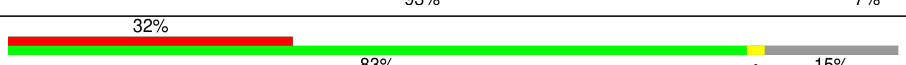
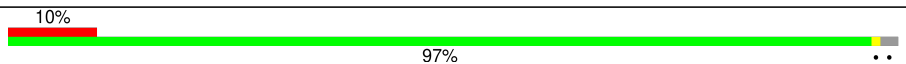

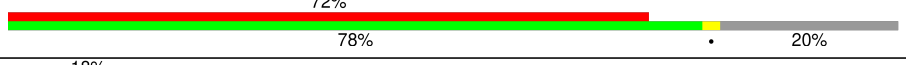







| Metric | Whole archive (#Entries) | EM structures (#Entries) |
|-----------------------|-----------------------------|-----------------------------|
| Ramachandran outliers | 207382 | 16835 |
| Sidechain outliers | 206894 | 16415 |
| RNA backbone | 6643 | 2191 |

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 | AA | 954 | |
| 2 | AB | 296 | |
| 3 | AC | 167 | |
| 4 | AE | 125 | |
| 5 | AI | 194 | |
| 6 | AJ | 138 | |
| 7 | AK | 128 | |
| 8 | AM | 137 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 9 | AN | 130 |  82% 18% |
| 10 | AO | 258 |  72% 26% |
| 11 | AP | 142 |  65% 32% |
| 12 | AQ | 87 |  98% |
| 13 | AT | 173 |  97% |
| 14 | AW | 187 |  51% 48% |
| 15 | AX | 398 |  19% 87% 11% |
| 16 | A2 | 118 |  14% 98% |
| 17 | AH | 201 |  15% 58% 39% |
| 18 | AL | 257 |  66% 32% |
| 19 | AR | 360 |  11% 81% 19% |
| 20 | AS | 190 |  5% 69% 29% |
| 21 | AU | 205 |  86% 14% |
| 22 | AV | 414 |  12% 86% 11% |
| 23 | AY | 395 |  15% 30% 70% |
| 24 | AZ | 106 |  34% 93% 7% |
| 25 | A1 | 323 |  32% 83% 15% |
| 26 | A0 | 218 |  10% 97% |
| 27 | A3 | 199 |  34% 64% |
| 28 | A4 | 689 |  72% 78% 20% |
| 29 | AD | 430 |  18% 78% 20% |
| 30 | AF | 242 |  13% 83% 14% |
| 31 | AG | 396 |  14% 78% 20% |
| 32 | A | 1559 |  75% 23% |
| 33 | B | 73 |  67% 10% 23% |







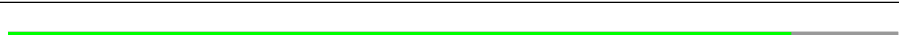
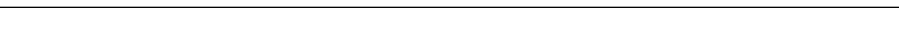
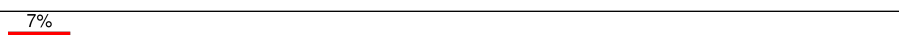
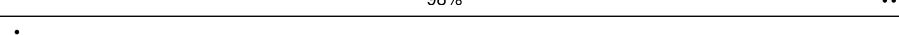
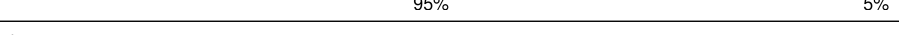
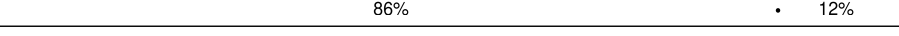











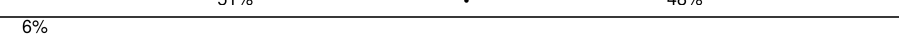

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 34 | D | 305 | 78% 22% |
| 35 | F | 311 | 78% 20% |
| 36 | H | 267 | 36% 63% |
| 37 | K | 178 | 96% |
| 38 | L | 145 | 78% 21% |
| 39 | M | 296 | 94% |
| 40 | O | 175 | 85% 13% |
| 41 | R | 149 | 89% 6% |
| 42 | S | 205 | 73% 24% |
| 43 | T | 212 | 75% 22% |
| 44 | W | 148 | 74% 25% |
| 45 | X | 256 | 90% 5% 5% |
| 46 | Y | 250 | 68% 30% |
| 47 | Z | 161 | 75% 25% |
| 48 | 0 | 188 | 56% 43% |
| 49 | 1 | 65 | 77% 20% |
| 50 | 2 | 92 | 49% 50% |
| 51 | 3 | 188 | 50% 49% |
| 52 | 4 | 103 | 37% 63% |
| 53 | 8 | 206 | 48% 52% |
| 54 | b | 155 | 94% 5% |
| 55 | e | 279 | 8% 77% 22% |
| 56 | g | 166 | 76% 20% |
| 57 | i | 128 | 75% 24% |
| 58 | j | 123 | 75% 24% |


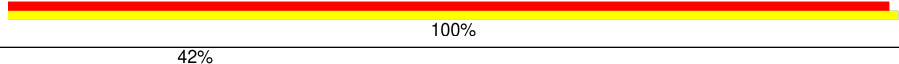
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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 59 | m | 128 |  |
| 60 | o | 102 |  |
| 61 | q | 222 |  |
| 62 | r | 196 |  |
| 63 | J | 192 |  |
| 64 | I | 261 |  |
| 65 | N | 251 |  |
| 66 | P | 179 |  |
| 67 | U | 153 |  |
| 68 | V | 216 |  |
| 69 | E | 348 |  |
| 70 | 5 | 423 |  |
| 71 | 6 | 380 |  |
| 72 | 7 | 338 |  |
| 73 | 9 | 137 |  |
| 74 | a | 142 |  |
| 75 | c | 332 |  |
| 76 | d | 306 |  |
| 77 | f | 194 |  |
| 78 | h | 158 |  |
| 79 | k | 112 |  |
| 80 | l | 138 |  |
| 81 | p | 206 |  |
| 82 | s | 439 |  |
| 83 | Q | 292 |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 84 | TA | 198 |  |
| 84 | TB | 198 |  |
| 84 | TC | 198 |  |
| 85 | u | 65 |  |
| 86 | v | 751 |  |
| 87 | A5 | 11 |  |
| 88 | A6 | 71 |  |
| 88 | A7 | 71 |  |

2 Entry composition [i](#)

There are 92 unique types of molecules in this entry. The entry contains 176217 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 12s rRNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|-----|---------|-------|
| | | | Total | C | N | O | P | | |
| 1 | AA | 944 | 20030 | 8980 | 3612 | 6494 | 944 | 0 | 0 |

- Molecule 2 is a protein called 28S ribosomal protein S2, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| | | | Total | C | N | O | S | | |
| 2 | AB | 220 | 1787 | 1141 | 324 | 312 | 10 | 0 | 0 |

- Molecule 3 is a protein called 28S ribosomal protein S24, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 3 | AC | 132 | 1082 | 699 | 195 | 184 | 4 | 0 | 0 |

- Molecule 4 is a protein called 28S ribosomal protein S6, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 4 | AE | 122 | 972 | 614 | 177 | 177 | 4 | 0 | 0 |

- Molecule 5 is a protein called 28S ribosomal protein S11, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 5 | AI | 136 | 1011 | 637 | 192 | 178 | 4 | 0 | 0 |

- Molecule 6 is a protein called 28S ribosomal protein S12, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 6 | AJ | 108 | 838 | 521 | 169 | 142 | 6 | 0 | 0 |

- Molecule 7 is a protein called 28S ribosomal protein S14, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 7 | AK | 101 | 861 | 537 | 179 | 140 | 5 | 0 | 0 |

- Molecule 8 is a protein called 28S ribosomal protein S16, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 8 | AM | 116 | 920 | 582 | 182 | 150 | 6 | 0 | 0 |

- Molecule 9 is a protein called 28S ribosomal protein S17, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 9 | AN | 107 | 846 | 549 | 153 | 141 | 3 | 0 | 0 |

- Molecule 10 is a protein called 28S ribosomal protein S18b, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 10 | AO | 190 | 1570 | 998 | 291 | 274 | 7 | 0 | 0 |

- Molecule 11 is a protein called 28S ribosomal protein S18c, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 11 | AP | 96 | 774 | 498 | 133 | 135 | 8 | 0 | 0 |

- Molecule 12 is a protein called 28S ribosomal protein S21, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 12 | AQ | 86 | 740 | 458 | 150 | 124 | 8 | 0 | 0 |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|---------|------------|
| AQ | 50 | ARG | CYS | variant | UNP P82921 |

- Molecule 13 is a protein called 28S ribosomal protein S25, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| | | | Total | C | N | O | S | | |
| 13 | AT | 168 | 1371 | 877 | 239 | 244 | 11 | 0 | 0 |

- Molecule 14 is a protein called 28S ribosomal protein S28, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 14 | AW | 97 | 766 | 486 | 137 | 139 | 4 | 0 | 0 |

- Molecule 15 is a protein called 28S ribosomal protein S29, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| | | | Total | C | N | O | S | | |
| 15 | AX | 353 | 2860 | 1828 | 503 | 518 | 11 | 0 | 0 |

- Molecule 16 is a protein called Coiled-coil-helix-coiled-coil-helix domain-containing protein 1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 16 | A2 | 116 | 925 | 574 | 181 | 162 | 8 | 0 | 0 |

- Molecule 17 is a protein called 28S ribosomal protein S10, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 17 | AH | 122 | 1014 | 656 | 172 | 183 | 3 | 0 | 0 |

- Molecule 18 is a protein called 28S ribosomal protein S15, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 18 | AL | 174 | 1451 | 924 | 271 | 249 | 7 | 0 | 0 |

- Molecule 19 is a protein called 28S ribosomal protein S22, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 19 | AR | 292 | 2388 | 1521 | 410 | 449 | 8 | 0 | 0 |

- Molecule 20 is a protein called 28S ribosomal protein S23, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 20 | AS | 135 | 1111 | 716 | 198 | 196 | 1 | 0 | 0 |

- Molecule 21 is a protein called 28S ribosomal protein S26, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 21 | AU | 177 | 1499 | 922 | 305 | 268 | 4 | 0 | 0 |

- Molecule 22 is a protein called 28S ribosomal protein S27, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| | | | Total | C | N | O | S | | |
| 22 | AV | 367 | 3009 | 1931 | 502 | 564 | 12 | 0 | 0 |

- Molecule 23 is a protein called 28S ribosomal protein S31, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 23 | AY | 120 | 1016 | 657 | 167 | 190 | 2 | 0 | 0 |

- Molecule 24 is a protein called 28S ribosomal protein S33, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 24 | AZ | 99 | 833 | 531 | 152 | 146 | 4 | 0 | 0 |

- Molecule 25 is a protein called 28S ribosomal protein S35, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| | | | Total | C | N | O | S | | |
| 25 | A1 | 275 | 2231 | 1414 | 380 | 426 | 11 | 0 | 0 |

- Molecule 26 is a protein called 28S ribosomal protein S34, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 26 | A0 | 214 | 1781 | 1125 | 341 | 310 | 5 | 0 | 0 |

- Molecule 27 is a protein called Aurora kinase A-interacting protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 27 | A3 | 72 | 639 | 409 | 137 | 92 | 1 | 0 | 0 |

- Molecule 28 is a protein called Pentatricopeptide repeat domain-containing protein 3, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 28 | A4 | 549 | 3010 | 1841 | 573 | 593 | 3 | 0 | 0 |

- Molecule 29 is a protein called 28S ribosomal protein S5, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| | | | Total | C | N | O | S | | |
| 29 | AD | 343 | 2731 | 1713 | 518 | 487 | 13 | 0 | 0 |

- Molecule 30 is a protein called 28S ribosomal protein S7, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| | | | Total | C | N | O | S | | |
| 30 | AF | 208 | 1724 | 1103 | 312 | 298 | 11 | 0 | 0 |

- Molecule 31 is a protein called 28S ribosomal protein S9, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| | | | Total | C | N | O | S | | |
| 31 | AG | 315 | 2587 | 1640 | 462 | 471 | 14 | 0 | 0 |

- Molecule 32 is a RNA chain called 16s rRNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|-------|
| | | | Total | C | N | O | P | | |
| 32 | A | 1527 | 32395 | 14536 | 5844 | 10488 | 1527 | 0 | 0 |

- Molecule 33 is a RNA chain called tRNAval.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| | | | Total | C | N | O | P | | |
| 33 | B | 56 | 1191 | 534 | 214 | 387 | 56 | 0 | 0 |

- Molecule 34 is a protein called 39S ribosomal protein L2, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 34 | D | 239 | Total | C | N | O | S | 0 | 0 |
| | | | 1866 | 1162 | 377 | 318 | 9 | | |

- Molecule 35 is a protein called 39S ribosomal protein L4, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 35 | F | 250 | Total | C | N | O | S | 0 | 0 |
| | | | 2013 | 1294 | 365 | 348 | 6 | | |

- Molecule 36 is a protein called 39S ribosomal protein L9, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 36 | H | 98 | Total | C | N | O | 0 | 0 |
| | | | 806 | 510 | 156 | 140 | | |

- Molecule 37 is a protein called 39S ribosomal protein L13, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 37 | K | 177 | Total | C | N | O | S | 0 | 0 |
| | | | 1451 | 934 | 259 | 251 | 7 | | |

- Molecule 38 is a protein called 39S ribosomal protein L14, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 38 | L | 115 | Total | C | N | O | S | 0 | 0 |
| | | | 889 | 559 | 171 | 154 | 5 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 39 | M | 287 | Total | C | N | O | S | 0 | 0 |
| | | | 2305 | 1472 | 425 | 402 | 6 | | |

- Molecule 40 is a protein called 39S ribosomal protein L17, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 40 | O | 152 | Total | C | N | O | S | 0 | 0 |
| | | | 1245 | 784 | 239 | 215 | 7 | | |

- Molecule 41 is a protein called 39S ribosomal protein L20, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 41 | R | 140 | 1153 | 732 | 231 | 186 | 4 | 0 | 0 |

- Molecule 42 is a protein called 39S ribosomal protein L21, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 42 | S | 156 | 1251 | 806 | 222 | 219 | 4 | 0 | 0 |

- Molecule 43 is a protein called 39S ribosomal protein L22, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 43 | T | 166 | 1368 | 875 | 254 | 232 | 7 | 0 | 0 |

- Molecule 44 is a protein called 39S ribosomal protein L27, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 44 | W | 111 | 871 | 558 | 164 | 146 | 3 | 0 | 0 |

- Molecule 45 is a protein called 39S ribosomal protein L28, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 45 | X | 243 | 2027 | 1310 | 350 | 362 | 5 | 0 | 0 |

There are 3 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|---------|------------|
| X | 148 | ALA | THR | variant | UNP Q13084 |
| X | 149 | SER | PRO | variant | UNP Q13084 |
| X | 150 | GLY | LYS | variant | UNP Q13084 |

- Molecule 46 is a protein called 39S ribosomal protein L47, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 46 | Y | 176 | 1517 | 970 | 291 | 252 | 4 | 0 | 0 |

- Molecule 47 is a protein called 39S ribosomal protein L30, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 47 | Z | 120 | Total | C | N | O | S | 0 | 0 |
| | | | 978 | 626 | 183 | 166 | 3 | | |

- Molecule 48 is a protein called 39S ribosomal protein L32, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 48 | 0 | 108 | Total | C | N | O | S | 0 | 0 |
| | | | 880 | 545 | 172 | 157 | 6 | | |

- Molecule 49 is a protein called 39S ribosomal protein L33, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 49 | 1 | 52 | Total | C | N | O | S | 0 | 0 |
| | | | 433 | 278 | 83 | 70 | 2 | | |

- Molecule 50 is a protein called 39S ribosomal protein L34, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 50 | 2 | 46 | Total | C | N | O | S | 0 | 0 |
| | | | 376 | 233 | 83 | 59 | 1 | | |

- Molecule 51 is a protein called 39S ribosomal protein L35, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 51 | 3 | 95 | Total | C | N | O | S | 0 | 0 |
| | | | 831 | 539 | 162 | 127 | 3 | | |

- Molecule 52 is a protein called 39S ribosomal protein L36, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 52 | 4 | 38 | Total | C | N | O | S | 0 | 0 |
| | | | 342 | 217 | 72 | 49 | 4 | | |

- Molecule 53 is a protein called 39S ribosomal protein L40, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 53 | 8 | 99 | Total | C | N | O | S | 0 | 0 |
| | | | 836 | 535 | 144 | 155 | 2 | | |

- Molecule 54 is a protein called 39S ribosomal protein L43, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 54 | b | 148 | 1178 | 733 | 229 | 213 | 3 | 0 | 0 |

- Molecule 55 is a protein called 39S ribosomal protein L46, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 55 | e | 217 | 1762 | 1124 | 310 | 323 | 5 | 0 | 0 |

- Molecule 56 is a protein called 39S ribosomal protein L49, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 56 | g | 132 | 1096 | 709 | 191 | 194 | 2 | 0 | 0 |

- Molecule 57 is a protein called 39S ribosomal protein L51, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 57 | i | 97 | 827 | 532 | 165 | 126 | 4 | 0 | 0 |

- Molecule 58 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 |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 58 | j | 93 | 740 | 460 | 143 | 135 | 2 | 0 | 0 |

- Molecule 59 is a protein called 39S ribosomal protein L55, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 59 | m | 45 | 372 | 232 | 76 | 62 | 2 | 0 | 0 |

- Molecule 60 is a protein called Ribosomal protein 63, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 60 | o | 94 | 797 | 501 | 165 | 128 | 3 | 0 | 0 |

- Molecule 61 is a protein called Growth arrest and DNA damage-inducible proteins-interacting protein 1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 61 | q | 168 | 1294 | 801 | 255 | 233 | 5 | 0 | 0 |

- Molecule 62 is a protein called 39S ribosomal protein S18a, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 62 | r | 162 | 1322 | 839 | 252 | 223 | 8 | 0 | 0 |

- Molecule 63 is a protein called 39S ribosomal protein L11, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 63 | J | 175 | 1330 | 847 | 237 | 244 | 2 | 0 | 0 |

- Molecule 64 is a protein called 39S ribosomal protein L10, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| | | | Total | C | N | O | S | | |
| 64 | I | 179 | 1435 | 925 | 258 | 242 | 10 | 0 | 0 |

- Molecule 65 is a protein called 39S ribosomal protein L16, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| | | | Total | C | N | O | S | | |
| 65 | N | 222 | 1786 | 1143 | 326 | 307 | 10 | 0 | 0 |

- Molecule 66 is a protein called Mitochondrial ribosomal protein L18, isoform CRA_b.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 66 | P | 143 | 1165 | 729 | 223 | 208 | 5 | 0 | 0 |

- Molecule 67 is a protein called 39S ribosomal protein L23, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 67 | U | 152 | 1224 | 774 | 233 | 214 | 3 | 0 | 0 |

- Molecule 68 is a protein called 39S ribosomal protein L24, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 68 | V | 206 | 1682 | 1071 | 299 | 304 | 8 | 0 | 0 |

- Molecule 69 is a protein called 39S ribosomal protein L3, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| | | | Total | C | N | O | S | | |
| 69 | E | 306 | 2410 | 1547 | 419 | 433 | 11 | 0 | 0 |

- Molecule 70 is a protein called 39S ribosomal protein L37, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| | | | Total | C | N | O | S | | |
| 70 | 5 | 394 | 3210 | 2073 | 560 | 566 | 11 | 0 | 0 |

- Molecule 71 is a protein called 39S ribosomal protein L38, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 71 | 6 | 354 | 2948 | 1881 | 525 | 533 | 9 | 0 | 0 |

- Molecule 72 is a protein called 39S ribosomal protein L39, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| | | | Total | C | N | O | S | | |
| 72 | 7 | 297 | 2410 | 1540 | 409 | 443 | 18 | 0 | 0 |

- Molecule 73 is a protein called 39S ribosomal protein L41, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 73 | 9 | 124 | 997 | 644 | 170 | 181 | 2 | 0 | 0 |

- Molecule 74 is a protein called 39S ribosomal protein L42, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 74 | a | 108 | 896 | 560 | 162 | 169 | 5 | 0 | 0 |

- Molecule 75 is a protein called 39S ribosomal protein L44, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 75 | c | 289 | Total | C | N | O | S | 0 | 0 |
| | | | 2322 | 1483 | 400 | 430 | 9 | | |

- Molecule 76 is a protein called 39S ribosomal protein L45, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 76 | d | 257 | Total | C | N | O | S | 0 | 0 |
| | | | 2075 | 1326 | 363 | 372 | 14 | | |

- Molecule 77 is a protein called 39S ribosomal protein L48, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 77 | f | 146 | Total | C | N | O | S | 0 | 0 |
| | | | 1126 | 714 | 186 | 222 | 4 | | |

- Molecule 78 is a protein called 39S ribosomal protein L50, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 78 | h | 110 | Total | C | N | O | S | 0 | 0 |
| | | | 894 | 568 | 156 | 167 | 3 | | |

- Molecule 79 is a protein called 39S ribosomal protein L53, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 79 | k | 96 | Total | C | N | O | S | 0 | 0 |
| | | | 743 | 462 | 143 | 133 | 5 | | |

- Molecule 80 is a protein called 39S ribosomal protein L54, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 80 | l | 72 | Total | C | N | O | S | 0 | 0 |
| | | | 619 | 394 | 112 | 111 | 2 | | |

- Molecule 81 is a protein called Peptidyl-tRNA hydrolase ICT1, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 81 | p | 152 | Total | C | N | O | S | 0 | 0 |
| | | | 1227 | 762 | 232 | 229 | 4 | | |

- Molecule 82 is a protein called 39S ribosomal protein S30, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| | | | Total | C | N | O | S | | |
| 82 | s | 393 | 3178 | 2036 | 565 | 563 | 14 | 0 | 0 |

- Molecule 83 is a protein called 39S ribosomal protein L19, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 83 | Q | 240 | 1995 | 1280 | 354 | 352 | 9 | 0 | 0 |

- Molecule 84 is a protein called 39S ribosomal protein L12, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| | | | Total | C | N | O | | |
| 84 | TA | 45 | 345 | 222 | 54 | 69 | 0 | 0 |
| 84 | TB | 27 | 213 | 137 | 33 | 43 | 0 | 0 |
| 84 | TC | 71 | 352 | 210 | 71 | 71 | 0 | 0 |

- Molecule 85 is a protein called P-site finger.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| | | | Total | C | N | O | | |
| 85 | u | 65 | 325 | 195 | 65 | 65 | 0 | 0 |

- Molecule 86 is a protein called Elongation factor G, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|----|---------|-------|
| | | | Total | C | N | O | S | | |
| 86 | v | 712 | 5546 | 3494 | 957 | 1062 | 33 | 0 | 0 |

- Molecule 87 is a DNA chain called mRNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|----|---------|-------|
| | | | Total | C | N | O | P | | |
| 87 | A5 | 11 | 213 | 104 | 32 | 66 | 11 | 0 | 0 |

- Molecule 88 is a DNA chain called P-site and E-site tRNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| | | | Total | C | N | O | P | | |
| 88 | A6 | 71 | 1368 | 670 | 204 | 424 | 70 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| | | | Total | C | N | O | P | | |
| 88 | A7 | 62 | 1197 | 586 | 180 | 370 | 61 | 0 | 0 |

- Molecule 89 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------------|----------|---------|
| 89 | AA | 27 | Total 27 | Mg 27 | 0 |
| 89 | AC | 1 | Total 1 | Mg 1 | 0 |
| 89 | A | 97 | Total 97 | Mg 97 | 0 |
| 89 | D | 1 | Total 1 | Mg 1 | 0 |
| 89 | W | 1 | Total 1 | Mg 1 | 0 |
| 89 | g | 1 | Total 1 | Mg 1 | 0 |
| 89 | E | 1 | Total 1 | Mg 1 | 0 |
| 89 | v | 1 | Total 1 | Mg 1 | 0 |

- Molecule 90 is ZINC ION (three-letter code: ZN) (formula: Zn).

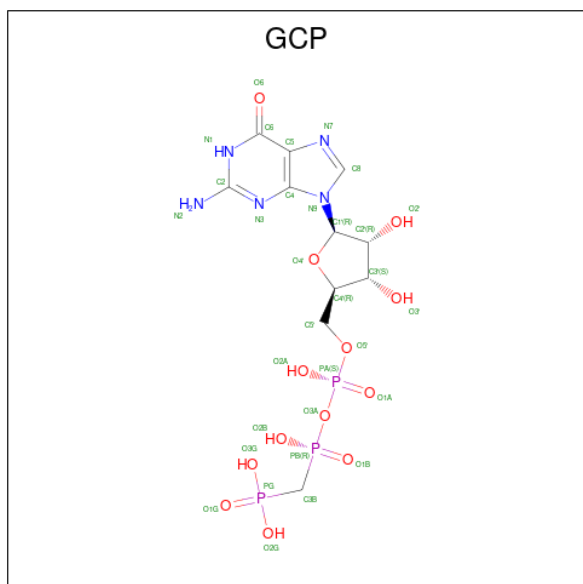
| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|------------|---------|---------|
| 90 | AB | 1 | Total 1 | Zn 1 | 0 |
| 90 | AO | 1 | Total 1 | Zn 1 | 0 |
| 90 | AP | 1 | Total 1 | Zn 1 | 0 |
| 90 | AT | 1 | Total 1 | Zn 1 | 0 |
| 90 | 0 | 1 | Total 1 | Zn 1 | 0 |
| 90 | 4 | 1 | Total 1 | Zn 1 | 0 |
| 90 | r | 1 | Total 1 | Zn 1 | 0 |

- Molecule 91 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| | | | Total | C | N | O | P | |
| 91 | AX | 1 | 28 | 10 | 5 | 11 | 2 | 0 |

- Molecule 92 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: GCP) (formula: $C_{11}H_{18}N_5O_{13}P_3$).

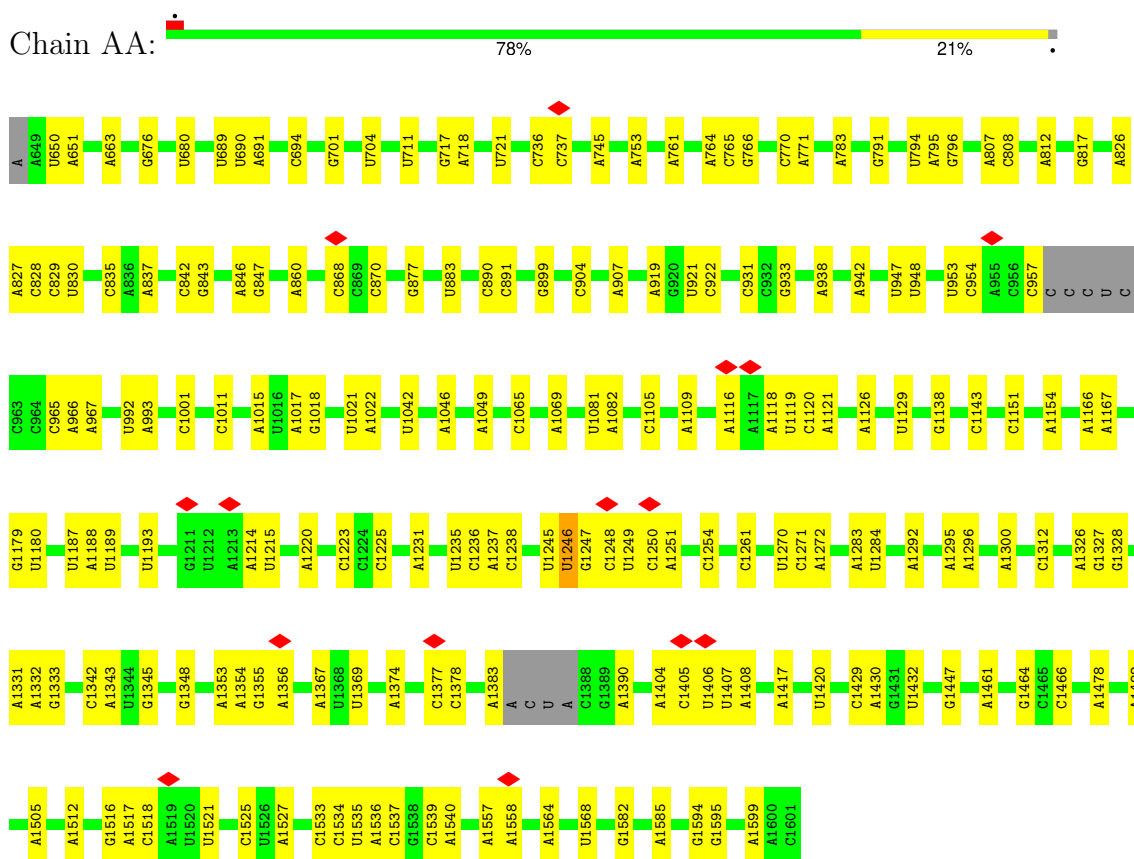


| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| | | | Total | C | N | O | P | |
| 92 | v | 1 | 32 | 11 | 5 | 13 | 3 | 0 |

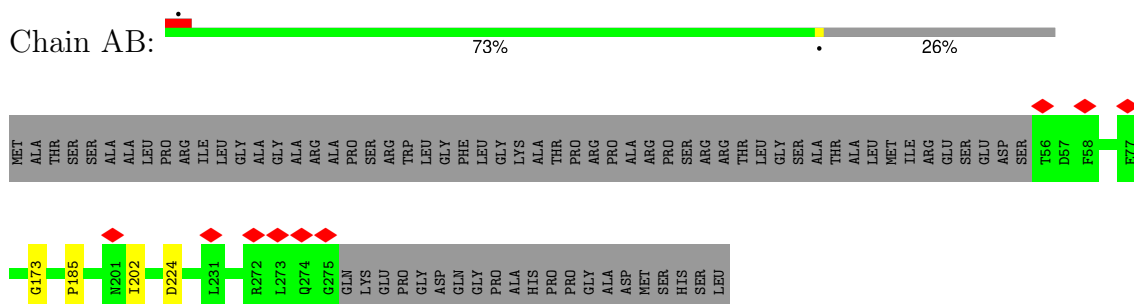
3 Residue-property plots [i](#)

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.

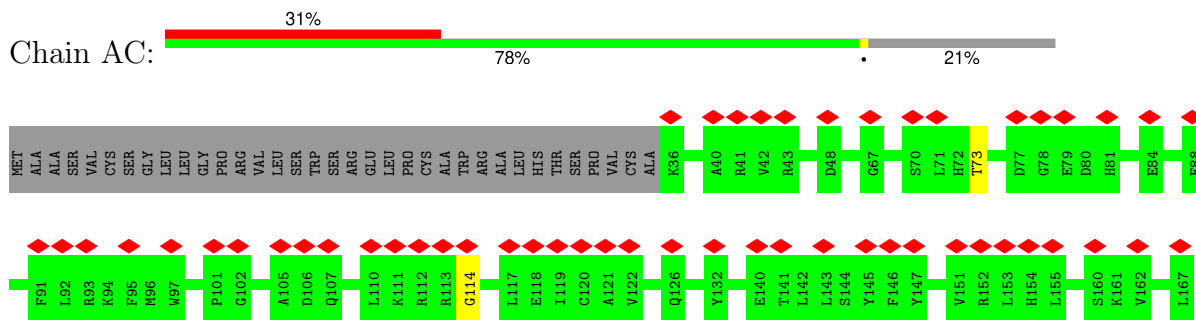
- Molecule 1: 12s rRNA



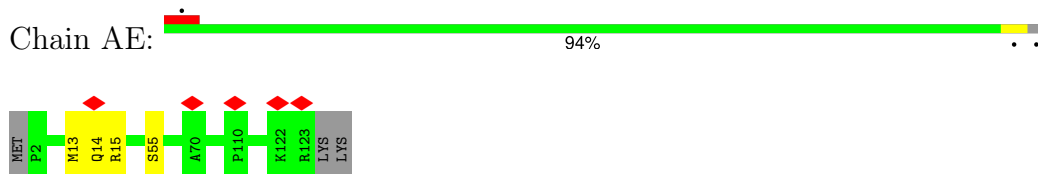
- Molecule 2: 28S ribosomal protein S2, mitochondrial



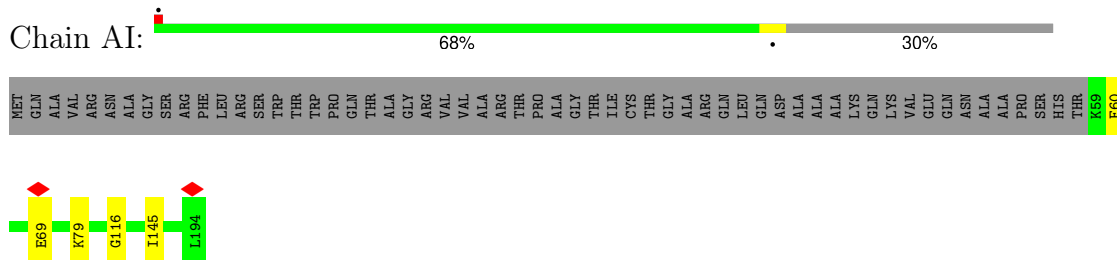
• Molecule 3: 28S ribosomal protein S24, mitochondrial



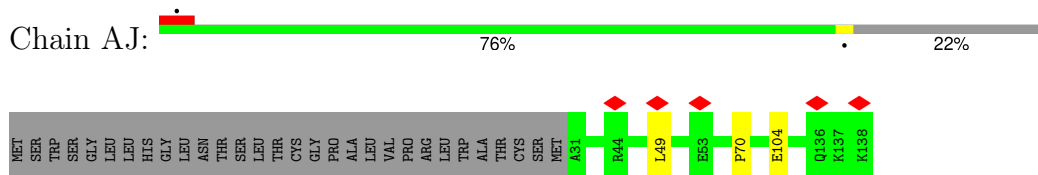
• Molecule 4: 28S ribosomal protein S6, mitochondrial



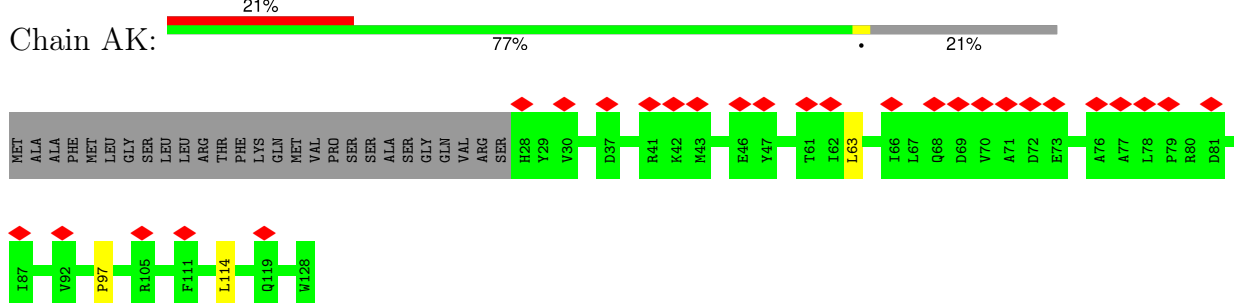
• Molecule 5: 28S ribosomal protein S11, mitochondrial




• Molecule 6: 28S ribosomal protein S12, mitochondrial

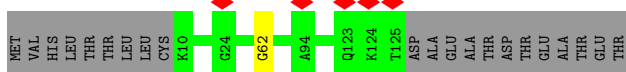


• Molecule 7: 28S ribosomal protein S14, mitochondrial




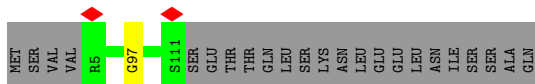
• Molecule 8: 28S ribosomal protein S16, mitochondrial

Chain AM:  84% 15%




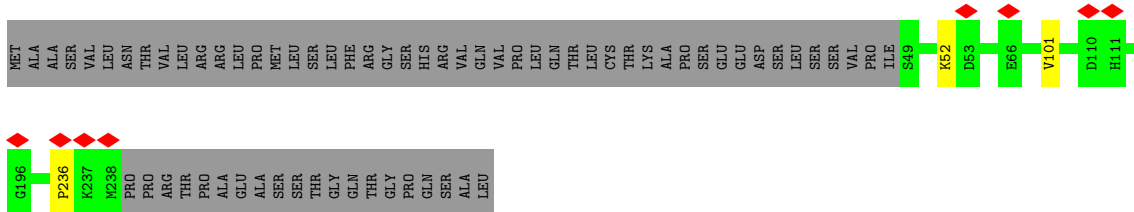
- Molecule 9: 28S ribosomal protein S17, mitochondrial

Chain AN:  82% 18%



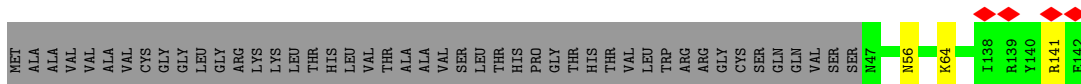
- Molecule 10: 28S ribosomal protein S18b, mitochondrial

Chain AO:  72% 26%



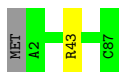
- Molecule 11: 28S ribosomal protein S18c, mitochondrial

Chain AP:  65% 32%



- Molecule 12: 28S ribosomal protein S21, mitochondrial

Chain AQ:  98% ..



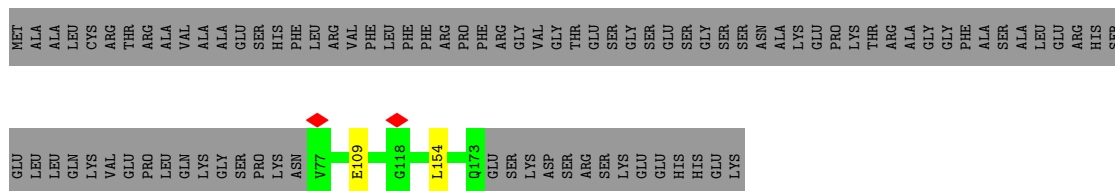
- Molecule 13: 28S ribosomal protein S25, mitochondrial

Chain AT:  97%

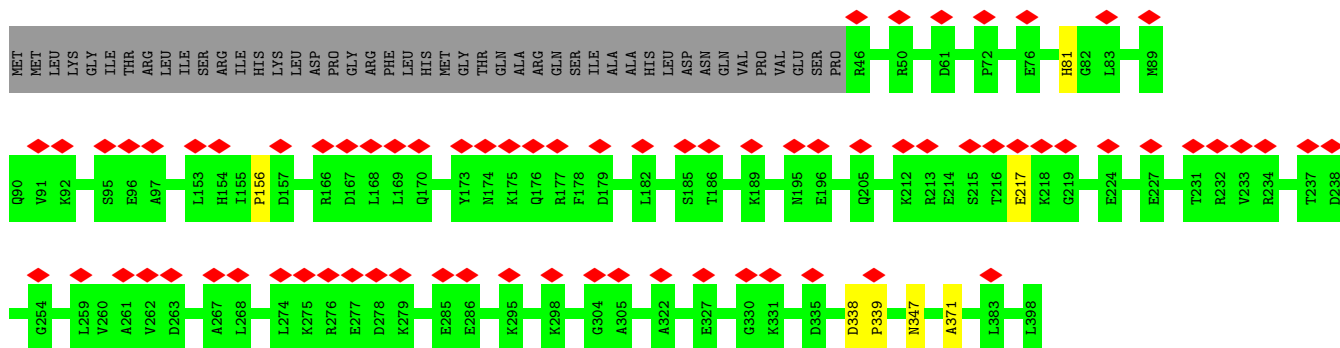
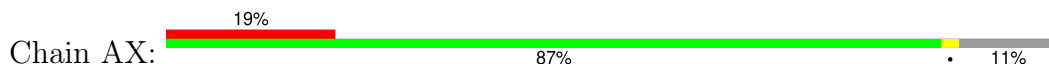


- Molecule 14: 28S ribosomal protein S28, mitochondrial

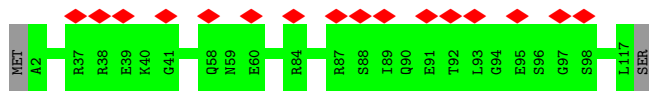
Chain AW:  51% 48%



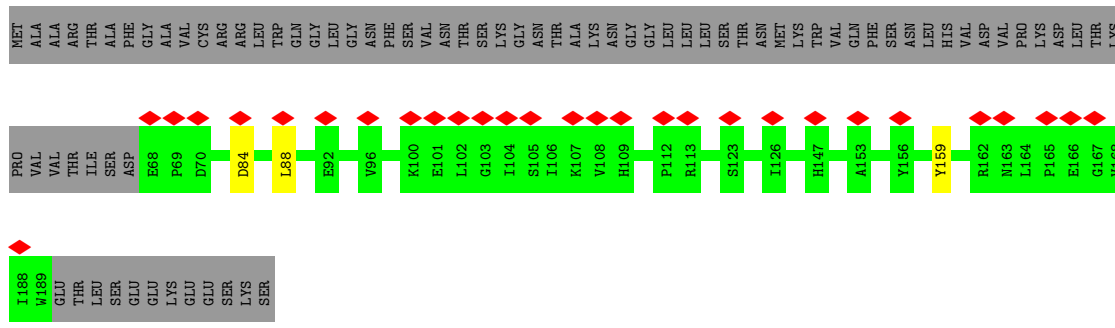
• Molecule 15: 28S ribosomal protein S29, mitochondrial



• Molecule 16: Coiled-coil-helix-coiled-coil-helix domain-containing protein 1

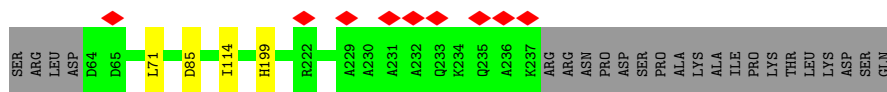


• Molecule 17: 28S ribosomal protein S10, mitochondrial

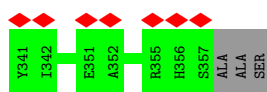
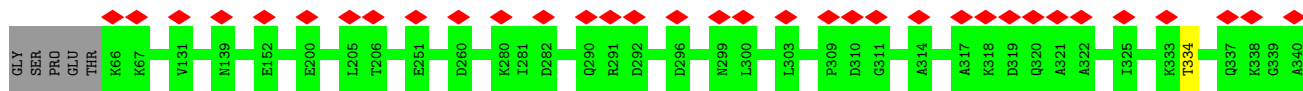
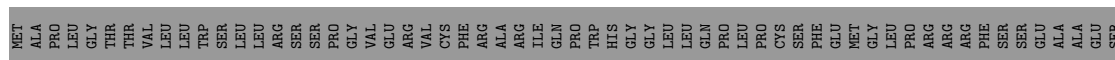
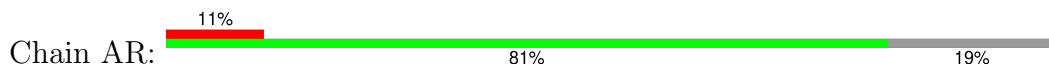


• Molecule 18: 28S ribosomal protein S15, mitochondrial

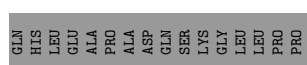
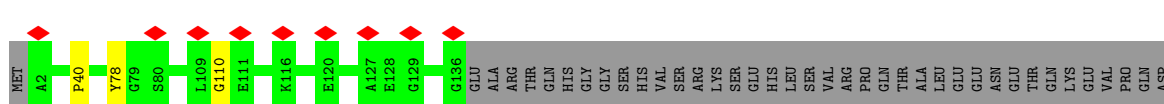




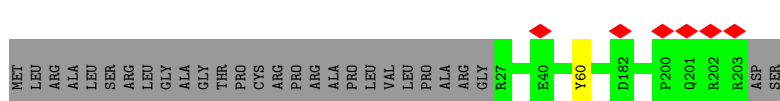
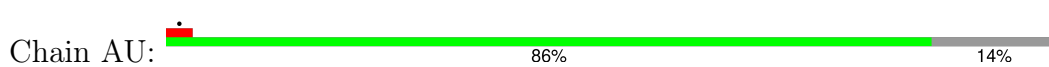
• Molecule 19: 28S ribosomal protein S22, mitochondrial



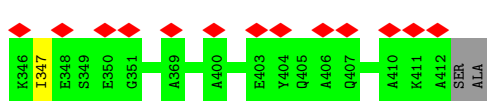
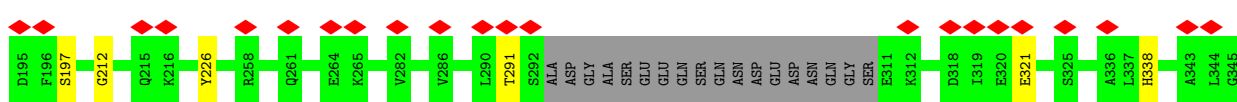
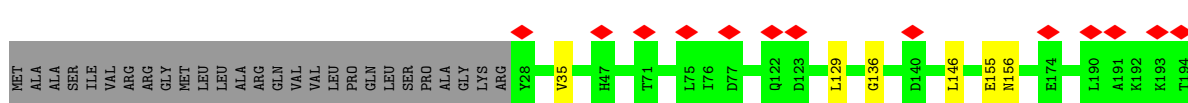
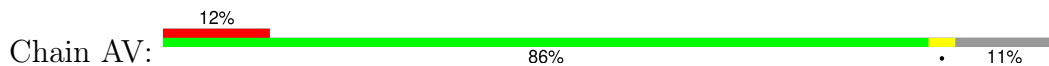
• Molecule 20: 28S ribosomal protein S23, mitochondrial



• Molecule 21: 28S ribosomal protein S26, mitochondrial

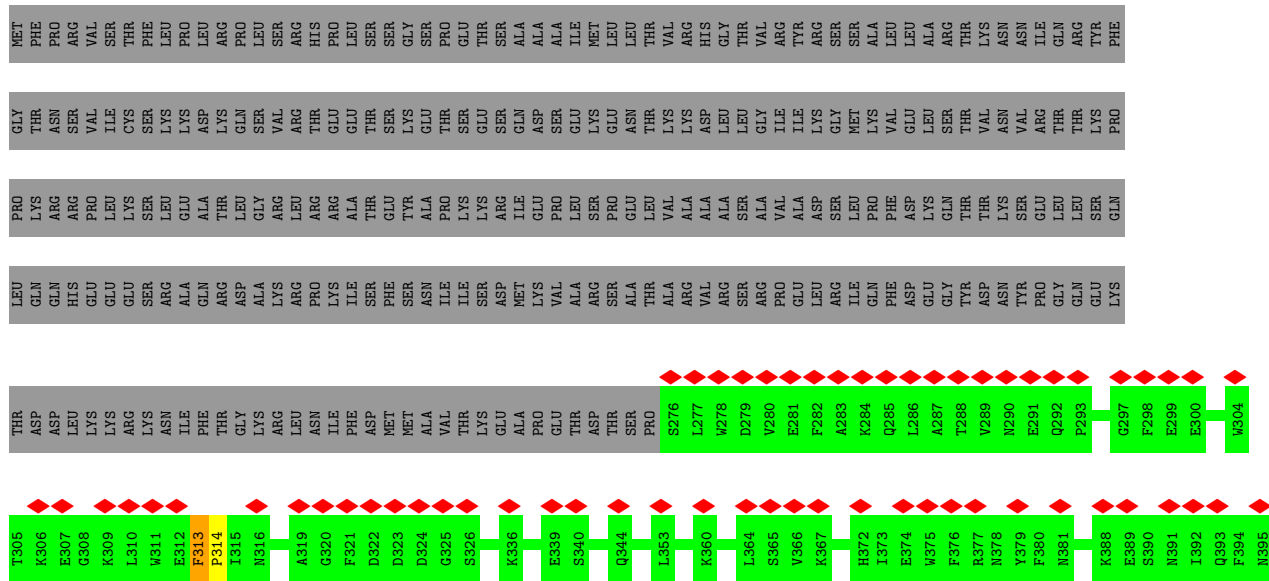


• Molecule 22: 28S ribosomal protein S27, mitochondrial



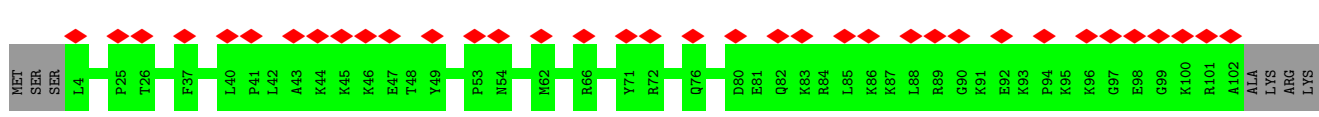
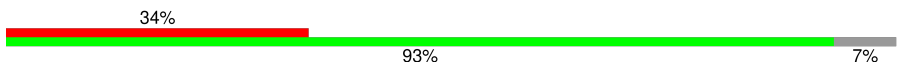
• Molecule 23: 28S ribosomal protein S31, mitochondrial

Chain AY:



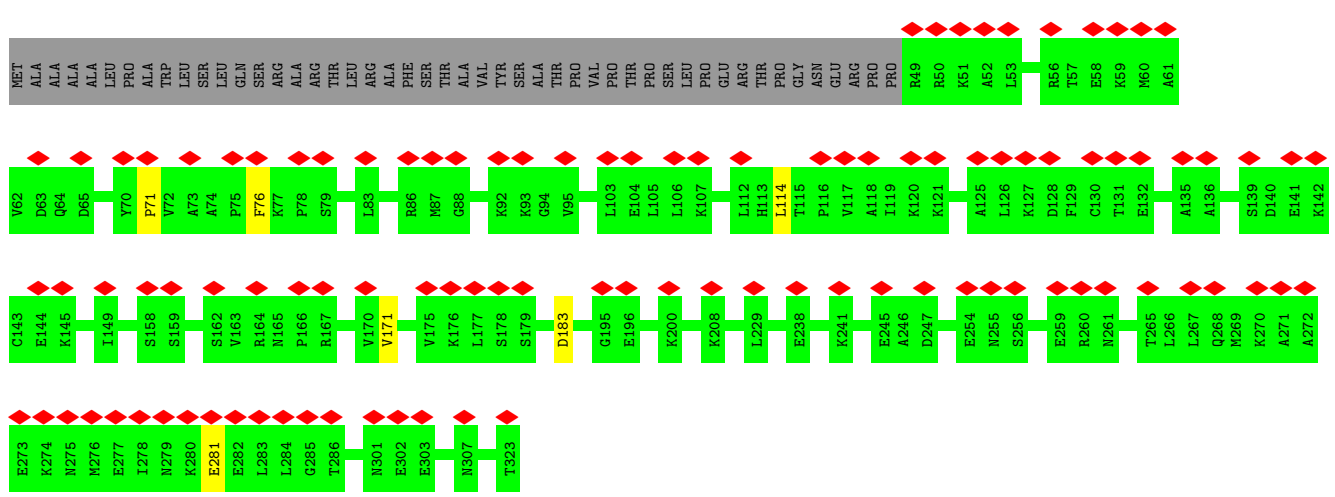
• Molecule 24: 28S ribosomal protein S33, mitochondrial

Chain AZ:



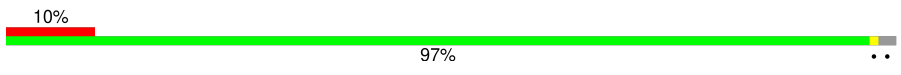
• Molecule 25: 28S ribosomal protein S35, mitochondrial

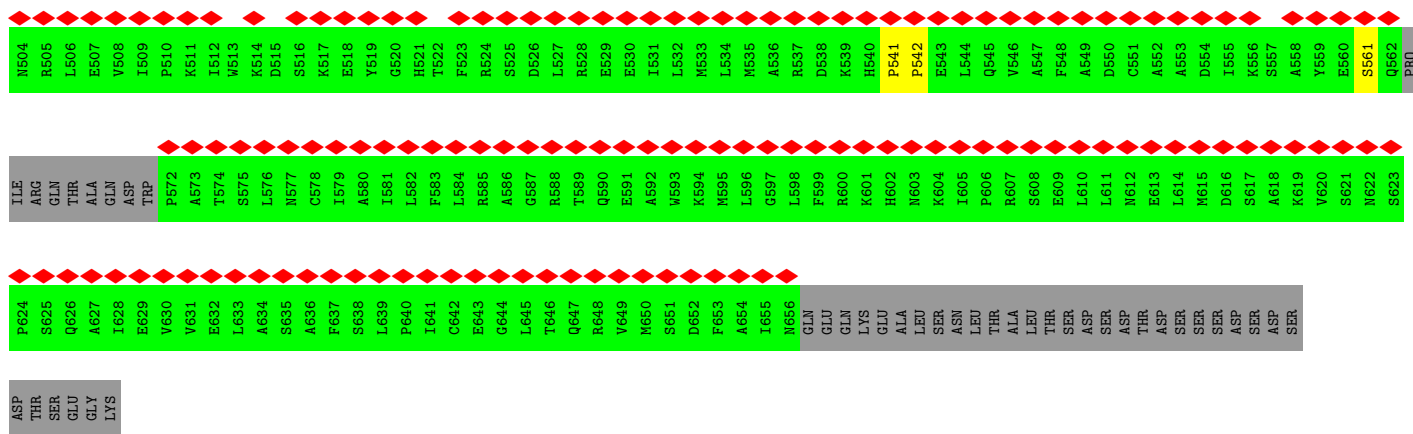
Chain A1:



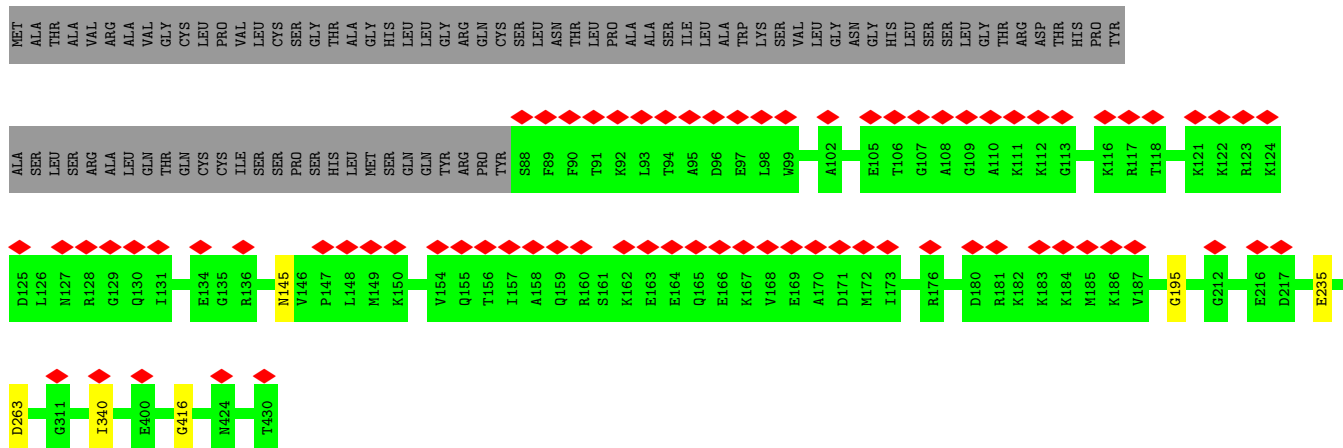
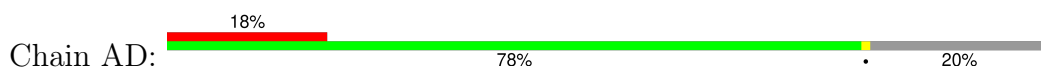
• Molecule 26: 28S ribosomal protein S34, mitochondrial

Chain A0:

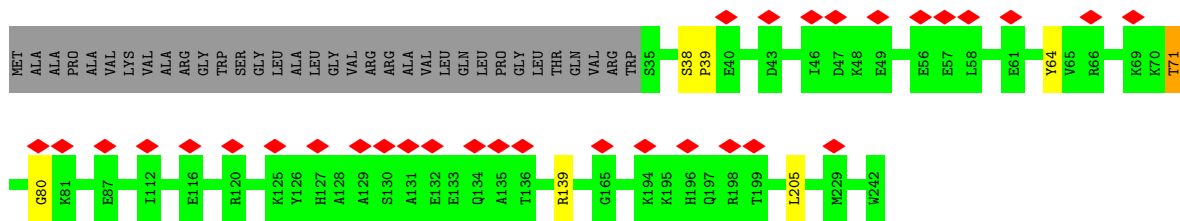
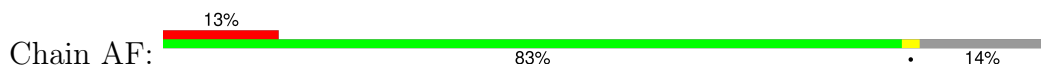




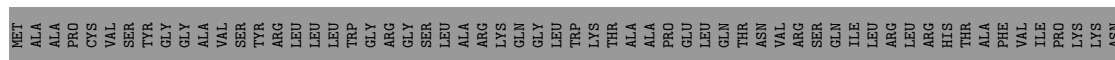
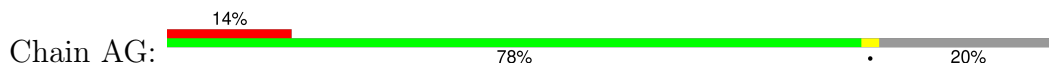
• Molecule 29: 28S ribosomal protein S5, mitochondrial

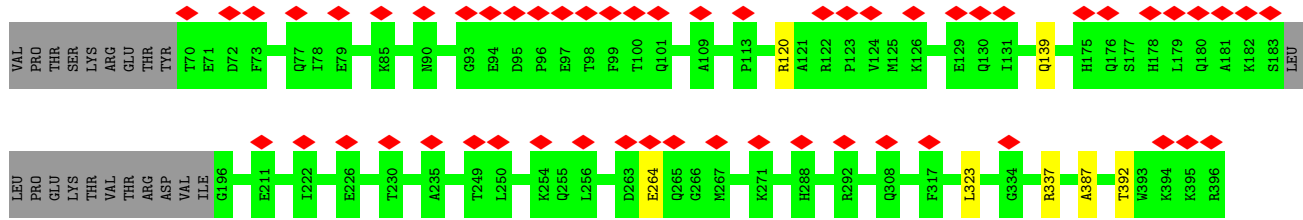


• Molecule 30: 28S ribosomal protein S7, mitochondrial

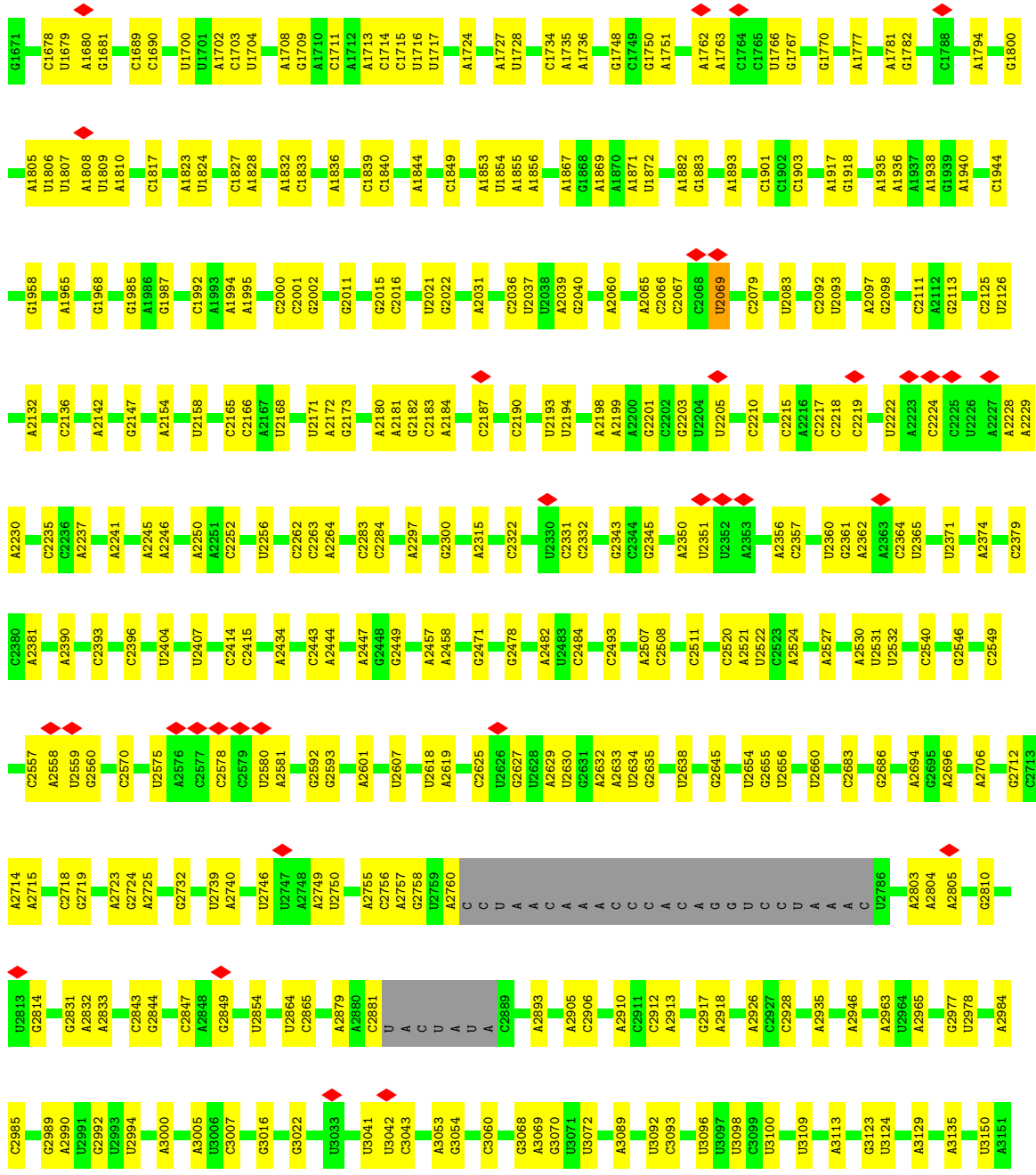


• Molecule 31: 28S ribosomal protein S9, mitochondrial



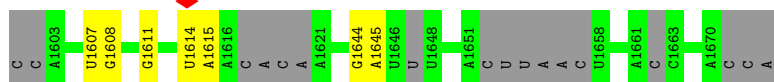


• Molecule 32: 16s rRNA

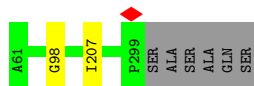
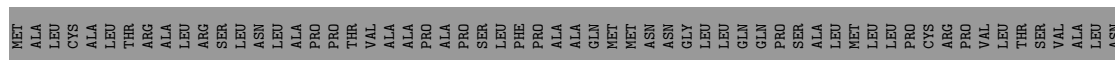




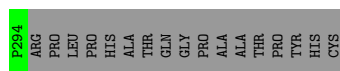
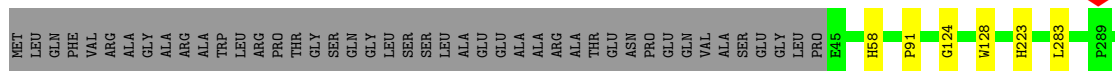
• Molecule 33: tRNA^{Val}



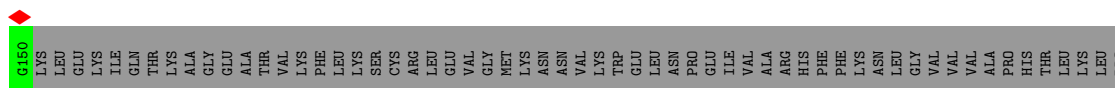
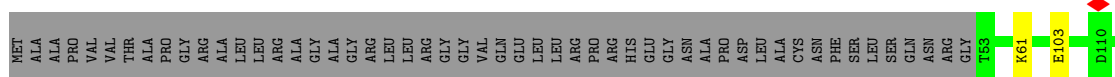
• Molecule 34: 39S ribosomal protein L2, mitochondrial



• Molecule 35: 39S ribosomal protein L4, mitochondrial



• Molecule 36: 39S ribosomal protein L9, mitochondrial

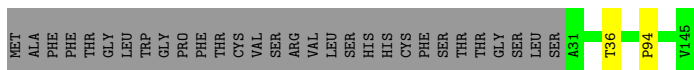
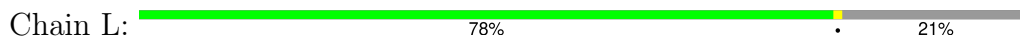


• Molecule 37: 39S ribosomal protein L13, mitochondrial





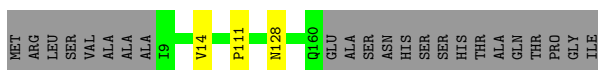
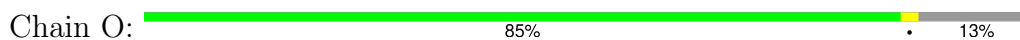
- Molecule 38: 39S ribosomal protein L14, mitochondrial



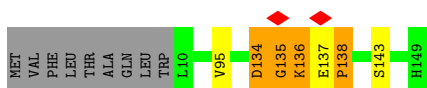
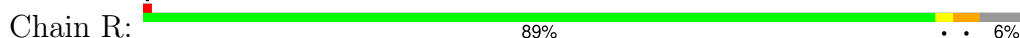
- Molecule 39: 39S ribosomal protein L15, mitochondrial



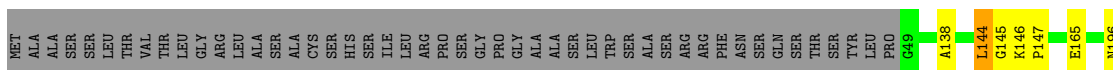
- Molecule 40: 39S ribosomal protein L17, mitochondrial



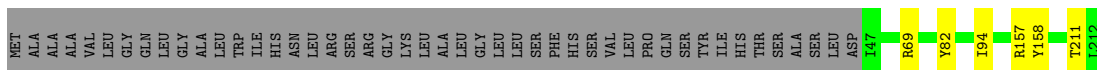
- Molecule 41: 39S ribosomal protein L20, mitochondrial



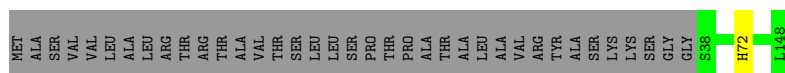
- Molecule 42: 39S ribosomal protein L21, mitochondrial



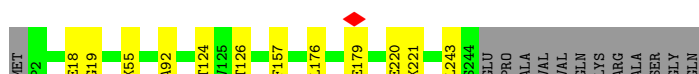
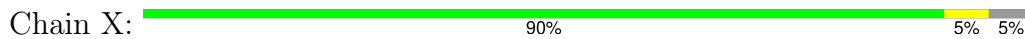
- Molecule 43: 39S ribosomal protein L22, mitochondrial



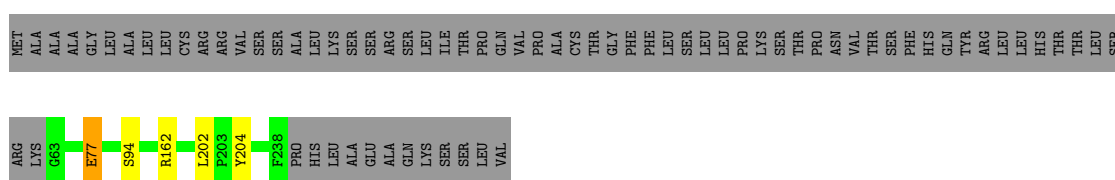
- Molecule 44: 39S ribosomal protein L27, mitochondrial



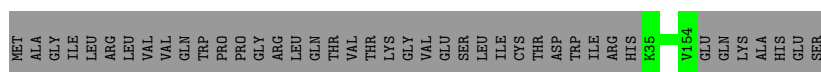
• Molecule 45: 39S ribosomal protein L28, mitochondrial



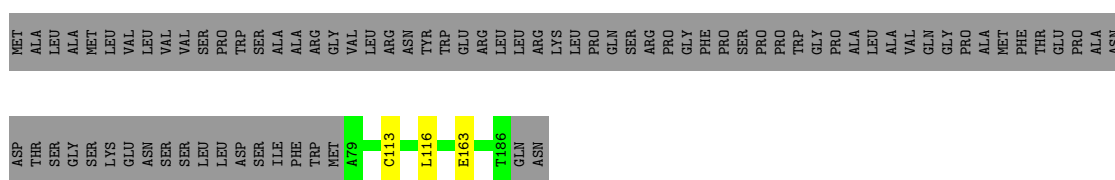
• Molecule 46: 39S ribosomal protein L47, mitochondrial



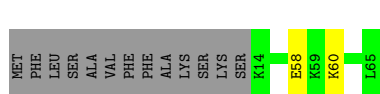
• Molecule 47: 39S ribosomal protein L30, mitochondrial



• Molecule 48: 39S ribosomal protein L32, mitochondrial

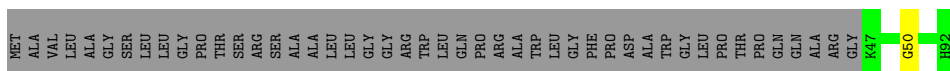


• Molecule 49: 39S ribosomal protein L33, mitochondrial

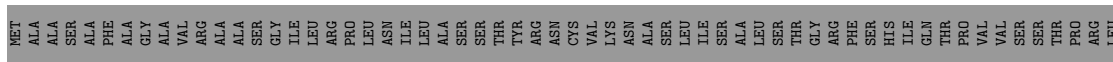


• Molecule 50: 39S ribosomal protein L34, mitochondrial

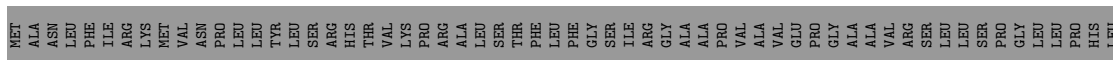




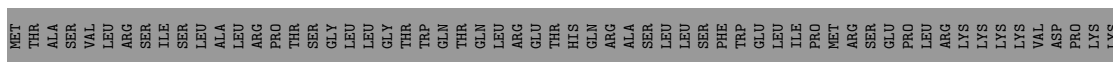
● Molecule 51: 39S ribosomal protein L35, mitochondrial



● Molecule 52: 39S ribosomal protein L36, mitochondrial



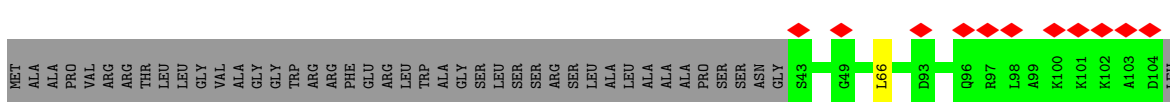
● Molecule 53: 39S ribosomal protein L40, mitochondrial

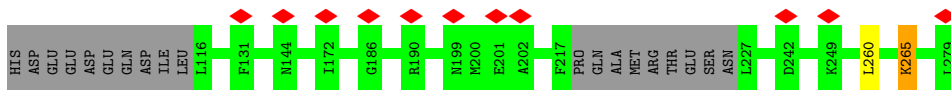


● Molecule 54: 39S ribosomal protein L43, mitochondrial

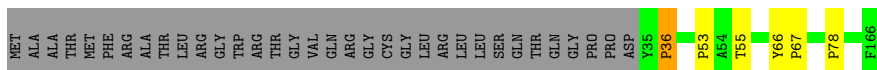


● Molecule 55: 39S ribosomal protein L46, mitochondrial

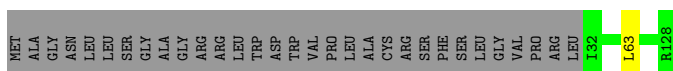




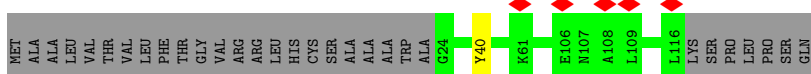
• Molecule 56: 39S ribosomal protein L49, mitochondrial



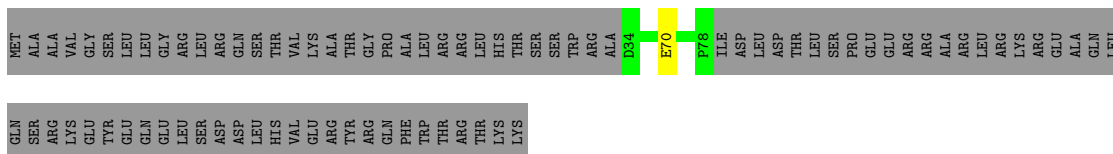
• Molecule 57: 39S ribosomal protein L51, mitochondrial



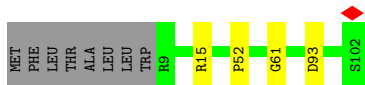
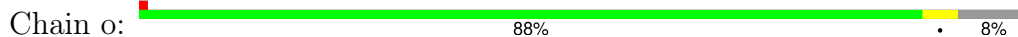
• Molecule 58: cDNA FLJ76418, highly similar to Homo sapiens mitochondrial ribosomal protein L52 (MRPL52), transcript variant 1, mRNA



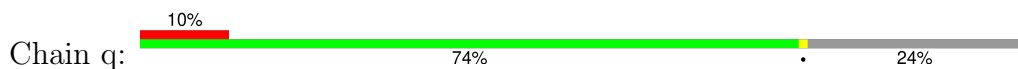
• Molecule 59: 39S ribosomal protein L55, mitochondrial

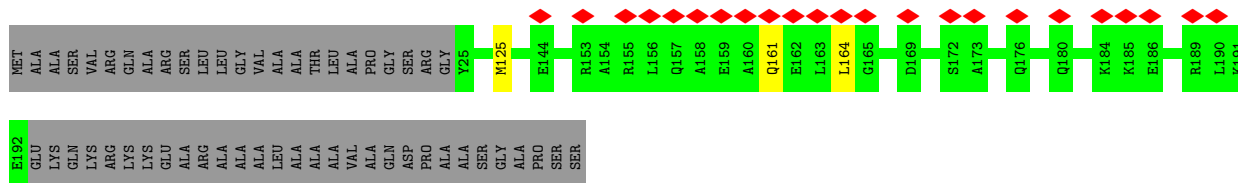


• Molecule 60: Ribosomal protein 63, mitochondrial

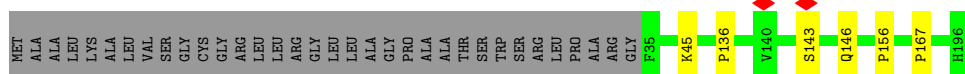
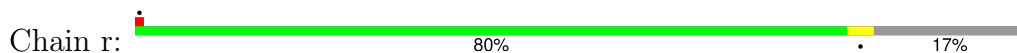


• Molecule 61: Growth arrest and DNA damage-inducible proteins-interacting protein 1

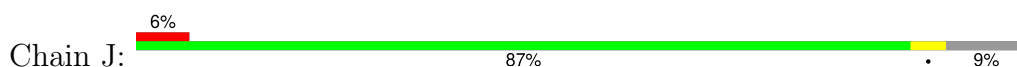




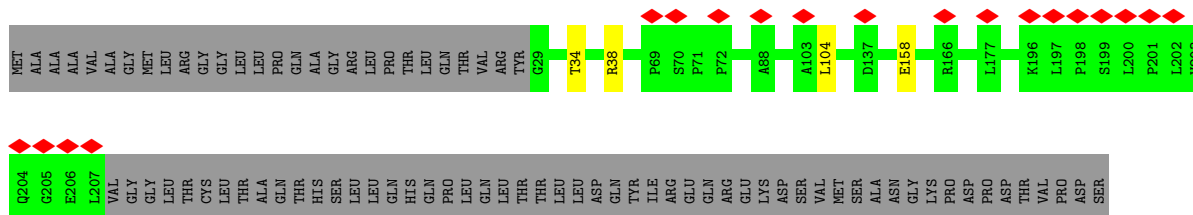
• Molecule 62: 39S ribosomal protein S18a, mitochondrial



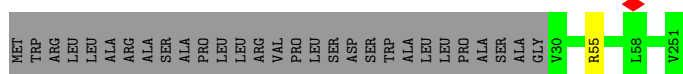
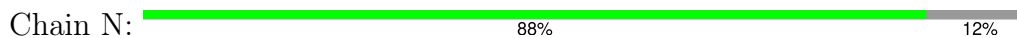
• Molecule 63: 39S ribosomal protein L11, mitochondrial



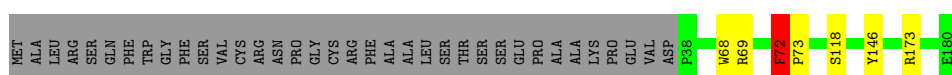
• Molecule 64: 39S ribosomal protein L10, mitochondrial



• Molecule 65: 39S ribosomal protein L16, mitochondrial



• Molecule 66: Mitochondrial ribosomal protein L18, isoform CRA_b

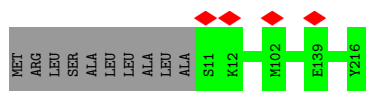


• Molecule 67: 39S ribosomal protein L23, mitochondrial

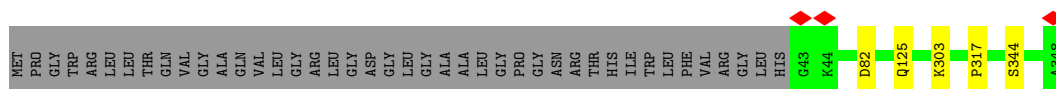
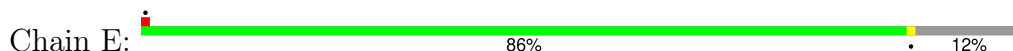




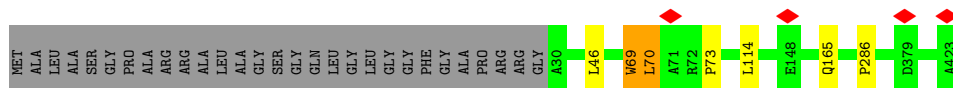
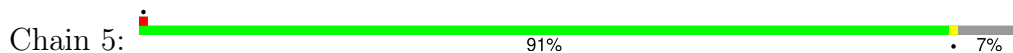
- Molecule 68: 39S ribosomal protein L24, mitochondrial



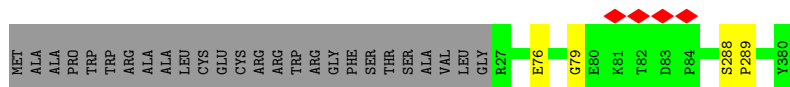
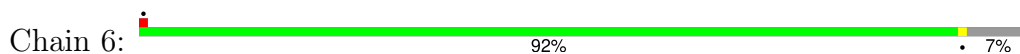
- Molecule 69: 39S ribosomal protein L3, mitochondrial



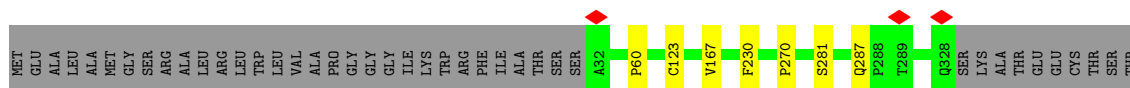
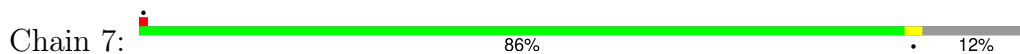
- Molecule 70: 39S ribosomal protein L37, mitochondrial



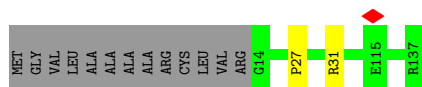
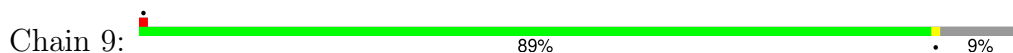
- Molecule 71: 39S ribosomal protein L38, mitochondrial



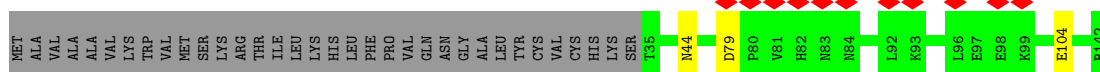
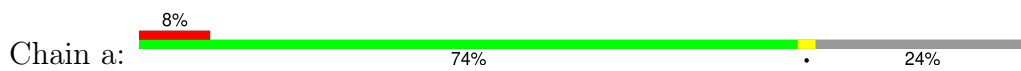
- Molecule 72: 39S ribosomal protein L39, mitochondrial



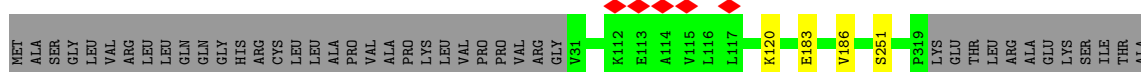
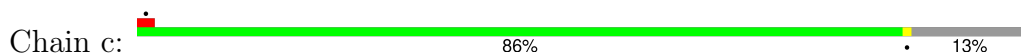
- Molecule 73: 39S ribosomal protein L41, mitochondrial



- Molecule 74: 39S ribosomal protein L42, mitochondrial

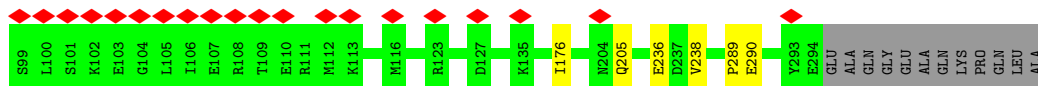
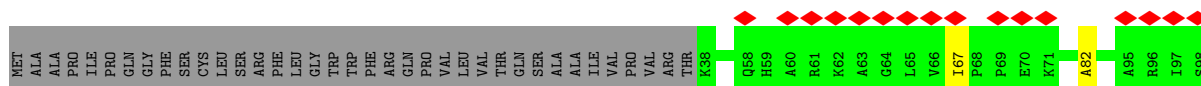
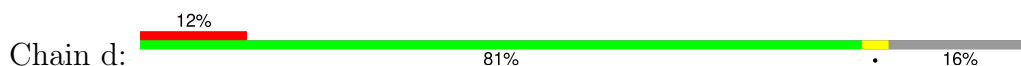


• Molecule 75: 39S ribosomal protein L44, mitochondrial

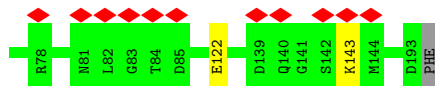
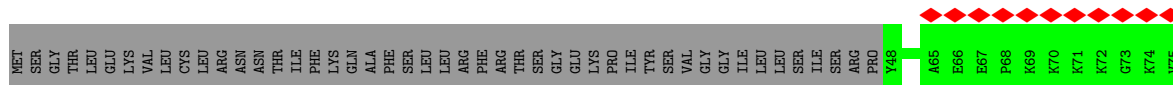


SER

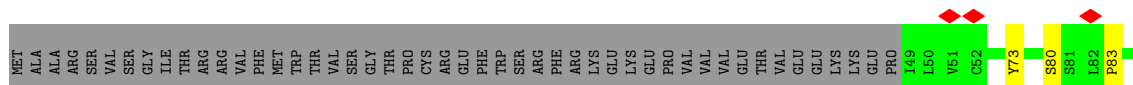
• Molecule 76: 39S ribosomal protein L45, mitochondrial



• Molecule 77: 39S ribosomal protein L48, mitochondrial

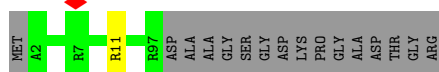
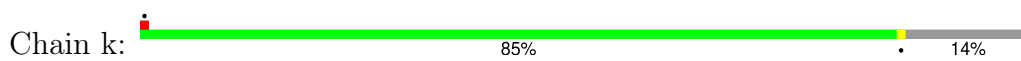


• Molecule 78: 39S ribosomal protein L50, mitochondrial

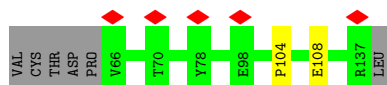


Y158

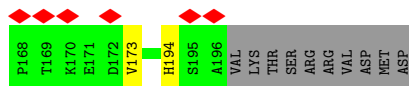
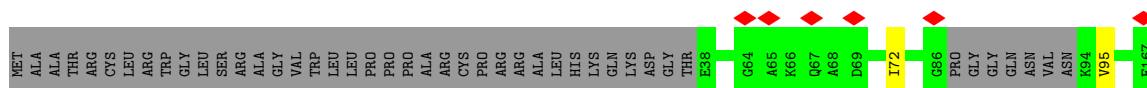
• Molecule 79: 39S ribosomal protein L53, mitochondrial



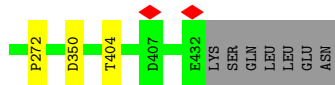
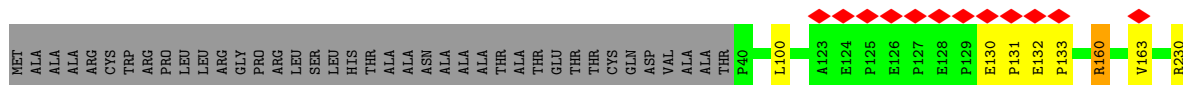
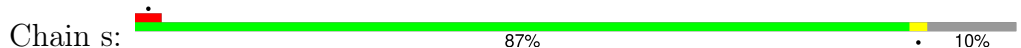
- Molecule 80: 39S ribosomal protein L54, mitochondrial



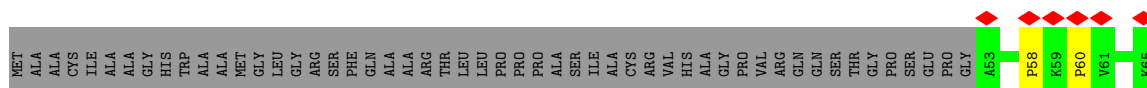
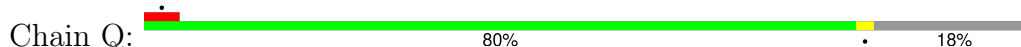
- Molecule 81: Peptidyl-tRNA hydrolase ICT1, mitochondrial

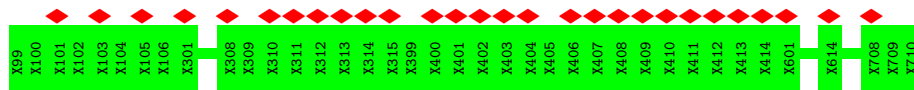


- Molecule 82: 39S ribosomal protein S30, mitochondrial



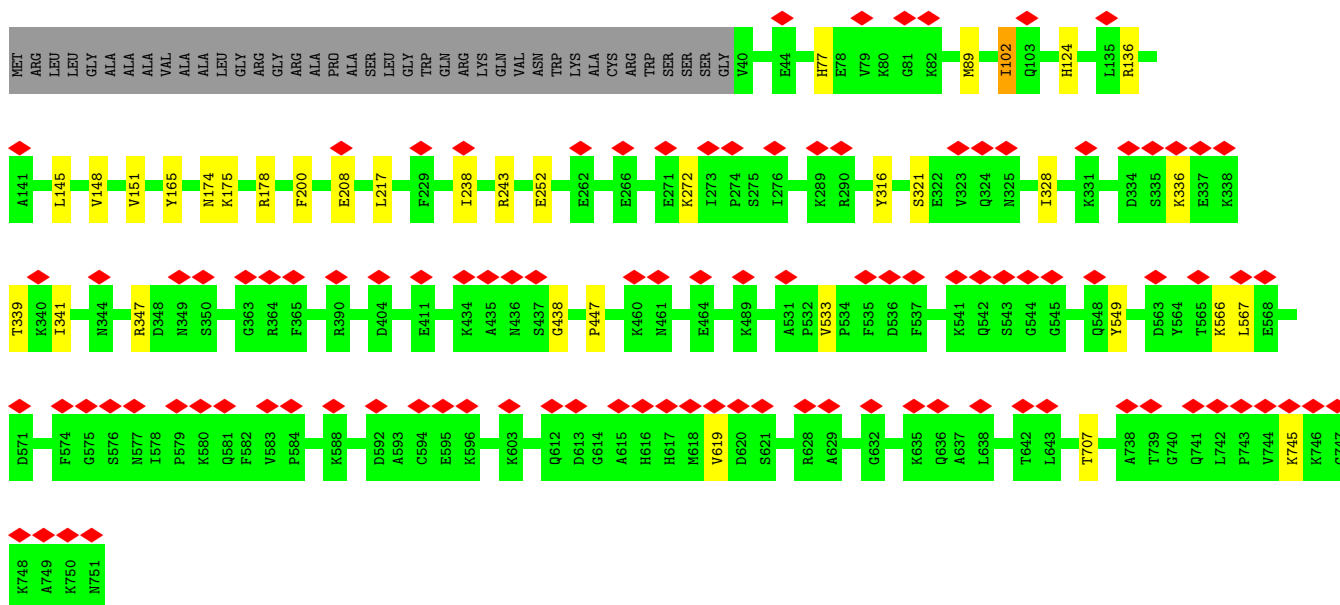
- Molecule 83: 39S ribosomal protein L19, mitochondrial





- Molecule 86: Elongation factor G, mitochondrial

Chain v: 14% 90% 5% 5%



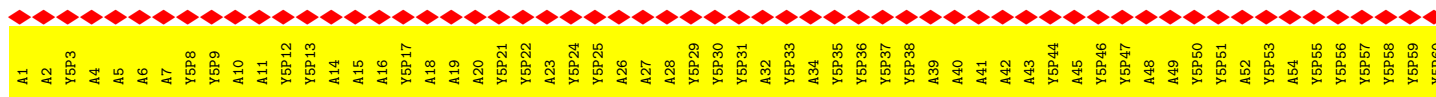
- Molecule 87: mRNA

Chain A5: 100% 100%



- Molecule 88: P-site and E-site tRNA

Chain A6: 99% 100%



- Molecule 88: P-site and E-site tRNA

Chain A7: 42% 87% 13%

4 Experimental information

| Property | Value | Source |
|--------------------------------------|---|-----------|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 150347 | 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 ($e^-/\text{\AA}^2$) | 69.2 | Depositor |
| Minimum defocus (nm) | Not provided | |
| Maximum defocus (nm) | Not provided | |
| Magnification | Not provided | |
| Image detector | GATAN K2 SUMMIT (4k x 4k) | Depositor |
| Maximum map value | 4.076 | Depositor |
| Minimum map value | -1.966 | Depositor |
| Average map value | 0.003 | Depositor |
| Map value standard deviation | 0.115 | Depositor |
| Recommended contour level | 0.267 | Depositor |
| Map size (\AA) | 438.44, 438.44, 438.44 | wwPDB |
| Map dimensions | 400, 400, 400 | wwPDB |
| Map angles ($^\circ$) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (\AA) | 1.0961, 1.0961, 1.0961 | Depositor |

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: Y5P, GDP, P5P, MG, GCP, ZN

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 | AA | 0.14 | 0/22406 | 0.73 | 6/34881 (0.0%) |
| 2 | AB | 0.23 | 0/1830 | 0.38 | 0/2477 |
| 3 | AC | 0.23 | 0/1112 | 0.40 | 0/1505 |
| 4 | AE | 0.23 | 0/989 | 0.42 | 0/1335 |
| 5 | AI | 0.24 | 0/1031 | 0.42 | 0/1390 |
| 6 | AJ | 0.23 | 0/854 | 0.42 | 0/1148 |
| 7 | AK | 0.21 | 0/879 | 0.38 | 0/1182 |
| 8 | AM | 0.23 | 0/941 | 0.39 | 0/1265 |
| 9 | AN | 0.23 | 0/864 | 0.41 | 0/1169 |
| 10 | AO | 0.23 | 0/1624 | 0.37 | 0/2209 |
| 11 | AP | 0.23 | 0/791 | 0.38 | 0/1062 |
| 12 | AQ | 0.22 | 0/752 | 0.35 | 0/1001 |
| 13 | AT | 0.24 | 0/1402 | 0.39 | 0/1883 |
| 14 | AW | 0.23 | 0/778 | 0.42 | 0/1048 |
| 15 | AX | 0.23 | 0/2932 | 0.39 | 0/3968 |
| 16 | A2 | 0.23 | 0/939 | 0.38 | 0/1256 |
| 17 | AH | 0.23 | 0/1037 | 0.39 | 0/1403 |
| 18 | AL | 0.23 | 0/1475 | 0.35 | 0/1970 |
| 19 | AR | 0.23 | 0/2435 | 0.36 | 0/3288 |
| 20 | AS | 0.24 | 0/1138 | 0.36 | 0/1533 |
| 21 | AU | 0.23 | 0/1521 | 0.35 | 0/2039 |
| 22 | AV | 0.23 | 0/3071 | 0.35 | 0/4147 |
| 23 | AY | 0.26 | 0/1046 | 0.43 | 1/1410 (0.1%) |
| 24 | AZ | 0.23 | 0/851 | 0.34 | 0/1133 |
| 25 | A1 | 0.23 | 0/2277 | 0.37 | 0/3079 |
| 26 | A0 | 0.22 | 0/1827 | 0.38 | 0/2473 |
| 27 | A3 | 0.23 | 0/650 | 0.36 | 0/855 |
| 28 | A4 | 0.23 | 0/3028 | 0.36 | 0/4197 |
| 29 | AD | 0.23 | 0/2783 | 0.38 | 0/3724 |
| 30 | AF | 0.23 | 0/1765 | 0.38 | 0/2369 |
| 31 | AG | 0.24 | 0/2642 | 0.38 | 0/3538 |
| 32 | A | 0.19 | 7/36246 (0.0%) | 0.78 | 23/56422 (0.0%) |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|---------------|-------------|---------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 33 | B | 0.13 | 0/1328 | 0.71 | 0/2056 |
| 34 | D | 0.23 | 0/1904 | 0.41 | 0/2561 |
| 35 | F | 0.23 | 0/2071 | 0.39 | 0/2817 |
| 36 | H | 0.22 | 0/820 | 0.41 | 0/1102 |
| 37 | K | 0.23 | 0/1495 | 0.37 | 0/2029 |
| 38 | L | 0.23 | 0/904 | 0.41 | 0/1218 |
| 39 | M | 0.24 | 0/2359 | 0.39 | 0/3185 |
| 40 | O | 0.23 | 0/1269 | 0.39 | 0/1708 |
| 41 | R | 0.23 | 0/1174 | 0.47 | 4/1572 (0.3%) |
| 42 | S | 0.24 | 0/1276 | 0.51 | 2/1729 (0.1%) |
| 43 | T | 0.23 | 0/1402 | 0.38 | 0/1886 |
| 44 | W | 0.24 | 0/893 | 0.42 | 0/1204 |
| 45 | X | 0.23 | 0/2081 | 0.37 | 0/2812 |
| 46 | Y | 0.23 | 0/1552 | 0.35 | 0/2079 |
| 47 | Z | 0.23 | 0/1003 | 0.39 | 0/1354 |
| 48 | 0 | 0.22 | 0/895 | 0.40 | 0/1201 |
| 49 | 1 | 0.23 | 0/438 | 0.41 | 0/583 |
| 50 | 2 | 0.22 | 0/382 | 0.38 | 0/507 |
| 51 | 3 | 0.23 | 0/852 | 0.38 | 0/1136 |
| 52 | 4 | 0.22 | 0/350 | 0.39 | 0/461 |
| 53 | 8 | 0.23 | 0/855 | 0.39 | 0/1152 |
| 54 | b | 0.23 | 0/1202 | 0.40 | 0/1626 |
| 55 | e | 0.23 | 0/1797 | 0.40 | 0/2422 |
| 56 | g | 0.25 | 0/1132 | 0.42 | 0/1543 |
| 57 | i | 0.23 | 0/849 | 0.35 | 0/1135 |
| 58 | j | 0.23 | 0/755 | 0.39 | 0/1016 |
| 59 | m | 0.22 | 0/379 | 0.41 | 0/510 |
| 60 | o | 0.22 | 0/818 | 0.35 | 0/1097 |
| 61 | q | 0.23 | 0/1325 | 0.41 | 1/1799 (0.1%) |
| 62 | r | 0.22 | 0/1362 | 0.38 | 0/1846 |
| 63 | J | 0.30 | 0/1348 | 0.47 | 0/1813 |
| 64 | I | 0.23 | 0/1467 | 0.42 | 0/1984 |
| 65 | N | 0.24 | 0/1833 | 0.39 | 0/2468 |
| 66 | P | 0.29 | 0/1191 | 0.53 | 3/1611 (0.2%) |
| 67 | U | 0.24 | 0/1254 | 0.38 | 0/1700 |
| 68 | V | 0.23 | 0/1727 | 0.39 | 0/2341 |
| 69 | E | 0.23 | 0/2479 | 0.40 | 0/3360 |
| 70 | 5 | 0.29 | 1/3305 (0.0%) | 0.43 | 0/4502 |
| 71 | 6 | 0.24 | 0/3043 | 0.39 | 0/4140 |
| 72 | 7 | 0.23 | 0/2467 | 0.39 | 0/3337 |
| 73 | 9 | 0.25 | 0/1025 | 0.40 | 0/1379 |
| 74 | a | 0.22 | 0/923 | 0.39 | 0/1254 |
| 75 | c | 0.24 | 0/2371 | 0.37 | 0/3205 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|------------------|-------------|------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 76 | d | 0.24 | 0/2132 | 0.40 | 0/2887 |
| 77 | f | 0.23 | 0/1144 | 0.43 | 0/1551 |
| 78 | h | 0.23 | 0/917 | 0.38 | 0/1249 |
| 79 | k | 0.23 | 0/754 | 0.40 | 0/1017 |
| 80 | l | 0.23 | 0/636 | 0.37 | 0/860 |
| 81 | p | 0.23 | 0/1246 | 0.40 | 0/1675 |
| 82 | s | 0.24 | 0/3262 | 0.43 | 1/4435 (0.0%) |
| 83 | Q | 0.25 | 0/2044 | 0.39 | 0/2757 |
| 84 | TA | 0.23 | 0/349 | 0.41 | 0/475 |
| 84 | TB | 0.21 | 0/212 | 0.39 | 0/286 |
| 84 | TC | 0.24 | 0/351 | 0.48 | 0/488 |
| 86 | v | 0.28 | 2/5647 (0.0%) | 0.51 | 6/7623 (0.1%) |
| All | All | 0.22 | 10/181965 (0.0%) | 0.56 | 47/258102 (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 |
|-----|-------|---------------------|---------------------|
| 23 | AY | 0 | 1 |
| 41 | R | 0 | 1 |
| 42 | S | 0 | 1 |
| 66 | P | 0 | 1 |
| 82 | s | 0 | 1 |
| 84 | TC | 0 | 1 |
| 86 | v | 0 | 1 |
| All | All | 0 | 7 |

The worst 5 of 10 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|--------|-------------|----------|
| 32 | A | 3089 | A | C5-C4 | -10.46 | 1.31 | 1.38 |
| 32 | A | 3089 | A | N9-C4 | 10.01 | 1.43 | 1.37 |
| 32 | A | 3089 | A | C2'-C1' | -7.28 | 1.45 | 1.53 |
| 86 | v | 174 | ASN | C-N | 7.27 | 1.50 | 1.34 |
| 32 | A | 3089 | A | C3'-O3' | -6.64 | 1.32 | 1.42 |

The worst 5 of 47 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 32 | A | 3089 | A | C2-N3-C4 | 26.44 | 123.82 | 110.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 32 | A | 3089 | A | N1-C6-N6 | -19.00 | 107.20 | 118.60 |
| 32 | A | 3089 | A | C5-C6-N1 | 17.36 | 126.38 | 117.70 |
| 32 | A | 3089 | A | N3-C4-C5 | -14.89 | 116.37 | 126.80 |
| 32 | A | 3089 | A | C5-N7-C8 | 14.31 | 111.06 | 103.90 |

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 23 | AY | 313 | PHE | Peptide |
| 66 | P | 72 | PHE | Peptide |
| 41 | R | 134 | ASP | Peptide |
| 42 | S | 144 | LEU | Peptide |
| 82 | s | 160 | ARG | Peptide |

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 2 | AB | 218/296 (74%) | 193 (88%) | 21 (10%) | 4 (2%) | 7 | 20 |
| 3 | AC | 130/167 (78%) | 110 (85%) | 19 (15%) | 1 (1%) | 16 | 39 |
| 4 | AE | 120/125 (96%) | 102 (85%) | 15 (12%) | 3 (2%) | 4 | 13 |
| 5 | AI | 134/194 (69%) | 117 (87%) | 12 (9%) | 5 (4%) | 2 | 6 |
| 6 | AJ | 106/138 (77%) | 88 (83%) | 15 (14%) | 3 (3%) | 4 | 11 |
| 7 | AK | 99/128 (77%) | 87 (88%) | 10 (10%) | 2 (2%) | 6 | 17 |
| 8 | AM | 114/137 (83%) | 101 (89%) | 12 (10%) | 1 (1%) | 14 | 35 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 9 | AN | 105/130 (81%) | 83 (79%) | 21 (20%) | 1 (1%) | 13 | 33 |
| 10 | AO | 188/258 (73%) | 170 (90%) | 15 (8%) | 3 (2%) | 8 | 22 |
| 11 | AP | 94/142 (66%) | 79 (84%) | 12 (13%) | 3 (3%) | 3 | 8 |
| 12 | AQ | 84/87 (97%) | 75 (89%) | 9 (11%) | 0 | 100 | 100 |
| 13 | AT | 166/173 (96%) | 149 (90%) | 17 (10%) | 0 | 100 | 100 |
| 14 | AW | 95/187 (51%) | 78 (82%) | 15 (16%) | 2 (2%) | 5 | 16 |
| 15 | AX | 351/398 (88%) | 318 (91%) | 27 (8%) | 6 (2%) | 7 | 21 |
| 16 | A2 | 114/118 (97%) | 102 (90%) | 12 (10%) | 0 | 100 | 100 |
| 17 | AH | 120/201 (60%) | 96 (80%) | 20 (17%) | 4 (3%) | 3 | 8 |
| 18 | AL | 172/257 (67%) | 151 (88%) | 17 (10%) | 4 (2%) | 5 | 14 |
| 19 | AR | 290/360 (81%) | 253 (87%) | 36 (12%) | 1 (0%) | 37 | 60 |
| 20 | AS | 133/190 (70%) | 122 (92%) | 8 (6%) | 3 (2%) | 5 | 14 |
| 21 | AU | 175/205 (85%) | 164 (94%) | 11 (6%) | 0 | 100 | 100 |
| 22 | AV | 363/414 (88%) | 312 (86%) | 42 (12%) | 9 (2%) | 4 | 13 |
| 23 | AY | 118/395 (30%) | 105 (89%) | 12 (10%) | 1 (1%) | 16 | 39 |
| 24 | AZ | 97/106 (92%) | 89 (92%) | 8 (8%) | 0 | 100 | 100 |
| 25 | A1 | 273/323 (84%) | 247 (90%) | 23 (8%) | 3 (1%) | 12 | 31 |
| 26 | A0 | 212/218 (97%) | 183 (86%) | 27 (13%) | 2 (1%) | 14 | 35 |
| 27 | A3 | 70/199 (35%) | 65 (93%) | 4 (6%) | 1 (1%) | 9 | 25 |
| 28 | A4 | 541/689 (78%) | 468 (86%) | 61 (11%) | 12 (2%) | 5 | 15 |
| 29 | AD | 341/430 (79%) | 298 (87%) | 38 (11%) | 5 (2%) | 8 | 24 |
| 30 | AF | 206/242 (85%) | 184 (89%) | 19 (9%) | 3 (2%) | 8 | 24 |
| 31 | AG | 311/396 (78%) | 274 (88%) | 35 (11%) | 2 (1%) | 22 | 46 |
| 34 | D | 237/305 (78%) | 207 (87%) | 28 (12%) | 2 (1%) | 16 | 39 |
| 35 | F | 248/311 (80%) | 217 (88%) | 26 (10%) | 5 (2%) | 6 | 17 |
| 36 | H | 96/267 (36%) | 83 (86%) | 11 (12%) | 2 (2%) | 5 | 16 |
| 37 | K | 175/178 (98%) | 153 (87%) | 16 (9%) | 6 (3%) | 3 | 7 |
| 38 | L | 113/145 (78%) | 101 (89%) | 11 (10%) | 1 (1%) | 14 | 35 |
| 39 | M | 285/296 (96%) | 252 (88%) | 26 (9%) | 7 (2%) | 4 | 13 |
| 40 | O | 150/175 (86%) | 128 (85%) | 19 (13%) | 3 (2%) | 6 | 17 |
| 41 | R | 138/149 (93%) | 124 (90%) | 9 (6%) | 5 (4%) | 3 | 6 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 42 | S | 154/205 (75%) | 135 (88%) | 15 (10%) | 4 (3%) | 4 | 13 |
| 43 | T | 164/212 (77%) | 148 (90%) | 13 (8%) | 3 (2%) | 7 | 20 |
| 44 | W | 109/148 (74%) | 96 (88%) | 12 (11%) | 1 (1%) | 14 | 35 |
| 45 | X | 241/256 (94%) | 213 (88%) | 22 (9%) | 6 (2%) | 4 | 13 |
| 46 | Y | 174/250 (70%) | 161 (92%) | 8 (5%) | 5 (3%) | 3 | 10 |
| 47 | Z | 118/161 (73%) | 106 (90%) | 12 (10%) | 0 | 100 | 100 |
| 48 | 0 | 106/188 (56%) | 93 (88%) | 10 (9%) | 3 (3%) | 4 | 11 |
| 49 | 1 | 50/65 (77%) | 42 (84%) | 7 (14%) | 1 (2%) | 6 | 17 |
| 50 | 2 | 44/92 (48%) | 41 (93%) | 2 (4%) | 1 (2%) | 5 | 14 |
| 51 | 3 | 93/188 (50%) | 84 (90%) | 8 (9%) | 1 (1%) | 12 | 31 |
| 52 | 4 | 36/103 (35%) | 33 (92%) | 3 (8%) | 0 | 100 | 100 |
| 53 | 8 | 97/206 (47%) | 84 (87%) | 13 (13%) | 0 | 100 | 100 |
| 54 | b | 146/155 (94%) | 129 (88%) | 14 (10%) | 3 (2%) | 5 | 16 |
| 55 | e | 211/279 (76%) | 188 (89%) | 22 (10%) | 1 (0%) | 25 | 50 |
| 56 | g | 130/166 (78%) | 111 (85%) | 14 (11%) | 5 (4%) | 2 | 6 |
| 57 | i | 95/128 (74%) | 75 (79%) | 20 (21%) | 0 | 100 | 100 |
| 58 | j | 91/123 (74%) | 83 (91%) | 7 (8%) | 1 (1%) | 12 | 31 |
| 59 | m | 43/128 (34%) | 34 (79%) | 8 (19%) | 1 (2%) | 5 | 14 |
| 60 | o | 92/102 (90%) | 78 (85%) | 11 (12%) | 3 (3%) | 3 | 8 |
| 61 | q | 166/222 (75%) | 154 (93%) | 10 (6%) | 2 (1%) | 11 | 29 |
| 62 | r | 160/196 (82%) | 139 (87%) | 17 (11%) | 4 (2%) | 4 | 13 |
| 63 | J | 173/192 (90%) | 152 (88%) | 15 (9%) | 6 (4%) | 3 | 7 |
| 64 | I | 177/261 (68%) | 164 (93%) | 12 (7%) | 1 (1%) | 22 | 46 |
| 65 | N | 220/251 (88%) | 203 (92%) | 16 (7%) | 1 (0%) | 25 | 50 |
| 66 | P | 141/179 (79%) | 123 (87%) | 13 (9%) | 5 (4%) | 3 | 7 |
| 67 | U | 150/153 (98%) | 121 (81%) | 27 (18%) | 2 (1%) | 10 | 27 |
| 68 | V | 204/216 (94%) | 179 (88%) | 25 (12%) | 0 | 100 | 100 |
| 69 | E | 304/348 (87%) | 268 (88%) | 32 (10%) | 4 (1%) | 10 | 27 |
| 70 | 5 | 392/423 (93%) | 347 (88%) | 41 (10%) | 4 (1%) | 13 | 33 |
| 71 | 6 | 352/380 (93%) | 302 (86%) | 47 (13%) | 3 (1%) | 14 | 35 |
| 72 | 7 | 295/338 (87%) | 260 (88%) | 28 (10%) | 7 (2%) | 5 | 13 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-------------------|-------------|------------|----------|-------------|-----|
| 73 | 9 | 122/137 (89%) | 106 (87%) | 15 (12%) | 1 (1%) | 16 | 39 |
| 74 | a | 106/142 (75%) | 95 (90%) | 8 (8%) | 3 (3%) | 4 | 11 |
| 75 | c | 287/332 (86%) | 266 (93%) | 17 (6%) | 4 (1%) | 9 | 25 |
| 76 | d | 255/306 (83%) | 215 (84%) | 34 (13%) | 6 (2%) | 5 | 13 |
| 77 | f | 144/194 (74%) | 122 (85%) | 21 (15%) | 1 (1%) | 19 | 41 |
| 78 | h | 108/158 (68%) | 93 (86%) | 13 (12%) | 2 (2%) | 6 | 18 |
| 79 | k | 94/112 (84%) | 86 (92%) | 8 (8%) | 0 | 100 | 100 |
| 80 | l | 70/138 (51%) | 62 (89%) | 7 (10%) | 1 (1%) | 9 | 25 |
| 81 | p | 148/206 (72%) | 130 (88%) | 16 (11%) | 2 (1%) | 9 | 25 |
| 82 | s | 391/439 (89%) | 342 (88%) | 40 (10%) | 9 (2%) | 5 | 14 |
| 83 | Q | 238/292 (82%) | 216 (91%) | 16 (7%) | 6 (2%) | 4 | 13 |
| 84 | TA | 43/198 (22%) | 32 (74%) | 11 (26%) | 0 | 100 | 100 |
| 84 | TB | 25/198 (13%) | 24 (96%) | 1 (4%) | 0 | 100 | 100 |
| 84 | TC | 69/198 (35%) | 57 (83%) | 11 (16%) | 1 (1%) | 9 | 25 |
| 86 | v | 710/751 (94%) | 565 (80%) | 128 (18%) | 17 (2%) | 5 | 13 |
| All | All | 14720/19244 (76%) | 12885 (88%) | 1589 (11%) | 246 (2%) | 10 | 21 |

5 of 246 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 18 | AL | 71 | LEU |
| 23 | AY | 314 | PRO |
| 28 | A4 | 252 | PRO |
| 28 | A4 | 450 | PRO |
| 28 | A4 | 542 | PRO |

5.3.2 Protein sidechains [i](#)

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|---------------|------------|----------|-------------|-----|
| 2 | AB | 193/249 (78%) | 193 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|---------------|------------|----------|-------------|-----|
| 3 | AC | 115/143 (80%) | 114 (99%) | 1 (1%) | 75 | 86 |
| 4 | AE | 104/107 (97%) | 103 (99%) | 1 (1%) | 73 | 85 |
| 5 | AI | 104/147 (71%) | 104 (100%) | 0 | 100 | 100 |
| 6 | AJ | 93/118 (79%) | 93 (100%) | 0 | 100 | 100 |
| 7 | AK | 91/113 (80%) | 90 (99%) | 1 (1%) | 70 | 83 |
| 8 | AM | 95/113 (84%) | 95 (100%) | 0 | 100 | 100 |
| 9 | AN | 93/115 (81%) | 93 (100%) | 0 | 100 | 100 |
| 10 | AO | 171/230 (74%) | 171 (100%) | 0 | 100 | 100 |
| 11 | AP | 87/123 (71%) | 87 (100%) | 0 | 100 | 100 |
| 12 | AQ | 78/79 (99%) | 77 (99%) | 1 (1%) | 65 | 80 |
| 13 | AT | 153/157 (98%) | 153 (100%) | 0 | 100 | 100 |
| 14 | AW | 84/158 (53%) | 84 (100%) | 0 | 100 | 100 |
| 15 | AX | 312/351 (89%) | 311 (100%) | 1 (0%) | 91 | 96 |
| 16 | A2 | 99/101 (98%) | 99 (100%) | 0 | 100 | 100 |
| 17 | AH | 112/180 (62%) | 110 (98%) | 2 (2%) | 54 | 75 |
| 18 | AL | 157/226 (70%) | 157 (100%) | 0 | 100 | 100 |
| 19 | AR | 262/318 (82%) | 262 (100%) | 0 | 100 | 100 |
| 20 | AS | 116/164 (71%) | 116 (100%) | 0 | 100 | 100 |
| 21 | AU | 153/174 (88%) | 152 (99%) | 1 (1%) | 81 | 90 |
| 22 | AV | 328/364 (90%) | 324 (99%) | 4 (1%) | 67 | 82 |
| 23 | AY | 111/357 (31%) | 111 (100%) | 0 | 100 | 100 |
| 24 | AZ | 89/95 (94%) | 89 (100%) | 0 | 100 | 100 |
| 25 | A1 | 253/291 (87%) | 250 (99%) | 3 (1%) | 67 | 82 |
| 26 | A0 | 186/190 (98%) | 185 (100%) | 1 (0%) | 86 | 93 |
| 27 | A3 | 66/166 (40%) | 63 (96%) | 3 (4%) | 23 | 48 |
| 28 | A4 | 83/609 (14%) | 83 (100%) | 0 | 100 | 100 |
| 29 | AD | 286/357 (80%) | 285 (100%) | 1 (0%) | 91 | 96 |
| 30 | AF | 185/209 (88%) | 180 (97%) | 5 (3%) | 40 | 64 |
| 31 | AG | 273/342 (80%) | 268 (98%) | 5 (2%) | 54 | 75 |
| 34 | D | 193/245 (79%) | 193 (100%) | 0 | 100 | 100 |
| 35 | F | 217/262 (83%) | 216 (100%) | 1 (0%) | 86 | 93 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|---------------|------------|----------|-------------|-----|
| 36 | H | 88/228 (39%) | 88 (100%) | 0 | 100 | 100 |
| 37 | K | 155/156 (99%) | 155 (100%) | 0 | 100 | 100 |
| 38 | L | 98/124 (79%) | 97 (99%) | 1 (1%) | 73 | 85 |
| 39 | M | 245/249 (98%) | 242 (99%) | 3 (1%) | 67 | 82 |
| 40 | O | 133/150 (89%) | 133 (100%) | 0 | 100 | 100 |
| 41 | R | 118/126 (94%) | 117 (99%) | 1 (1%) | 79 | 88 |
| 42 | S | 141/180 (78%) | 140 (99%) | 1 (1%) | 81 | 90 |
| 43 | T | 146/182 (80%) | 143 (98%) | 3 (2%) | 48 | 70 |
| 44 | W | 91/119 (76%) | 91 (100%) | 0 | 100 | 100 |
| 45 | X | 217/227 (96%) | 211 (97%) | 6 (3%) | 38 | 63 |
| 46 | Y | 159/223 (71%) | 158 (99%) | 1 (1%) | 84 | 91 |
| 47 | Z | 111/147 (76%) | 111 (100%) | 0 | 100 | 100 |
| 48 | 0 | 97/164 (59%) | 97 (100%) | 0 | 100 | 100 |
| 49 | 1 | 49/60 (82%) | 48 (98%) | 1 (2%) | 50 | 72 |
| 50 | 2 | 40/72 (56%) | 40 (100%) | 0 | 100 | 100 |
| 51 | 3 | 88/166 (53%) | 88 (100%) | 0 | 100 | 100 |
| 52 | 4 | 37/89 (42%) | 37 (100%) | 0 | 100 | 100 |
| 53 | 8 | 91/190 (48%) | 91 (100%) | 0 | 100 | 100 |
| 54 | b | 130/135 (96%) | 130 (100%) | 0 | 100 | 100 |
| 55 | e | 188/236 (80%) | 185 (98%) | 3 (2%) | 58 | 77 |
| 56 | g | 122/148 (82%) | 120 (98%) | 2 (2%) | 58 | 77 |
| 57 | i | 86/110 (78%) | 85 (99%) | 1 (1%) | 67 | 82 |
| 58 | j | 74/97 (76%) | 74 (100%) | 0 | 100 | 100 |
| 59 | m | 40/113 (35%) | 40 (100%) | 0 | 100 | 100 |
| 60 | o | 80/87 (92%) | 79 (99%) | 1 (1%) | 65 | 80 |
| 61 | q | 114/178 (64%) | 114 (100%) | 0 | 100 | 100 |
| 62 | r | 147/169 (87%) | 145 (99%) | 2 (1%) | 62 | 79 |
| 63 | J | 138/150 (92%) | 136 (99%) | 2 (1%) | 62 | 79 |
| 64 | I | 164/232 (71%) | 161 (98%) | 3 (2%) | 54 | 75 |
| 65 | N | 189/211 (90%) | 189 (100%) | 0 | 100 | 100 |
| 66 | P | 125/154 (81%) | 123 (98%) | 2 (2%) | 58 | 77 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-------------------|-------------|----------|-------------|-----|
| 67 | U | 126/135 (93%) | 126 (100%) | 0 | 100 | 100 |
| 68 | V | 184/191 (96%) | 184 (100%) | 0 | 100 | 100 |
| 69 | E | 260/290 (90%) | 259 (100%) | 1 (0%) | 89 | 95 |
| 70 | 5 | 353/368 (96%) | 349 (99%) | 4 (1%) | 70 | 83 |
| 71 | 6 | 313/332 (94%) | 312 (100%) | 1 (0%) | 91 | 96 |
| 72 | 7 | 272/303 (90%) | 272 (100%) | 0 | 100 | 100 |
| 73 | 9 | 104/112 (93%) | 103 (99%) | 1 (1%) | 73 | 85 |
| 74 | a | 101/133 (76%) | 101 (100%) | 0 | 100 | 100 |
| 75 | c | 253/288 (88%) | 253 (100%) | 0 | 100 | 100 |
| 76 | d | 224/274 (82%) | 222 (99%) | 2 (1%) | 75 | 86 |
| 77 | f | 122/173 (70%) | 121 (99%) | 1 (1%) | 79 | 88 |
| 78 | h | 104/148 (70%) | 103 (99%) | 1 (1%) | 73 | 85 |
| 79 | k | 81/90 (90%) | 80 (99%) | 1 (1%) | 67 | 82 |
| 80 | l | 67/116 (58%) | 66 (98%) | 1 (2%) | 60 | 78 |
| 81 | p | 134/181 (74%) | 132 (98%) | 2 (2%) | 60 | 78 |
| 82 | s | 336/381 (88%) | 335 (100%) | 1 (0%) | 91 | 96 |
| 83 | Q | 221/256 (86%) | 220 (100%) | 1 (0%) | 86 | 93 |
| 84 | TA | 39/158 (25%) | 39 (100%) | 0 | 100 | 100 |
| 84 | TB | 26/158 (16%) | 26 (100%) | 0 | 100 | 100 |
| 86 | v | 598/630 (95%) | 584 (98%) | 14 (2%) | 45 | 69 |
| All | All | 12561/16442 (76%) | 12466 (99%) | 95 (1%) | 77 | 88 |

5 of 95 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 63 | J | 126 | GLN |
| 76 | d | 205 | GLN |
| 64 | I | 34 | THR |
| 70 | 5 | 46 | LEU |
| 79 | k | 11 | ARG |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 201 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 56 | g | 73 | GLN |
| 67 | U | 74 | HIS |
| 86 | v | 506 | GLN |
| 58 | j | 36 | ASN |
| 62 | r | 146 | GLN |

5.3.3 RNA [i](#)

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1 | AA | 940/954 (98%) | 190 (20%) | 10 (1%) |
| 32 | A | 1523/1559 (97%) | 345 (22%) | 18 (1%) |
| 33 | B | 51/73 (69%) | 6 (11%) | 1 (1%) |
| All | All | 2514/2586 (97%) | 541 (21%) | 29 (1%) |

5 of 541 RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | AA | 650 | U |
| 1 | AA | 651 | A |
| 1 | AA | 663 | A |
| 1 | AA | 676 | G |
| 1 | AA | 680 | U |

5 of 29 RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 32 | A | 1823 | A |
| 32 | A | 3196 | G |
| 32 | A | 2165 | C |
| 32 | A | 2989 | G |
| 32 | A | 1994 | A |

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

144 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 |
| 88 | Y5P | A6 | 13 | 88 | 14,19,20 | 4.26 | 2 (14%) | 18,26,29 | 1.28 | 2 (11%) |
| 88 | Y5P | A7 | 69 | 88 | 14,19,20 | 4.66 | 2 (14%) | 18,26,29 | 1.46 | 3 (16%) |
| 88 | P5P | A6 | 14 | 88 | 15,23,24 | 1.47 | 3 (20%) | 10,33,36 | 0.82 | 0 |
| 88 | Y5P | A6 | 31 | 88 | 14,19,20 | 4.59 | 2 (14%) | 18,26,29 | 1.45 | 3 (16%) |
| 88 | Y5P | A6 | 58 | 88 | 14,19,20 | 4.55 | 2 (14%) | 18,26,29 | 1.41 | 3 (16%) |
| 88 | P5P | A7 | 14 | 88 | 15,23,24 | 1.44 | 3 (20%) | 10,33,36 | 0.79 | 0 |
| 87 | P5P | A5 | 6 | 87 | 15,23,24 | 1.40 | 2 (13%) | 10,33,36 | 1.12 | 1 (10%) |
| 87 | P5P | A5 | 11 | 87 | 15,23,24 | 1.38 | 2 (13%) | 10,33,36 | 0.89 | 1 (10%) |
| 88 | P5P | A6 | 40 | 88 | 15,23,24 | 1.35 | 2 (13%) | 10,33,36 | 1.04 | 1 (10%) |
| 88 | Y5P | A6 | 50 | 88 | 14,19,20 | 4.60 | 2 (14%) | 18,26,29 | 1.38 | 2 (11%) |
| 88 | Y5P | A6 | 65 | 88 | 14,19,20 | 4.42 | 2 (14%) | 18,26,29 | 1.42 | 3 (16%) |
| 88 | P5P | A6 | 6 | 88 | 15,23,24 | 1.42 | 2 (13%) | 10,33,36 | 0.99 | 1 (10%) |
| 88 | P5P | A6 | 11 | 88 | 15,23,24 | 1.37 | 1 (6%) | 10,33,36 | 0.97 | 1 (10%) |
| 88 | Y5P | A6 | 46 | 88 | 14,19,20 | 4.49 | 2 (14%) | 18,26,29 | 1.46 | 3 (16%) |
| 88 | P5P | A6 | 1 | 88 | 15,20,24 | 1.49 | 2 (13%) | 11,29,36 | 0.77 | 0 |
| 88 | Y5P | A7 | 37 | 88 | 14,19,20 | 4.37 | 2 (14%) | 18,26,29 | 1.41 | 3 (16%) |
| 88 | Y5P | A7 | 25 | 88 | 14,19,20 | 4.31 | 2 (14%) | 18,26,29 | 1.39 | 3 (16%) |
| 88 | P5P | A7 | 20 | 88 | 15,23,24 | 1.39 | 2 (13%) | 10,33,36 | 1.09 | 1 (10%) |
| 88 | P5P | A6 | 27 | 88 | 15,23,24 | 1.35 | 1 (6%) | 10,33,36 | 0.80 | 0 |
| 88 | Y5P | A7 | 21 | 88 | 14,19,20 | 4.36 | 2 (14%) | 18,26,29 | 1.45 | 3 (16%) |
| 88 | P5P | A6 | 39 | 88 | 15,23,24 | 1.38 | 2 (13%) | 10,33,36 | 1.07 | 1 (10%) |
| 88 | P5P | A7 | 43 | 88 | 15,23,24 | 1.54 | 2 (13%) | 10,33,36 | 1.16 | 1 (10%) |
| 88 | Y5P | A6 | 68 | 88 | 14,19,20 | 4.78 | 2 (14%) | 18,26,29 | 1.71 | 4 (22%) |
| 88 | Y5P | A6 | 30 | 88 | 14,19,20 | 4.48 | 2 (14%) | 18,26,29 | 1.47 | 3 (16%) |
| 88 | P5P | A6 | 32 | 88 | 15,23,24 | 1.30 | 2 (13%) | 10,33,36 | 0.86 | 0 |
| 88 | Y5P | A7 | 8 | 88 | 14,19,20 | 4.65 | 2 (14%) | 18,26,29 | 1.41 | 3 (16%) |
| 88 | P5P | A7 | 5 | 88 | 15,23,24 | 1.40 | 1 (6%) | 10,33,36 | 0.85 | 1 (10%) |
| 88 | P5P | A7 | 2 | 88 | 15,23,24 | 1.60 | 3 (20%) | 10,33,36 | 0.93 | 1 (10%) |
| 88 | Y5P | A6 | 37 | 88 | 14,19,20 | 4.37 | 2 (14%) | 18,26,29 | 1.40 | 3 (16%) |
| 88 | Y5P | A6 | 38 | 88 | 14,19,20 | 4.33 | 2 (14%) | 18,26,29 | 1.41 | 3 (16%) |
| 88 | Y5P | A6 | 67 | 88 | 14,19,20 | 4.68 | 2 (14%) | 18,26,29 | 1.52 | 3 (16%) |
| 87 | Y5P | A5 | 10 | 87 | 14,19,20 | 4.49 | 2 (14%) | 18,26,29 | 1.46 | 3 (16%) |
| 88 | Y5P | A6 | 66 | 88 | 14,19,20 | 4.54 | 2 (14%) | 18,26,29 | 1.48 | 3 (16%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 88 | P5P | A6 | 7 | 88 | 15,23,24 | 1.44 | 2 (13%) | 10,33,36 | 0.77 | 0 |
| 88 | P5P | A6 | 48 | 88 | 15,23,24 | 1.39 | 2 (13%) | 10,33,36 | 1.38 | 1 (10%) |
| 88 | P5P | A6 | 23 | 88 | 15,23,24 | 1.38 | 2 (13%) | 10,33,36 | 0.84 | 1 (10%) |
| 88 | Y5P | A6 | 53 | 88 | 14,19,20 | 4.69 | 2 (14%) | 18,26,29 | 1.50 | 4 (22%) |
| 88 | Y5P | A6 | 36 | 88 | 14,19,20 | 4.42 | 2 (14%) | 18,26,29 | 1.36 | 3 (16%) |
| 87 | Y5P | A5 | 7 | 87 | 14,19,20 | 4.58 | 2 (14%) | 18,26,29 | 1.43 | 3 (16%) |
| 88 | Y5P | A6 | 12 | 88 | 14,19,20 | 4.33 | 2 (14%) | 18,26,29 | 1.40 | 3 (16%) |
| 87 | Y5P | A5 | 3 | 87 | 14,19,20 | 4.49 | 2 (14%) | 18,26,29 | 1.62 | 3 (16%) |
| 88 | Y5P | A6 | 8 | 88 | 14,19,20 | 4.63 | 2 (14%) | 18,26,29 | 1.40 | 3 (16%) |
| 88 | P5P | A7 | 40 | 88 | 15,23,24 | 1.37 | 2 (13%) | 10,33,36 | 1.02 | 1 (10%) |
| 88 | P5P | A7 | 26 | 88 | 15,23,24 | 1.42 | 2 (13%) | 10,33,36 | 1.11 | 1 (10%) |
| 88 | Y5P | A6 | 29 | 88 | 14,19,20 | 4.37 | 2 (14%) | 18,26,29 | 1.40 | 3 (16%) |
| 88 | Y5P | A7 | 65 | 88 | 14,19,20 | 4.61 | 2 (14%) | 18,26,29 | 1.46 | 3 (16%) |
| 87 | P5P | A5 | 9 | 87 | 15,23,24 | 1.37 | 2 (13%) | 10,33,36 | 0.76 | 0 |
| 88 | Y5P | A6 | 3 | 88 | 14,19,20 | 4.43 | 2 (14%) | 18,26,29 | 1.50 | 3 (16%) |
| 88 | P5P | A7 | 19 | 88 | 15,23,24 | 1.40 | 2 (13%) | 10,33,36 | 1.43 | 2 (20%) |
| 87 | Y5P | A5 | 1 | 87 | 14,19,20 | 4.80 | 2 (14%) | 18,26,29 | 1.85 | 3 (16%) |
| 88 | P5P | A6 | 52 | 88 | 15,23,24 | 1.46 | 2 (13%) | 10,33,36 | 1.35 | 1 (10%) |
| 88 | Y5P | A7 | 61 | 88 | 14,19,20 | 4.46 | 2 (14%) | 18,26,29 | 1.42 | 3 (16%) |
| 88 | P5P | A6 | 19 | 88 | 15,23,24 | 1.37 | 2 (13%) | 10,33,36 | 1.41 | 2 (20%) |
| 88 | P5P | A7 | 41 | 88 | 15,23,24 | 1.41 | 2 (13%) | 10,33,36 | 1.04 | 1 (10%) |
| 88 | Y5P | A6 | 70 | 88 | 14,19,20 | 4.52 | 2 (14%) | 18,26,29 | 1.46 | 2 (11%) |
| 88 | Y5P | A6 | 17 | 88 | 14,19,20 | 4.65 | 2 (14%) | 18,26,29 | 1.42 | 2 (11%) |
| 88 | P5P | A6 | 20 | 88 | 15,23,24 | 1.38 | 2 (13%) | 10,33,36 | 1.10 | 1 (10%) |
| 88 | Y5P | A7 | 64 | 88 | 14,19,20 | 4.53 | 2 (14%) | 18,26,29 | 1.34 | 2 (11%) |
| 88 | Y5P | A6 | 51 | 88 | 14,19,20 | 4.42 | 2 (14%) | 18,26,29 | 1.40 | 3 (16%) |
| 88 | Y5P | A7 | 68 | 88 | 14,19,20 | 4.72 | 2 (14%) | 18,26,29 | 1.69 | 4 (22%) |
| 88 | Y5P | A6 | 9 | 88 | 14,19,20 | 4.66 | 2 (14%) | 18,26,29 | 1.78 | 4 (22%) |
| 88 | Y5P | A6 | 69 | 88 | 14,19,20 | 4.64 | 2 (14%) | 18,26,29 | 1.96 | 6 (33%) |
| 88 | P5P | A7 | 42 | 88 | 15,23,24 | 1.37 | 2 (13%) | 10,33,36 | 1.10 | 0 |
| 88 | Y5P | A7 | 70 | 88 | 14,19,20 | 4.51 | 2 (14%) | 18,26,29 | 1.45 | 2 (11%) |
| 88 | Y5P | A7 | 58 | 88 | 14,19,20 | 4.59 | 2 (14%) | 18,26,29 | 1.48 | 3 (16%) |
| 88 | Y5P | A7 | 24 | 88 | 14,19,20 | 4.16 | 2 (14%) | 18,26,29 | 1.36 | 2 (11%) |
| 88 | P5P | A6 | 10 | 88 | 15,23,24 | 1.40 | 2 (13%) | 10,33,36 | 0.78 | 1 (10%) |
| 88 | Y5P | A6 | 35 | 88 | 14,19,20 | 4.40 | 2 (14%) | 18,26,29 | 1.40 | 3 (16%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|-------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 88 | Y5P | A6 | 63 | 88 | 14,19,20 | 4.62 | 2 (14%) | 18,26,29 | 1.52 | 3 (16%) |
| 88 | P5P | A7 | 27 | 88 | 15,23,24 | 1.36 | 2 (13%) | 10,33,36 | 0.81 | 0 |
| 88 | P5P | A7 | 71 | 88 | 15,23,24 | 1.39 | 2 (13%) | 10,33,36 | 0.92 | 0 |
| 88 | P5P | A6 | 5 | 88 | 15,23,24 | 1.35 | 2 (13%) | 10,33,36 | 0.72 | 0 |
| 88 | Y5P | A7 | 63 | 88 | 14,19,20 | 4.53 | 2 (14%) | 18,26,29 | 1.49 | 3 (16%) |
| 88 | P5P | A7 | 15 | 88 | 15,23,24 | 1.47 | 3 (20%) | 10,33,36 | 1.07 | 1 (10%) |
| 88 | Y5P | A6 | 60 | 88 | 14,19,20 | 4.51 | 2 (14%) | 18,26,29 | 1.54 | 3 (16%) |
| 88 | Y5P | A7 | 67 | 88 | 14,19,20 | 4.66 | 2 (14%) | 18,26,29 | 1.61 | 3 (16%) |
| 88 | Y5P | A7 | 59 | 88 | 14,19,20 | 4.76 | 2 (14%) | 18,26,29 | 1.46 | 3 (16%) |
| 88 | Y5P | A6 | 47 | 88 | 14,19,20 | 4.58 | 2 (14%) | 18,26,29 | 1.51 | 3 (16%) |
| 88 | P5P | A7 | 39 | 88 | 15,23,24 | 1.38 | 2 (13%) | 10,33,36 | 1.08 | 1 (10%) |
| 88 | P5P | A6 | 54 | 88 | 15,23,24 | 1.46 | 2 (13%) | 10,33,36 | 0.98 | 1 (10%) |
| 88 | Y5P | A7 | 47 | 88 | 14,19,20 | 4.59 | 2 (14%) | 18,26,29 | 1.53 | 3 (16%) |
| 88 | P5P | A6 | 4 | 88 | 15,23,24 | 1.38 | 2 (13%) | 10,33,36 | 1.00 | 1 (10%) |
| 88 | Y5P | A7 | 17 | 88 | 14,19,20 | 4.61 | 2 (14%) | 18,26,29 | 1.42 | 2 (11%) |
| 88 | P5P | A6 | 16 | 88 | 15,23,24 | 1.50 | 3 (20%) | 10,33,36 | 1.44 | 2 (20%) |
| 88 | P5P | A6 | 34 | 88 | 15,23,24 | 1.39 | 3 (20%) | 10,33,36 | 0.61 | 0 |
| 88 | P5P | A6 | 42 | 88 | 15,23,24 | 1.36 | 2 (13%) | 10,33,36 | 1.03 | 0 |
| 88 | P5P | A6 | 43 | 88 | 15,23,24 | 1.48 | 2 (13%) | 10,33,36 | 1.08 | 0 |
| 88 | P5P | A7 | 4 | 88 | 15,23,24 | 1.38 | 2 (13%) | 10,33,36 | 1.36 | 2 (20%) |
| 88 | Y5P | A7 | 3 | 88 | 14,19,20 | 4.38 | 2 (14%) | 18,26,29 | 1.50 | 3 (16%) |
| 88 | Y5P | A6 | 64 | 88 | 14,19,20 | 4.52 | 2 (14%) | 18,26,29 | 1.41 | 3 (16%) |
| 87 | Y5P | A5 | 8 | 87 | 14,19,20 | 4.64 | 2 (14%) | 18,26,29 | 1.45 | 3 (16%) |
| 88 | Y5P | A7 | 56 | 88 | 14,19,20 | 4.54 | 2 (14%) | 18,26,29 | 1.48 | 3 (16%) |
| 88 | Y5P | A6 | 59 | 88 | 14,19,20 | 4.79 | 2 (14%) | 18,26,29 | 1.45 | 3 (16%) |
| 88 | P5P | A7 | 18 | 88 | 15,23,24 | 1.50 | 2 (13%) | 10,33,36 | 0.86 | 0 |
| 88 | P5P | A7 | 23 | 88 | 15,23,24 | 1.39 | 2 (13%) | 10,33,36 | 0.86 | 1 (10%) |
| 88 | P5P | A6 | 28 | 88 | 15,23,24 | 1.39 | 2 (13%) | 10,33,36 | 0.98 | 1 (10%) |
| 88 | Y5P | A7 | 12 | 88 | 14,19,20 | 4.27 | 2 (14%) | 18,26,29 | 1.39 | 3 (16%) |
| 88 | P5P | A6 | 71 | 32,88 | 15,23,24 | 1.39 | 2 (13%) | 10,33,36 | 0.73 | 0 |
| 88 | Y5P | A7 | 44 | 88 | 14,19,20 | 4.69 | 2 (14%) | 18,26,29 | 1.45 | 2 (11%) |
| 88 | Y5P | A7 | 62 | 88 | 14,19,20 | 4.40 | 2 (14%) | 18,26,29 | 1.49 | 3 (16%) |
| 88 | P5P | A7 | 54 | 88 | 15,23,24 | 1.46 | 2 (13%) | 10,33,36 | 0.92 | 1 (10%) |
| 88 | Y5P | A7 | 66 | 88 | 14,19,20 | 4.58 | 2 (14%) | 18,26,29 | 1.47 | 2 (11%) |
| 88 | Y5P | A6 | 57 | 88 | 14,19,20 | 4.48 | 2 (14%) | 18,26,29 | 1.42 | 3 (16%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 88 | Y5P | A7 | 55 | 88 | 14,19,20 | 4.47 | 2 (14%) | 18,26,29 | 1.50 | 3 (16%) |
| 88 | Y5P | A7 | 51 | 88 | 14,19,20 | 4.36 | 2 (14%) | 18,26,29 | 1.43 | 3 (16%) |
| 88 | Y5P | A6 | 56 | 88 | 14,19,20 | 4.56 | 2 (14%) | 18,26,29 | 1.45 | 3 (16%) |
| 88 | P5P | A7 | 10 | 88 | 15,23,24 | 1.37 | 2 (13%) | 10,33,36 | 0.81 | 1 (10%) |
| 88 | P5P | A7 | 1 | 88 | 15,20,24 | 1.49 | 2 (13%) | 11,29,36 | 0.64 | 0 |
| 88 | Y5P | A6 | 62 | 88 | 14,19,20 | 4.57 | 2 (14%) | 18,26,29 | 1.50 | 3 (16%) |
| 87 | P5P | A5 | 5 | 87 | 15,23,24 | 1.41 | 2 (13%) | 10,33,36 | 0.81 | 0 |
| 88 | P5P | A6 | 26 | 88 | 15,23,24 | 1.44 | 2 (13%) | 10,33,36 | 1.12 | 1 (10%) |
| 88 | Y5P | A6 | 55 | 88 | 14,19,20 | 4.52 | 2 (14%) | 18,26,29 | 1.52 | 3 (16%) |
| 88 | Y5P | A6 | 33 | 88 | 14,19,20 | 4.41 | 2 (14%) | 18,26,29 | 1.44 | 3 (16%) |
| 88 | Y5P | A7 | 60 | 88 | 14,19,20 | 4.45 | 2 (14%) | 18,26,29 | 1.56 | 2 (11%) |
| 88 | P5P | A7 | 48 | 88 | 15,23,24 | 1.41 | 2 (13%) | 10,33,36 | 1.57 | 2 (20%) |
| 88 | Y5P | A6 | 61 | 88 | 14,19,20 | 4.57 | 2 (14%) | 18,26,29 | 1.48 | 3 (16%) |
| 88 | P5P | A7 | 6 | 88 | 15,23,24 | 1.38 | 2 (13%) | 10,33,36 | 1.63 | 2 (20%) |
| 88 | Y5P | A6 | 24 | 88 | 14,19,20 | 4.16 | 2 (14%) | 18,26,29 | 1.36 | 2 (11%) |
| 88 | Y5P | A7 | 9 | 88 | 14,19,20 | 4.67 | 2 (14%) | 18,26,29 | 1.78 | 3 (16%) |
| 88 | Y5P | A6 | 22 | 88 | 14,19,20 | 4.29 | 2 (14%) | 18,26,29 | 1.40 | 3 (16%) |
| 87 | P5P | A5 | 2 | 87 | 15,23,24 | 1.50 | 2 (13%) | 10,33,36 | 0.92 | 1 (10%) |
| 88 | P5P | A6 | 18 | 88 | 15,23,24 | 1.49 | 2 (13%) | 10,33,36 | 0.90 | 0 |
| 88 | P5P | A7 | 7 | 88 | 15,23,24 | 1.39 | 2 (13%) | 10,33,36 | 1.11 | 1 (10%) |
| 88 | Y5P | A7 | 22 | 88 | 14,19,20 | 4.29 | 2 (14%) | 18,26,29 | 1.42 | 3 (16%) |
| 88 | P5P | A6 | 15 | 88 | 15,23,24 | 1.46 | 3 (20%) | 10,33,36 | 1.17 | 1 (10%) |
| 88 | Y5P | A7 | 57 | 88 | 14,19,20 | 4.46 | 2 (14%) | 18,26,29 | 1.45 | 3 (16%) |
| 88 | P5P | A6 | 2 | 88 | 15,23,24 | 1.45 | 2 (13%) | 10,33,36 | 0.86 | 1 (10%) |
| 88 | Y5P | A7 | 46 | 88 | 14,19,20 | 4.51 | 2 (14%) | 18,26,29 | 1.48 | 3 (16%) |
| 88 | P5P | A7 | 52 | 88 | 15,23,24 | 1.45 | 2 (13%) | 10,33,36 | 1.32 | 1 (10%) |
| 88 | Y5P | A6 | 44 | 88 | 14,19,20 | 4.68 | 2 (14%) | 18,26,29 | 1.46 | 2 (11%) |
| 88 | Y5P | A7 | 50 | 88 | 14,19,20 | 4.54 | 2 (14%) | 18,26,29 | 1.39 | 2 (11%) |
| 88 | Y5P | A7 | 13 | 88 | 14,19,20 | 4.20 | 2 (14%) | 18,26,29 | 1.28 | 2 (11%) |
| 88 | P5P | A6 | 45 | 88 | 15,23,24 | 1.36 | 2 (13%) | 10,33,36 | 0.97 | 0 |
| 88 | P5P | A7 | 49 | 88 | 15,23,24 | 1.41 | 2 (13%) | 10,33,36 | 1.04 | 1 (10%) |
| 88 | P5P | A7 | 11 | 88 | 15,23,24 | 1.40 | 2 (13%) | 10,33,36 | 1.01 | 1 (10%) |
| 88 | P5P | A7 | 16 | 88 | 15,23,24 | 1.48 | 3 (20%) | 10,33,36 | 1.48 | 2 (20%) |
| 88 | P5P | A7 | 45 | 88 | 15,23,24 | 1.36 | 2 (13%) | 10,33,36 | 0.87 | 0 |
| 88 | Y5P | A6 | 25 | 88 | 14,19,20 | 4.34 | 2 (14%) | 18,26,29 | 1.40 | 3 (16%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 88 | Y5P | A7 | 53 | 88 | 14,19,20 | 4.66 | 2 (14%) | 18,26,29 | 1.55 | 3 (16%) |
| 87 | Y5P | A5 | 4 | 87 | 14,19,20 | 4.79 | 2 (14%) | 18,26,29 | 1.82 | 3 (16%) |
| 88 | Y5P | A7 | 38 | 88 | 14,19,20 | 4.36 | 2 (14%) | 18,26,29 | 1.40 | 3 (16%) |
| 88 | Y5P | A6 | 21 | 88 | 14,19,20 | 4.38 | 2 (14%) | 18,26,29 | 1.38 | 3 (16%) |
| 88 | P5P | A6 | 49 | 88 | 15,23,24 | 1.39 | 2 (13%) | 10,33,36 | 1.15 | 1 (10%) |
| 88 | P5P | A6 | 41 | 88 | 15,23,24 | 1.39 | 2 (13%) | 10,33,36 | 1.01 | 1 (10%) |

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 |
|-----|------|-------|-----|------|---------|-----------|---------|
| 88 | Y5P | A6 | 13 | 88 | - | 3/7/33/34 | 0/2/2/2 |
| 88 | Y5P | A7 | 69 | 88 | - | 1/7/33/34 | 0/2/2/2 |
| 88 | P5P | A6 | 14 | 88 | - | 2/3/25/26 | 0/3/3/3 |
| 88 | Y5P | A6 | 31 | 88 | - | 1/7/33/34 | 0/2/2/2 |
| 88 | Y5P | A6 | 58 | 88 | - | 3/7/33/34 | 0/2/2/2 |
| 88 | P5P | A7 | 14 | 88 | - | 2/3/25/26 | 0/3/3/3 |
| 87 | P5P | A5 | 6 | 87 | - | 0/3/25/26 | 0/3/3/3 |
| 87 | P5P | A5 | 11 | 87 | - | 0/3/25/26 | 0/3/3/3 |
| 88 | P5P | A6 | 40 | 88 | - | 0/3/25/26 | 0/3/3/3 |
| 88 | Y5P | A6 | 50 | 88 | - | 4/7/33/34 | 0/2/2/2 |
| 88 | Y5P | A6 | 65 | 88 | - | 1/7/33/34 | 0/2/2/2 |
| 88 | P5P | A6 | 6 | 88 | - | 3/3/25/26 | 0/3/3/3 |
| 88 | P5P | A6 | 11 | 88 | - | 0/3/25/26 | 0/3/3/3 |
| 88 | Y5P | A6 | 46 | 88 | - | 3/7/33/34 | 0/2/2/2 |
| 88 | P5P | A6 | 1 | 88 | - | 0/2/22/26 | 0/3/3/3 |
| 88 | Y5P | A7 | 37 | 88 | - | 1/7/33/34 | 0/2/2/2 |
| 88 | Y5P | A7 | 25 | 88 | - | 1/7/33/34 | 0/2/2/2 |
| 88 | P5P | A7 | 20 | 88 | - | 0/3/25/26 | 0/3/3/3 |
| 88 | P5P | A6 | 27 | 88 | - | 0/3/25/26 | 0/3/3/3 |
| 88 | Y5P | A7 | 21 | 88 | - | 3/7/33/34 | 0/2/2/2 |
| 88 | P5P | A6 | 39 | 88 | - | 0/3/25/26 | 0/3/3/3 |
| 88 | P5P | A7 | 43 | 88 | - | 3/3/25/26 | 0/3/3/3 |
| 88 | Y5P | A6 | 68 | 88 | - | 1/7/33/34 | 0/2/2/2 |
| 88 | Y5P | A6 | 30 | 88 | - | 1/7/33/34 | 0/2/2/2 |
| 88 | P5P | A6 | 32 | 88 | - | 0/3/25/26 | 0/3/3/3 |
| 88 | Y5P | A7 | 8 | 88 | - | 1/7/33/34 | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|-----------|---------|
| 88 | P5P | A7 | 5 | 88 | - | 2/3/25/26 | 0/3/3/3 |
| 88 | P5P | A7 | 2 | 88 | - | 0/3/25/26 | 0/3/3/3 |
| 88 | Y5P | A6 | 37 | 88 | - | 1/7/33/34 | 0/2/2/2 |
| 88 | Y5P | A6 | 38 | 88 | - | 1/7/33/34 | 0/2/2/2 |
| 88 | Y5P | A6 | 67 | 88 | - | 1/7/33/34 | 0/2/2/2 |
| 87 | Y5P | A5 | 10 | 87 | - | 1/7/33/34 | 0/2/2/2 |
| 88 | Y5P | A6 | 66 | 88 | - | 1/7/33/34 | 0/2/2/2 |
| 88 | P5P | A6 | 7 | 88 | - | 3/3/25/26 | 0/3/3/3 |
| 88 | P5P | A6 | 48 | 88 | - | 0/3/25/26 | 0/3/3/3 |
| 88 | P5P | A6 | 23 | 88 | - | 0/3/25/26 | 0/3/3/3 |
| 88 | Y5P | A6 | 53 | 88 | - | 3/7/33/34 | 0/2/2/2 |
| 88 | Y5P | A6 | 36 | 88 | - | 1/7/33/34 | 0/2/2/2 |
| 87 | Y5P | A5 | 7 | 87 | - | 3/7/33/34 | 0/2/2/2 |
| 88 | Y5P | A6 | 12 | 88 | - | 3/7/33/34 | 0/2/2/2 |
| 87 | Y5P | A5 | 3 | 87 | - | 4/7/33/34 | 0/2/2/2 |
| 88 | Y5P | A6 | 8 | 88 | - | 1/7/33/34 | 0/2/2/2 |
| 88 | P5P | A7 | 40 | 88 | - | 0/3/25/26 | 0/3/3/3 |
| 88 | P5P | A7 | 26 | 88 | - | 0/3/25/26 | 0/3/3/3 |
| 88 | Y5P | A6 | 29 | 88 | - | 1/7/33/34 | 0/2/2/2 |
| 88 | Y5P | A7 | 65 | 88 | - | 2/7/33/34 | 0/2/2/2 |
| 87 | P5P | A5 | 9 | 87 | - | 0/3/25/26 | 0/3/3/3 |
| 88 | Y5P | A6 | 3 | 88 | - | 1/7/33/34 | 0/2/2/2 |
| 88 | P5P | A7 | 19 | 88 | - | 0/3/25/26 | 0/3/3/3 |
| 87 | Y5P | A5 | 1 | 87 | - | 7/7/33/34 | 0/2/2/2 |
| 88 | P5P | A6 | 52 | 88 | - | 3/3/25/26 | 0/3/3/3 |
| 88 | Y5P | A7 | 61 | 88 | - | 1/7/33/34 | 0/2/2/2 |
| 88 | P5P | A6 | 19 | 88 | - | 0/3/25/26 | 0/3/3/3 |
| 88 | P5P | A7 | 41 | 88 | - | 0/3/25/26 | 0/3/3/3 |
| 88 | Y5P | A6 | 70 | 88 | - | 3/7/33/34 | 0/2/2/2 |
| 88 | Y5P | A6 | 17 | 88 | - | 3/7/33/34 | 0/2/2/2 |
| 88 | P5P | A6 | 20 | 88 | - | 0/3/25/26 | 0/3/3/3 |
| 88 | Y5P | A7 | 64 | 88 | - | 3/7/33/34 | 0/2/2/2 |
| 88 | Y5P | A6 | 51 | 88 | - | 2/7/33/34 | 0/2/2/2 |
| 88 | Y5P | A7 | 68 | 88 | - | 1/7/33/34 | 0/2/2/2 |
| 88 | Y5P | A6 | 9 | 88 | - | 5/7/33/34 | 0/2/2/2 |
| 88 | Y5P | A6 | 69 | 88 | - | 3/7/33/34 | 0/2/2/2 |
| 88 | P5P | A7 | 42 | 88 | - | 0/3/25/26 | 0/3/3/3 |
| 88 | Y5P | A7 | 70 | 88 | - | 3/7/33/34 | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|-------|---------|-----------|---------|
| 88 | Y5P | A7 | 58 | 88 | - | 3/7/33/34 | 0/2/2/2 |
| 88 | Y5P | A7 | 24 | 88 | - | 1/7/33/34 | 0/2/2/2 |
| 88 | P5P | A6 | 10 | 88 | - | 0/3/25/26 | 0/3/3/3 |
| 88 | Y5P | A6 | 35 | 88 | - | 1/7/33/34 | 0/2/2/2 |
| 88 | Y5P | A6 | 63 | 88 | - | 1/7/33/34 | 0/2/2/2 |
| 88 | P5P | A7 | 27 | 88 | - | 1/3/25/26 | 0/3/3/3 |
| 88 | P5P | A7 | 71 | 88 | - | 1/3/25/26 | 0/3/3/3 |
| 88 | P5P | A6 | 5 | 88 | - | 2/3/25/26 | 0/3/3/3 |
| 88 | Y5P | A7 | 63 | 88 | - | 1/7/33/34 | 0/2/2/2 |
| 88 | P5P | A7 | 15 | 88 | - | 0/3/25/26 | 0/3/3/3 |
| 88 | Y5P | A6 | 60 | 88 | - | 2/7/33/34 | 0/2/2/2 |
| 88 | Y5P | A7 | 67 | 88 | - | 1/7/33/34 | 0/2/2/2 |
| 88 | Y5P | A7 | 59 | 88 | - | 1/7/33/34 | 0/2/2/2 |
| 88 | Y5P | A6 | 47 | 88 | - | 1/7/33/34 | 0/2/2/2 |
| 88 | P5P | A7 | 39 | 88 | - | 0/3/25/26 | 0/3/3/3 |
| 88 | P5P | A6 | 54 | 88 | - | 1/3/25/26 | 0/3/3/3 |
| 88 | Y5P | A7 | 47 | 88 | - | 1/7/33/34 | 0/2/2/2 |
| 88 | P5P | A6 | 4 | 88 | - | 0/3/25/26 | 0/3/3/3 |
| 88 | Y5P | A7 | 17 | 88 | - | 2/7/33/34 | 0/2/2/2 |
| 88 | P5P | A6 | 16 | 88 | - | 2/3/25/26 | 0/3/3/3 |
| 88 | P5P | A6 | 34 | 88 | - | 0/3/25/26 | 0/3/3/3 |
| 88 | P5P | A6 | 42 | 88 | - | 0/3/25/26 | 0/3/3/3 |
| 88 | P5P | A6 | 43 | 88 | - | 3/3/25/26 | 0/3/3/3 |
| 88 | P5P | A7 | 4 | 88 | - | 0/3/25/26 | 0/3/3/3 |
| 88 | Y5P | A7 | 3 | 88 | - | 1/7/33/34 | 0/2/2/2 |
| 88 | Y5P | A6 | 64 | 88 | - | 1/7/33/34 | 0/2/2/2 |
| 87 | Y5P | A5 | 8 | 87 | - | 3/7/33/34 | 0/2/2/2 |
| 88 | Y5P | A7 | 56 | 88 | - | 4/7/33/34 | 0/2/2/2 |
| 88 | Y5P | A6 | 59 | 88 | - | 1/7/33/34 | 0/2/2/2 |
| 88 | P5P | A7 | 18 | 88 | - | 1/3/25/26 | 0/3/3/3 |
| 88 | P5P | A7 | 23 | 88 | - | 0/3/25/26 | 0/3/3/3 |
| 88 | P5P | A6 | 28 | 88 | - | 2/3/25/26 | 0/3/3/3 |
| 88 | Y5P | A7 | 12 | 88 | - | 3/7/33/34 | 0/2/2/2 |
| 88 | P5P | A6 | 71 | 32,88 | - | 1/3/25/26 | 0/3/3/3 |
| 88 | Y5P | A7 | 44 | 88 | - | 2/7/33/34 | 0/2/2/2 |
| 88 | Y5P | A7 | 62 | 88 | - | 1/7/33/34 | 0/2/2/2 |
| 88 | P5P | A7 | 54 | 88 | - | 1/3/25/26 | 0/3/3/3 |
| 88 | Y5P | A7 | 66 | 88 | - | 1/7/33/34 | 0/2/2/2 |
| 88 | Y5P | A6 | 57 | 88 | - | 1/7/33/34 | 0/2/2/2 |
| 88 | Y5P | A7 | 55 | 88 | - | 1/7/33/34 | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|-----------|---------|
| 88 | Y5P | A7 | 51 | 88 | - | 2/7/33/34 | 0/2/2/2 |
| 88 | Y5P | A6 | 56 | 88 | - | 4/7/33/34 | 0/2/2/2 |
| 88 | P5P | A7 | 10 | 88 | - | 0/3/25/26 | 0/3/3/3 |
| 88 | P5P | A7 | 1 | 88 | - | 0/2/22/26 | 0/3/3/3 |
| 88 | Y5P | A6 | 62 | 88 | - | 1/7/33/34 | 0/2/2/2 |
| 87 | P5P | A5 | 5 | 87 | - | 2/3/25/26 | 0/3/3/3 |
| 88 | P5P | A6 | 26 | 88 | - | 0/3/25/26 | 0/3/3/3 |
| 88 | Y5P | A6 | 55 | 88 | - | 3/7/33/34 | 0/2/2/2 |
| 88 | Y5P | A6 | 33 | 88 | - | 3/7/33/34 | 0/2/2/2 |
| 88 | Y5P | A7 | 60 | 88 | - | 1/7/33/34 | 0/2/2/2 |
| 88 | P5P | A7 | 48 | 88 | - | 0/3/25/26 | 0/3/3/3 |
| 88 | Y5P | A6 | 61 | 88 | - | 1/7/33/34 | 0/2/2/2 |
| 88 | P5P | A7 | 6 | 88 | - | 3/3/25/26 | 0/3/3/3 |
| 88 | Y5P | A6 | 24 | 88 | - | 1/7/33/34 | 0/2/2/2 |
| 88 | Y5P | A7 | 9 | 88 | - | 3/7/33/34 | 0/2/2/2 |
| 88 | Y5P | A6 | 22 | 88 | - | 3/7/33/34 | 0/2/2/2 |
| 87 | P5P | A5 | 2 | 87 | - | 2/3/25/26 | 0/3/3/3 |
| 88 | P5P | A6 | 18 | 88 | - | 1/3/25/26 | 0/3/3/3 |
| 88 | P5P | A7 | 7 | 88 | - | 3/3/25/26 | 0/3/3/3 |
| 88 | Y5P | A7 | 22 | 88 | - | 3/7/33/34 | 0/2/2/2 |
| 88 | P5P | A6 | 15 | 88 | - | 0/3/25/26 | 0/3/3/3 |
| 88 | Y5P | A7 | 57 | 88 | - | 1/7/33/34 | 0/2/2/2 |
| 88 | P5P | A6 | 2 | 88 | - | 1/3/25/26 | 0/3/3/3 |
| 88 | Y5P | A7 | 46 | 88 | - | 3/7/33/34 | 0/2/2/2 |
| 88 | P5P | A7 | 52 | 88 | - | 3/3/25/26 | 0/3/3/3 |
| 88 | Y5P | A6 | 44 | 88 | - | 2/7/33/34 | 0/2/2/2 |
| 88 | Y5P | A7 | 50 | 88 | - | 4/7/33/34 | 0/2/2/2 |
| 88 | Y5P | A7 | 13 | 88 | - | 1/7/33/34 | 0/2/2/2 |
| 88 | P5P | A6 | 45 | 88 | - | 2/3/25/26 | 0/3/3/3 |
| 88 | P5P | A7 | 49 | 88 | - | 0/3/25/26 | 0/3/3/3 |
| 88 | P5P | A7 | 11 | 88 | - | 0/3/25/26 | 0/3/3/3 |
| 88 | P5P | A7 | 16 | 88 | - | 2/3/25/26 | 0/3/3/3 |
| 88 | P5P | A7 | 45 | 88 | - | 2/3/25/26 | 0/3/3/3 |
| 88 | Y5P | A6 | 25 | 88 | - | 1/7/33/34 | 0/2/2/2 |
| 88 | Y5P | A7 | 53 | 88 | - | 4/7/33/34 | 0/2/2/2 |
| 87 | Y5P | A5 | 4 | 87 | - | 7/7/33/34 | 0/2/2/2 |
| 88 | Y5P | A7 | 38 | 88 | - | 2/7/33/34 | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|-----------|---------|
| 88 | Y5P | A6 | 21 | 88 | - | 3/7/33/34 | 0/2/2/2 |
| 88 | P5P | A6 | 49 | 88 | - | 0/3/25/26 | 0/3/3/3 |
| 88 | P5P | A6 | 41 | 88 | - | 0/3/25/26 | 0/3/3/3 |

The worst 5 of 293 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 88 | A6 | 69 | Y5P | C4-N3 | -14.56 | 1.32 | 1.46 |
| 88 | A6 | 53 | Y5P | C4-N3 | -13.91 | 1.33 | 1.46 |
| 88 | A6 | 8 | Y5P | C4-N3 | -13.70 | 1.33 | 1.46 |
| 88 | A7 | 53 | Y5P | C4-N3 | -13.56 | 1.33 | 1.46 |
| 88 | A7 | 67 | Y5P | C4-N3 | -13.50 | 1.33 | 1.46 |

The worst 5 of 282 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|------|-------------|----------|
| 88 | A6 | 69 | Y5P | C5-C4-N3 | 5.02 | 122.24 | 114.15 |
| 88 | A6 | 67 | Y5P | C5-C4-N3 | 4.88 | 122.02 | 114.15 |
| 88 | A6 | 44 | Y5P | C5-C4-N3 | 4.85 | 121.96 | 114.15 |
| 88 | A7 | 44 | Y5P | C5-C4-N3 | 4.82 | 121.93 | 114.15 |
| 88 | A7 | 67 | Y5P | C5-C4-N3 | 4.82 | 121.92 | 114.15 |

There are no chirality outliers.

5 of 220 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 87 | A5 | 1 | Y5P | O4'-C4'-C5'-O5' |
| 87 | A5 | 1 | Y5P | C3'-C4'-C5'-O5' |
| 87 | A5 | 2 | P5P | O4'-C4'-C5'-O5' |
| 87 | A5 | 4 | Y5P | O4'-C4'-C5'-O5' |
| 87 | A5 | 4 | Y5P | C3'-C4'-C5'-O5' |

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [\(i\)](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 139 ligands modelled in this entry, 137 are monoatomic - leaving 2 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 |
| 92 | GCP | v | 802 | 89 | 27,34,34 | 1.81 | 5 (18%) | 35,54,54 | 2.39 | 10 (28%) |
| 91 | GDP | AX | 500 | - | 25,30,30 | 1.00 | 1 (4%) | 30,47,47 | 1.05 | 2 (6%) |

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 |
|-----|------|-------|-----|------|---------|------------|---------|
| 92 | GCP | v | 802 | 89 | - | 5/15/38/38 | 0/3/3/3 |
| 91 | GDP | AX | 500 | - | - | 1/12/32/32 | 0/3/3/3 |

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

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 92 | v | 802 | GCP | PG-O1G | 5.57 | 1.61 | 1.50 |
| 92 | v | 802 | GCP | C5-C6 | 4.39 | 1.49 | 1.41 |
| 92 | v | 802 | GCP | PG-O3G | 3.04 | 1.61 | 1.55 |
| 92 | v | 802 | GCP | PG-O2G | -2.64 | 1.49 | 1.55 |
| 91 | AX | 500 | GDP | C6-N1 | -2.23 | 1.34 | 1.37 |

The worst 5 of 12 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 92 | v | 802 | GCP | PB-O3A-PA | -5.90 | 113.11 | 132.37 |
| 92 | v | 802 | GCP | C2-N1-C6 | 5.26 | 123.27 | 115.96 |
| 92 | v | 802 | GCP | C2-N3-C4 | 4.77 | 120.62 | 115.48 |
| 92 | v | 802 | GCP | N3-C2-N1 | -4.14 | 121.95 | 127.21 |
| 92 | v | 802 | GCP | O4'-C1'-N9 | 4.10 | 114.18 | 108.75 |

There are no chirality outliers.

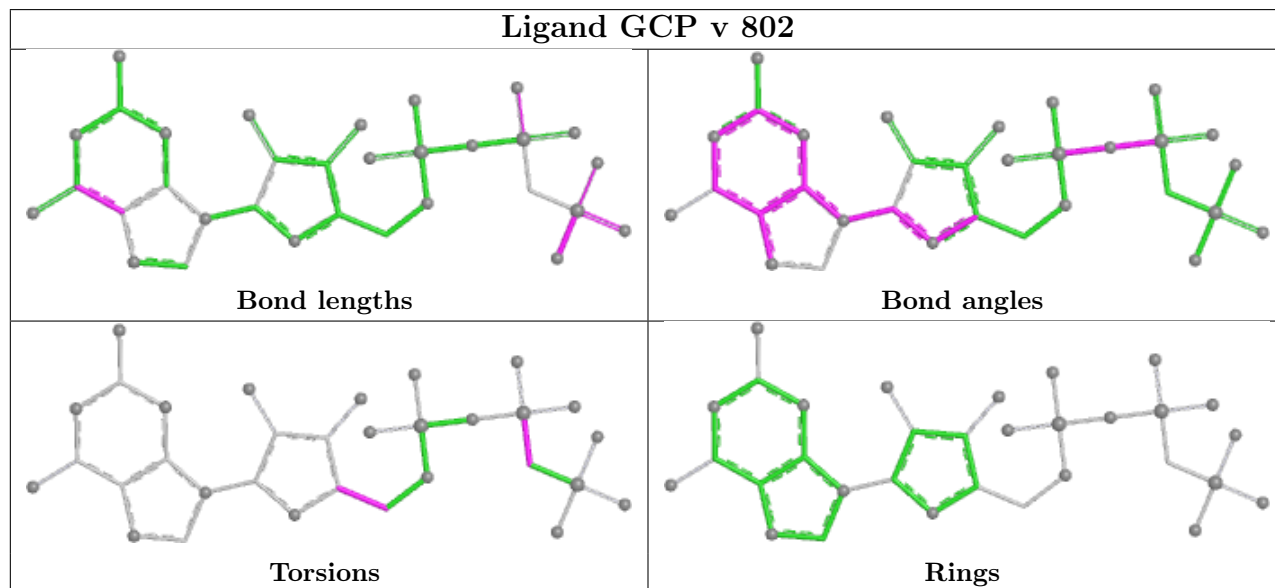
5 of 6 torsion outliers are listed below:

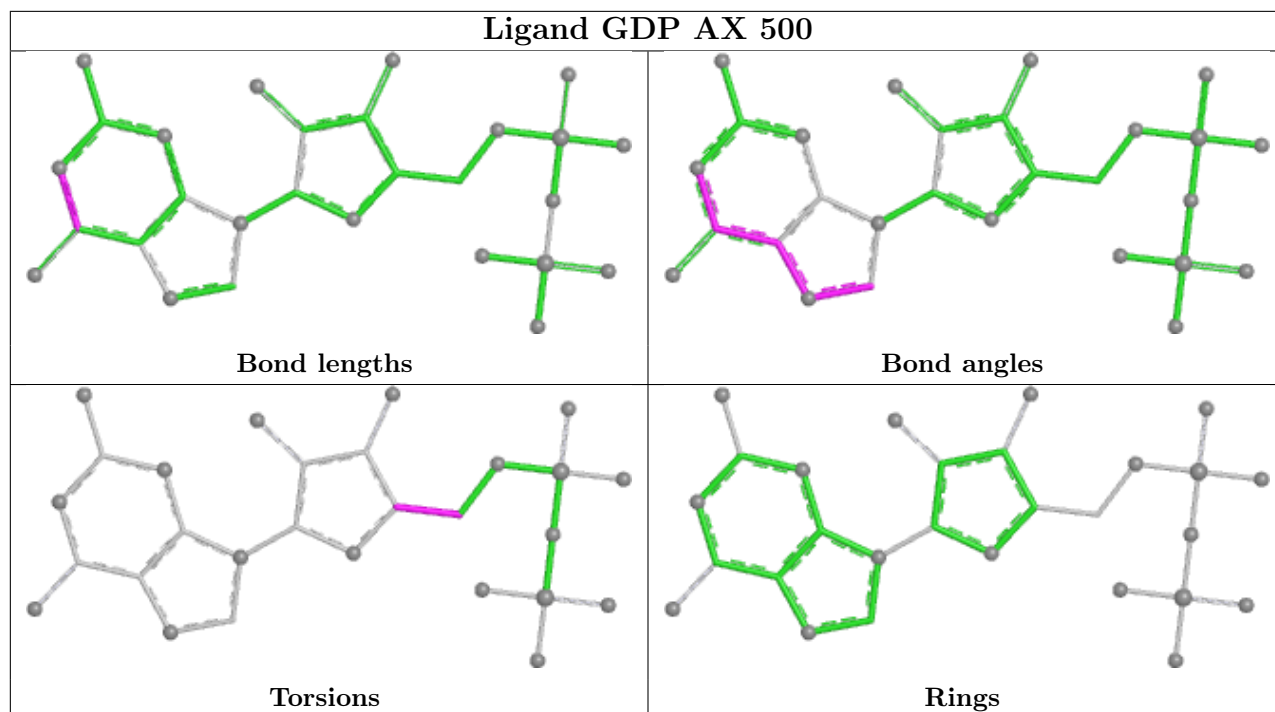
| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 92 | v | 802 | GCP | PG-C3B-PB-O1B |
| 92 | v | 802 | GCP | PG-C3B-PB-O3A |
| 92 | v | 802 | GCP | O4'-C4'-C5'-O5' |
| 92 | v | 802 | GCP | C3'-C4'-C5'-O5' |
| 92 | v | 802 | GCP | PG-C3B-PB-O2B |

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 |
|-----|-------|------------------|
| 85 | 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 | 48.04 |
| 1 | u | 106:UNK | C | 301:UNK | N | 30.88 |
| 1 | u | 315:UNK | C | 399:UNK | N | 19.09 |
| 1 | u | 615:UNK | C | 700:UNK | N | 18.25 |

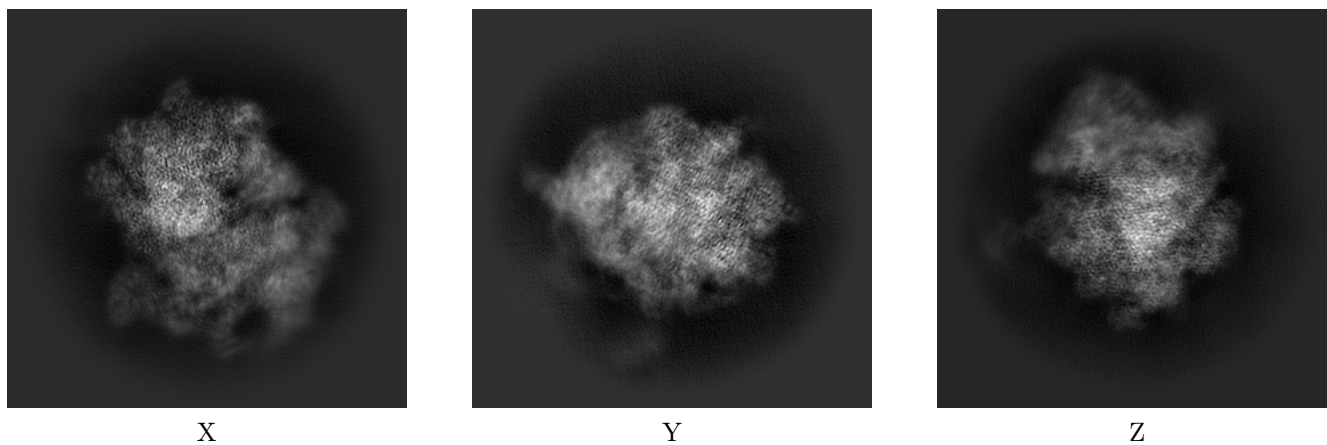
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21242. 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](#)

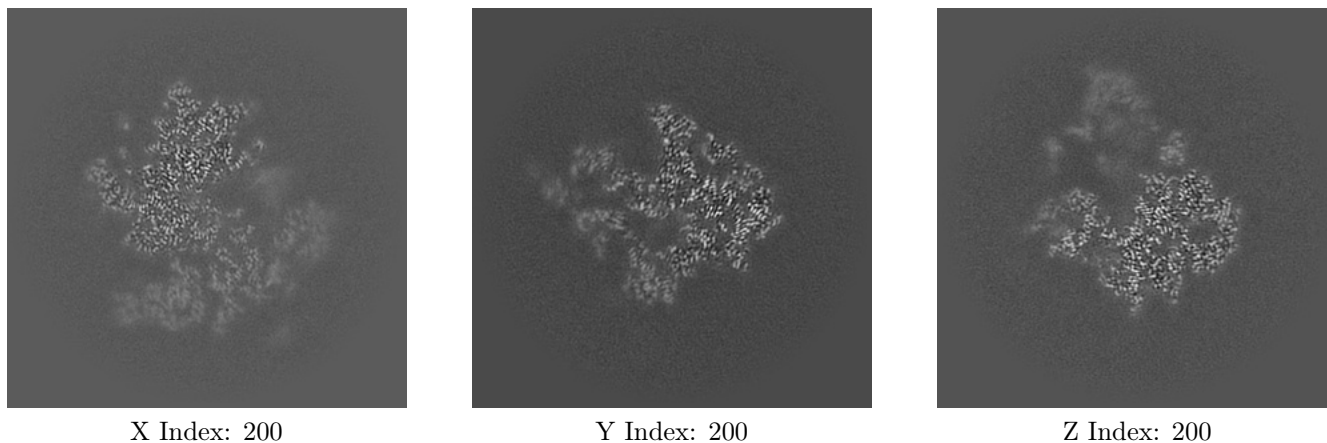
6.1.1 Primary map



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

6.2 Central slices [i](#)

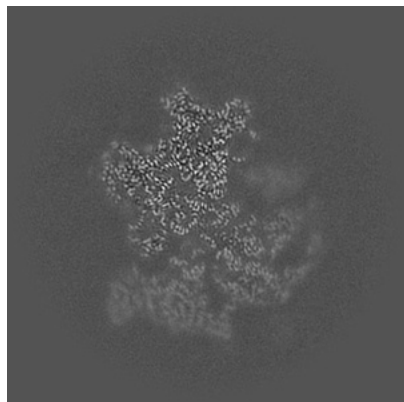
6.2.1 Primary map



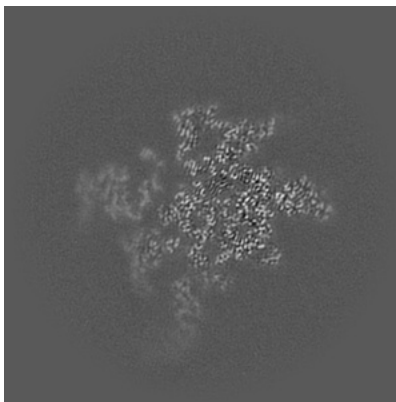
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

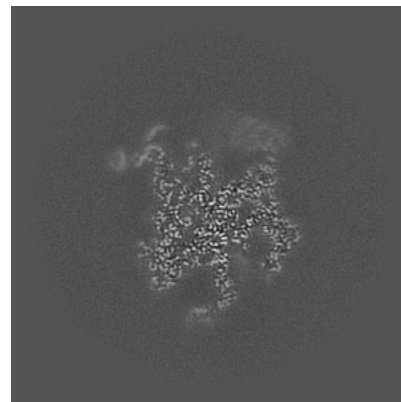
6.3.1 Primary map



X Index: 210



Y Index: 172

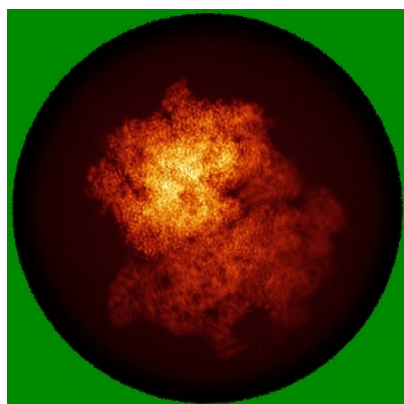


Z Index: 242

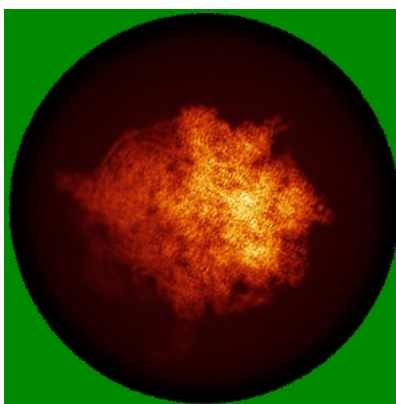
The images above show the largest variance slices of the map in three orthogonal directions.

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

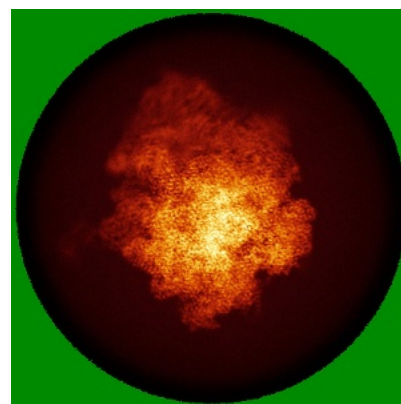
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.267. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

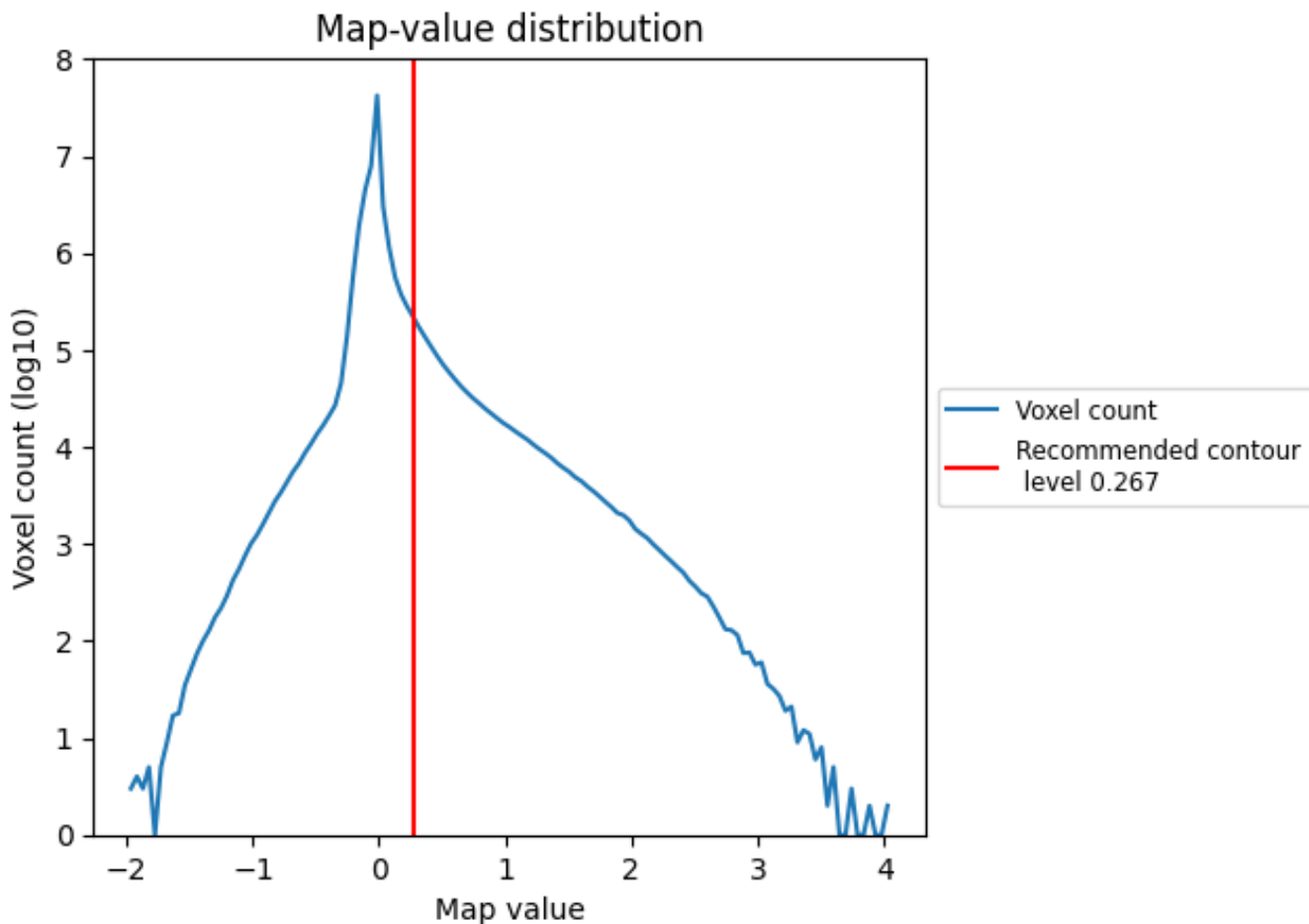
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

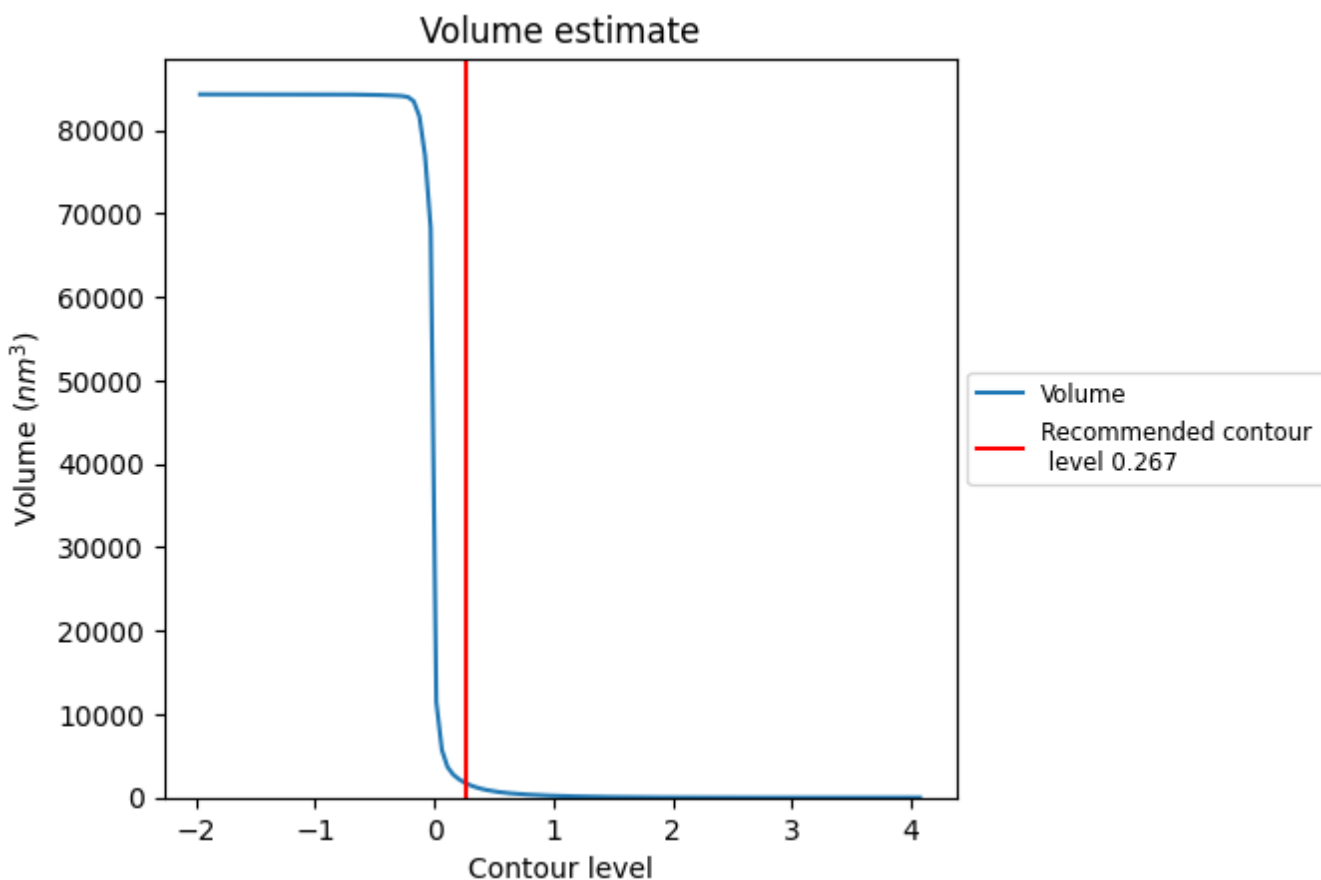
This section contains the results of statistical analysis of the map.

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.

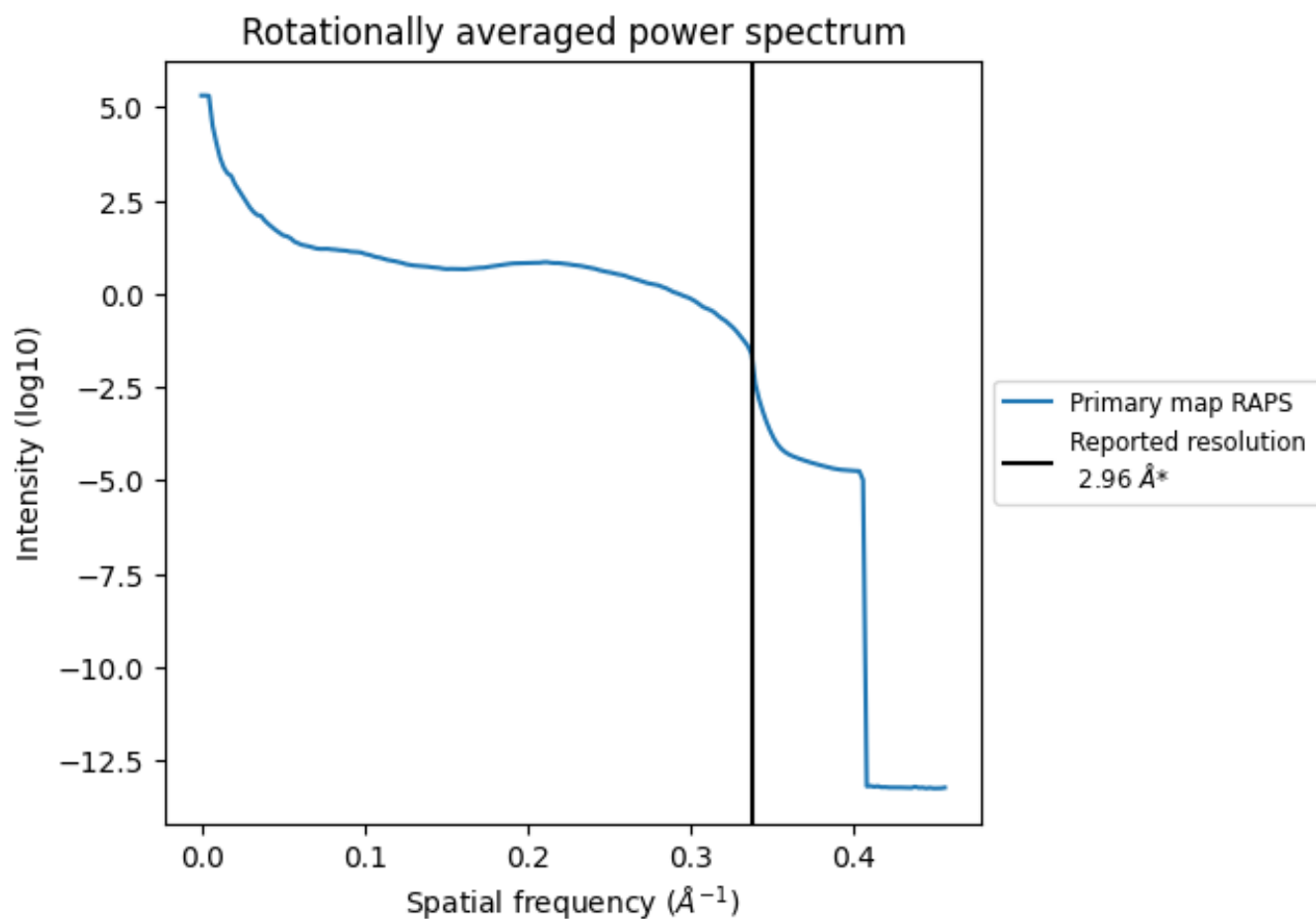
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1709 nm³; this corresponds to an approximate mass of 1544 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)



*Reported resolution corresponds to spatial frequency of 0.338 Å⁻¹

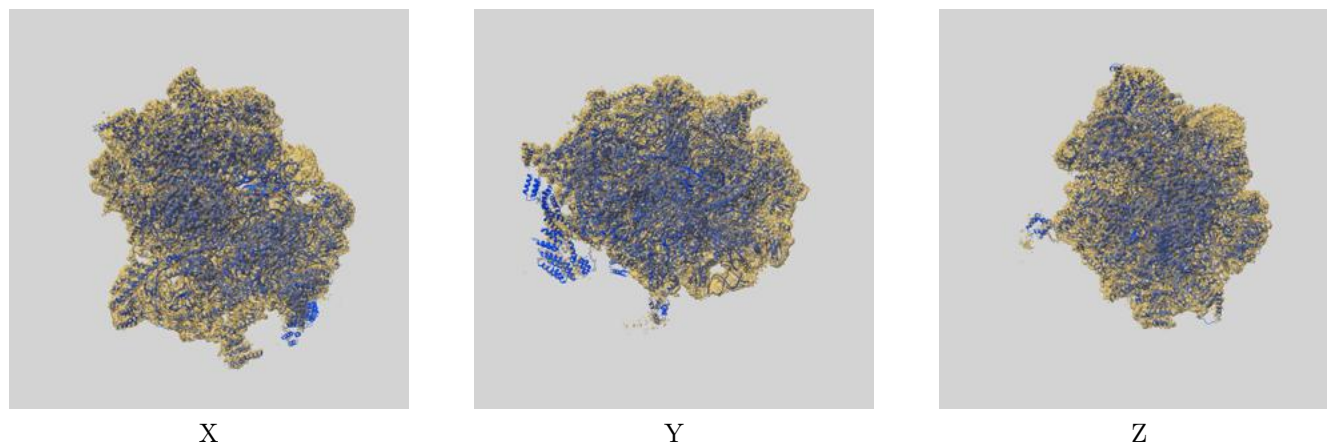
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

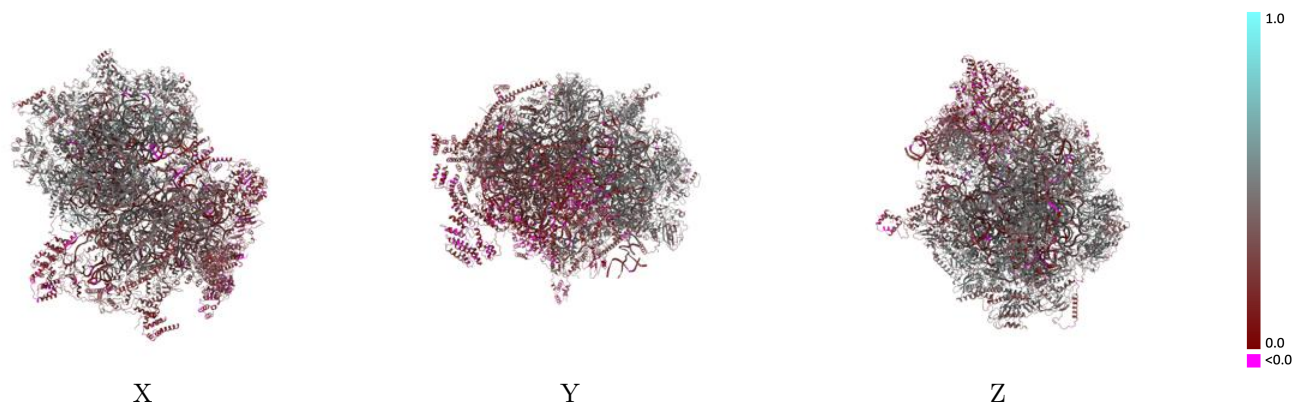
This section contains information regarding the fit between EMDB map EMD-21242 and PDB model 6VMI. Per-residue inclusion information can be found in section 3 on page 22.

9.1 Map-model overlay [i](#)



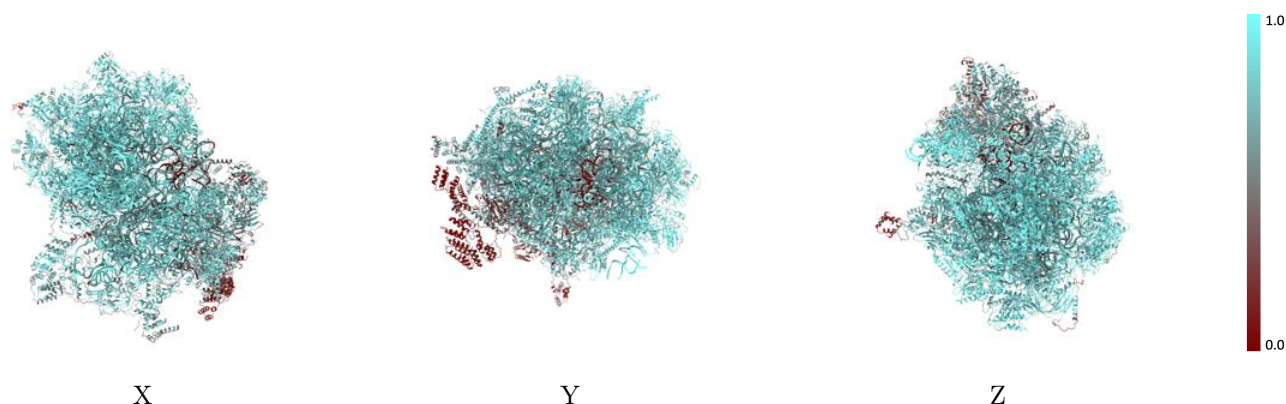
The images above show the 3D surface view of the map at the recommended contour level 0.267 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



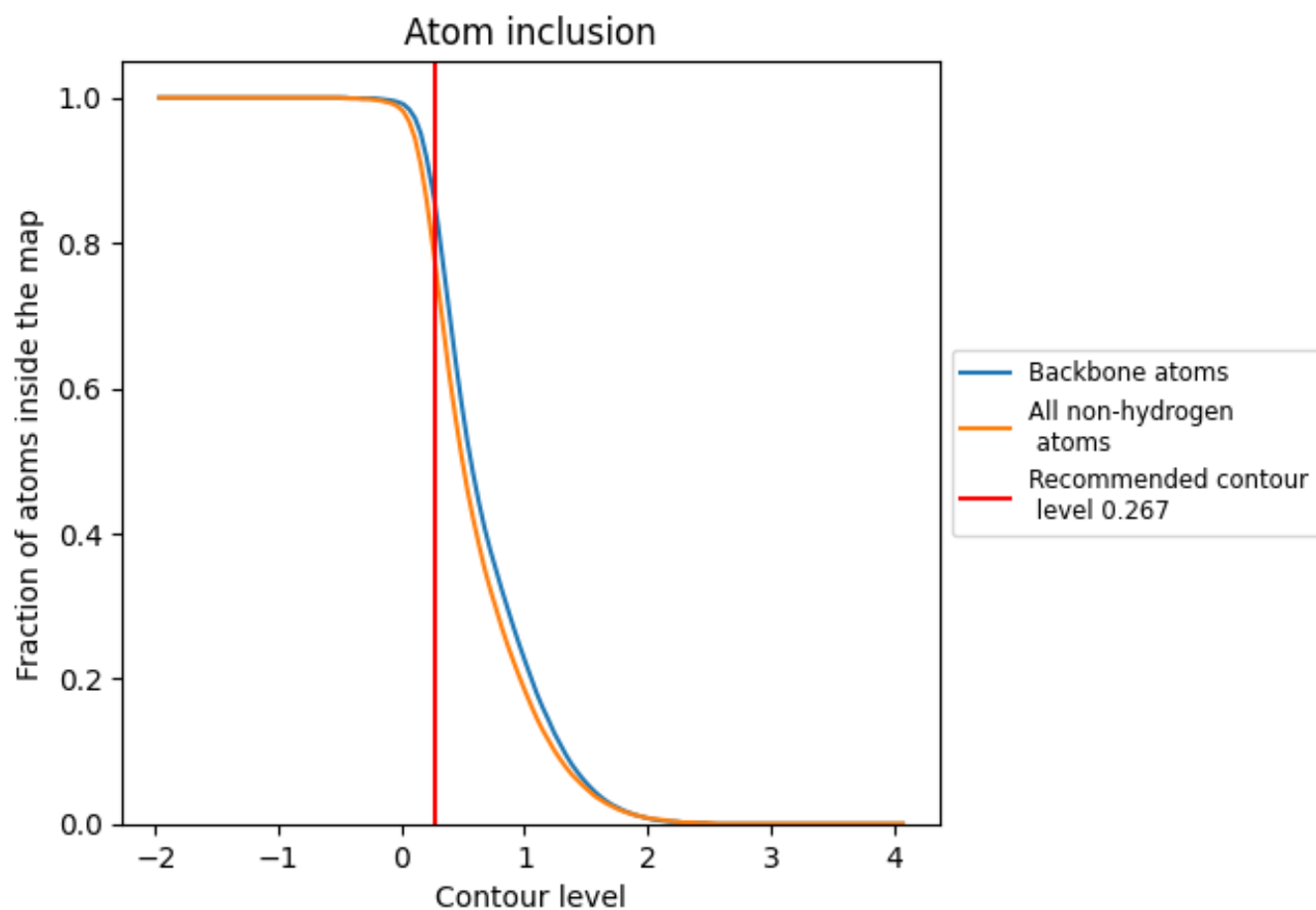
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.267).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 86% 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 (0.267) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|-------|--|--|
| All |  0.7820 |  0.3390 |
| 0 |  0.8790 |  0.4430 |
| 1 |  0.8550 |  0.4410 |
| 2 |  0.9060 |  0.4680 |
| 3 |  0.9010 |  0.5010 |
| 4 |  0.8990 |  0.4740 |
| 5 |  0.8980 |  0.4400 |
| 6 |  0.8850 |  0.4090 |
| 7 |  0.8660 |  0.4100 |
| 8 |  0.7540 |  0.2460 |
| 9 |  0.8800 |  0.4210 |
| A |  0.8460 |  0.3360 |
| A0 |  0.7340 |  0.2560 |
| A1 |  0.5090 |  0.1810 |
| A2 |  0.6550 |  0.3320 |
| A3 |  0.8090 |  0.4300 |
| A4 |  0.1430 |  0.1650 |
| A5 |  0.0470 |  0.0780 |
| A6 |  0.0270 |  0.0710 |
| A7 |  0.3890 |  0.1280 |
| AA |  0.8650 |  0.2980 |
| AB |  0.7760 |  0.3190 |
| AC |  0.5070 |  0.1970 |
| AD |  0.6200 |  0.3110 |
| AE |  0.7640 |  0.3890 |
| AF |  0.6420 |  0.2680 |
| AG |  0.6450 |  0.2300 |
| AH |  0.5830 |  0.2180 |
| AI |  0.8290 |  0.4060 |
| AJ |  0.7630 |  0.3750 |
| AK |  0.5980 |  0.1710 |
| AL |  0.7890 |  0.3790 |
| AM |  0.7740 |  0.2970 |
| AN |  0.8510 |  0.4030 |
| AO |  0.7700 |  0.2930 |

































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| Chain | Atom inclusion | Q-score |
|-------|--|--|
| AP |  0.7740 |  0.3830 |
| AQ |  0.8310 |  0.4000 |
| AR |  0.6720 |  0.2350 |
| AS |  0.7050 |  0.2830 |
| AT |  0.8030 |  0.3480 |
| AU |  0.7520 |  0.2540 |
| AV |  0.6780 |  0.1770 |
| AW |  0.7610 |  0.3350 |
| AX |  0.6230 |  0.1760 |
| AY |  0.4180 |  0.1470 |
| AZ |  0.4910 |  0.1800 |
| B |  0.9460 |  0.2990 |
| D |  0.8780 |  0.4520 |
| E |  0.8940 |  0.4620 |
| F |  0.8950 |  0.4560 |
| H |  0.8530 |  0.4040 |
| I |  0.7190 |  0.3300 |
| J |  0.7350 |  0.2970 |
| K |  0.9040 |  0.4710 |
| L |  0.8610 |  0.4600 |
| M |  0.8910 |  0.4540 |
| N |  0.8760 |  0.4560 |
| O |  0.8870 |  0.4420 |
| P |  0.9120 |  0.4350 |
| Q |  0.8490 |  0.4350 |
| R |  0.8930 |  0.4580 |
| S |  0.9030 |  0.4520 |
| T |  0.8850 |  0.4580 |
| TA |  0.1570 |  0.1180 |
| TB |  0.1830 |  0.1980 |
| TC |  0.0740 |  0.1600 |
| U |  0.8740 |  0.4430 |
| V |  0.8570 |  0.4170 |
| W |  0.8790 |  0.4580 |
| X |  0.8860 |  0.4460 |
| Y |  0.8940 |  0.4480 |
| Z |  0.8880 |  0.4580 |
| a |  0.7940 |  0.3920 |
| b |  0.8970 |  0.4720 |
| c |  0.8700 |  0.4230 |
| d |  0.7510 |  0.3760 |
| e |  0.7240 |  0.2060 |

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| Chain | Atom inclusion | Q-score |
|-------|--|--|
| f |  0.7180 |  0.3210 |
| g |  0.8820 |  0.4300 |
| h |  0.8410 |  0.3600 |
| i |  0.9070 |  0.4580 |
| j |  0.8450 |  0.4020 |
| k |  0.8040 |  0.3520 |
| l |  0.7710 |  0.3130 |
| m |  0.8020 |  0.2930 |
| o |  0.8560 |  0.4260 |
| p |  0.8200 |  0.3850 |
| q |  0.7930 |  0.3470 |
| r |  0.8850 |  0.4230 |
| s |  0.8910 |  0.4470 |
| u |  0.5290 |  0.1420 |
| v |  0.6750 |  0.3110 |