



Full wwPDB EM Validation Report ⓘ

Jul 23, 2024 – 12:36 am BST

PDB ID : 7QI4
EMDB ID : EMD-13980
Title : Human mitochondrial ribosome at 2.2 Å resolution (bound to partly built tRNAs and mRNA)
Authors : Singh, V.; Itoh, Y.; Amunts, A.
Deposited on : 2021-12-14
Resolution : 2.21 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The 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.dev92
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

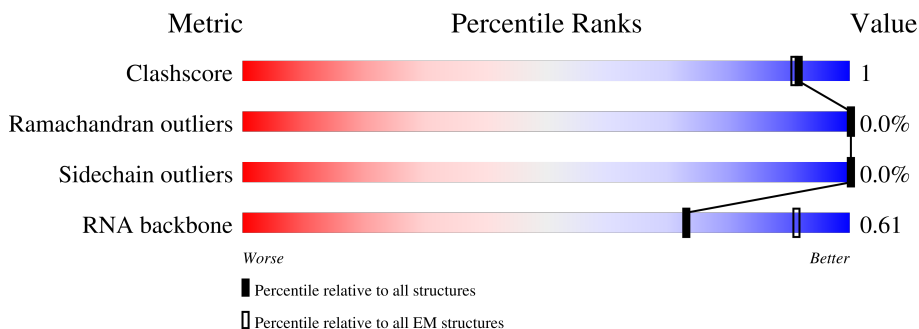
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.21 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



| Metric | Whole archive (#Entries) | EM structures (#Entries) |
|-----------------------|-----------------------------|-----------------------------|
| Clashscore | 158937 | 4297 |
| Ramachandran outliers | 154571 | 4023 |
| Sidechain outliers | 154315 | 3826 |
| RNA backbone | 4643 | 859 |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | AA | 954 | 82% 17% |
| 2 | AB | 296 | 75% 24% |
| 3 | AC | 167 | 74% 5% 21% |
| 4 | AD | 430 | 77% 20% |
| 5 | AE | 125 | 94% |
| 6 | AF | 242 | 81% 5% 14% |
| 7 | AG | 396 | 5% 79% 17% |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 8 | AH | 201 | |
| 9 | AI | 194 | |
| 10 | AJ | 138 | |
| 11 | AK | 128 | |
| 12 | AL | 257 | |
| 13 | AM | 137 | |
| 14 | AN | 130 | |
| 15 | AO | 258 | |
| 16 | AP | 142 | |
| 17 | AQ | 87 | |
| 18 | AR | 360 | |
| 19 | AS | 190 | |
| 20 | AT | 173 | |
| 21 | AU | 205 | |
| 22 | AV | 414 | |
| 23 | AW | 187 | |
| 24 | AX | 398 | |
| 25 | AY | 395 | |
| 26 | AZ | 106 | |
| 27 | A0 | 217 | |
| 28 | A1 | 323 | |
| 29 | A2 | 118 | |
| 30 | A3 | 199 | |
| 31 | A4 | 689 | |
| 32 | Aw | 22 | |




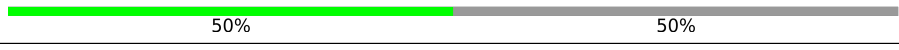

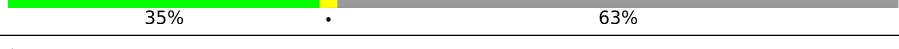
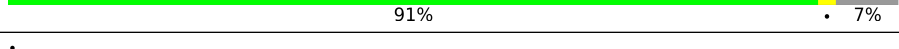
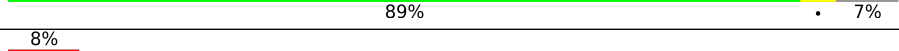
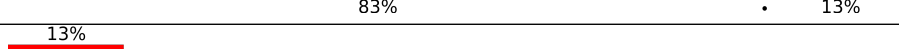
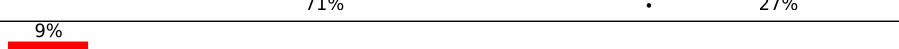
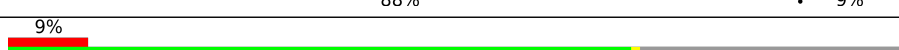

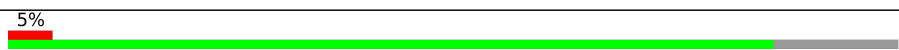

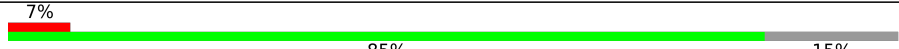





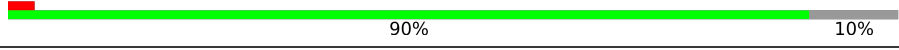
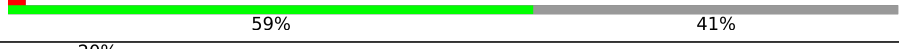



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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 33 | Ax | 70 | |
| 34 | Az | 34 | |
| 35 | A | 1558 | |
| 36 | B | 72 | |
| 37 | D | 305 | |
| 38 | E | 348 | |
| 39 | F | 311 | |
| 40 | H | 267 | |
| 41 | I | 261 | |
| 42 | J | 192 | |
| 43 | K | 178 | |
| 44 | L | 145 | |
| 45 | M | 296 | |
| 46 | N | 251 | |
| 47 | O | 175 | |
| 48 | P | 180 | |
| 49 | Q | 292 | |
| 50 | R | 149 | |
| 51 | S | 205 | |
| 52 | T | 206 | |
| 53 | U | 153 | |
| 54 | V | 216 | |
| 55 | W | 148 | |
| 56 | X | 256 | |
| 57 | Y | 250 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 58 | Z | 161 |  |
| 59 | 0 | 188 |  |
| 60 | 1 | 65 |  |
| 61 | 2 | 92 |  |
| 62 | 3 | 188 |  |
| 63 | 4 | 103 |  |
| 64 | 5 | 423 |  |
| 65 | 6 | 380 |  |
| 66 | 7 | 338 |  |
| 67 | 8 | 206 |  |
| 68 | 9 | 137 |  |
| 69 | a | 142 |  |
| 70 | b | 215 |  |
| 71 | c | 332 |  |
| 72 | d | 306 |  |
| 73 | e | 279 |  |
| 74 | f | 212 |  |
| 75 | g | 166 |  |
| 76 | h | 158 |  |
| 77 | i | 128 |  |
| 78 | j | 123 |  |
| 79 | k | 112 |  |
| 80 | l | 138 |  |
| 81 | m | 128 |  |
| 82 | o | 102 |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 83 | p | 206 | |
| 84 | q | 222 | |
| 85 | r | 196 | |
| 86 | s | 439 | |
| 87 | t | 198 | |
| 87 | u | 198 | |
| 87 | v | 198 | |
| 87 | w | 198 | |
| 87 | x | 198 | |
| 87 | y | 198 | |
| 88 | z | 325 | |
| 89 | Ay | 52 | |

2 Entry composition

There are 101 unique types of molecules in this entry. The entry contains 340116 atoms, of which 152427 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 mitochondrial rRNA.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-------|------|------|-----|---------|-------|
| 1 | AA | 954 | Total | C | H | N | O | P | 0 | 0 |
| | | | 30564 | 9088 | 10304 | 3647 | 6571 | 954 | | |

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

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|-------|
| 2 | AB | 225 | Total | C | H | N | O | S | 0 | 0 |
| | | | 3644 | 1164 | 1816 | 331 | 323 | 10 | | |

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

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 3 | AC | 132 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2172 | 699 | 1089 | 195 | 185 | 4 | | |

- Molecule 4 is a protein called 28S ribosomal protein S5, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|-------|
| 4 | AD | 343 | Total | C | H | N | O | S | 0 | 0 |
| | | | 5536 | 1713 | 2805 | 518 | 487 | 13 | | |

- Molecule 5 is a protein called 28S ribosomal protein S6, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 5 | AE | 122 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1972 | 614 | 1000 | 177 | 177 | 4 | | |

- Molecule 6 is a protein called 28S ribosomal protein S7, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|-------|
| 6 | AF | 208 | Total | C | H | N | O | S | 0 | 0 |
| | | | 3496 | 1104 | 1771 | 312 | 298 | 11 | | |

- Molecule 7 is a protein called 28S ribosomal protein S9, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|-------|
| 7 | AG | 327 | Total | C | H | N | O | S | 0 | 0 |
| | | | 5377 | 1710 | 2689 | 477 | 487 | 14 | | |

- Molecule 8 is a protein called 28S ribosomal protein S10, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 8 | AH | 140 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2339 | 745 | 1187 | 194 | 210 | 3 | | |

- Molecule 9 is a protein called 28S ribosomal protein S11, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 9 | AI | 137 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2081 | 642 | 1061 | 192 | 182 | 4 | | |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| AI | 184 | 5F0 | ASN | conflict | UNP P82912 |

- Molecule 10 is a protein called 28S ribosomal protein S12, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 10 | AJ | 108 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1727 | 521 | 888 | 169 | 143 | 6 | | |

- Molecule 11 is a protein called 28S ribosomal protein S14, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 11 | AK | 101 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1748 | 537 | 886 | 179 | 141 | 5 | | |

- Molecule 12 is a protein called 28S ribosomal protein S15, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 12 | AL | 174 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2994 | 925 | 1541 | 270 | 251 | 7 | | |

- Molecule 13 is a protein called 28S ribosomal protein S16, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 13 | AM | 119 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1908 | 594 | 966 | 185 | 157 | 6 | | |

- Molecule 14 is a protein called 28S ribosomal protein S17, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 14 | AN | 110 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1797 | 562 | 929 | 156 | 147 | 3 | | |

- Molecule 15 is a protein called 28S ribosomal protein S18b, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|---------|-------|
| 15 | AO | 193 | Total | C | H | N | O | S | 0 | 0 |
| | | | 3149 | 1014 | 1557 | 294 | 277 | 7 | | |

- Molecule 16 is a protein called 28S ribosomal protein S18c, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 16 | AP | 97 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1587 | 501 | 806 | 134 | 138 | 8 | | |

- Molecule 17 is a protein called MRPS21 isoform 1.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 17 | AQ | 86 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1502 | 460 | 758 | 150 | 126 | 8 | | |

- Molecule 18 is a protein called 28S ribosomal protein S22, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|---------|-------|
| 18 | AR | 295 | Total | C | H | N | O | S | 0 | 0 |
| | | | 4839 | 1533 | 2430 | 413 | 455 | 8 | | |

- Molecule 19 is a protein called 28S ribosomal protein S23, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 19 | AS | 135 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2227 | 716 | 1116 | 198 | 196 | 1 | | |

- Molecule 20 is a protein called 28S ribosomal protein S25, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|----|---------|-------|
| 20 | AT | 168 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2764 | 877 | 1393 | 239 | 244 | 11 | | |

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

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 21 | AU | 176 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2989 | 916 | 1501 | 301 | 267 | 4 | | |

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

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|-------|
| 22 | AV | 362 | Total | C | H | N | O | S | 0 | 0 |
| | | | 5933 | 1904 | 2964 | 495 | 558 | 12 | | |

- Molecule 23 is a protein called 28S ribosomal protein S28, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 23 | AW | 100 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1593 | 498 | 804 | 141 | 146 | 4 | | |

- Molecule 24 is a protein called 28S ribosomal protein S29, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|-------|
| 24 | AX | 352 | Total | C | H | N | O | S | 0 | 0 |
| | | | 5694 | 1822 | 2845 | 499 | 517 | 11 | | |

- Molecule 25 is a protein called 28S ribosomal protein S31, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 25 | AY | 149 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2444 | 801 | 1198 | 207 | 234 | 4 | | |

- Molecule 26 is a protein called 28S ribosomal protein S33, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 26 | AZ | 100 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1698 | 534 | 859 | 153 | 148 | 4 | | |

- Molecule 27 is a protein called 28S ribosomal protein S34, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|---------|-------|
| 27 | A0 | 215 | Total | C | H | N | O | S | 0 | 0 |
| | | | 3584 | 1130 | 1797 | 339 | 313 | 5 | | |

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

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|-------|
| 28 | A1 | 279 | Total | C | H | N | O | S | 0 | 0 |
| | | | 4561 | 1435 | 2296 | 387 | 432 | 11 | | |

- Molecule 29 is a protein called Coiled-coil-helix-coiled-coil-helix domain-containing protein 1.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 29 | A2 | 117 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1906 | 579 | 971 | 182 | 166 | 8 | | |

- Molecule 30 is a protein called Aurora kinase A-interacting protein.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---|---------|-------|
| 30 | A3 | 70 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1326 | 401 | 701 | 134 | 89 | 1 | | |

- Molecule 31 is a protein called Pentatricopeptide repeat domain-containing protein 3, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|-------|
| 31 | A4 | 588 | Total | C | H | N | O | S | 0 | 0 |
| | | | 9538 | 3053 | 4770 | 808 | 879 | 28 | | |

- Molecule 32 is a RNA chain called A/A-tRNA.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|-----|----|---------|-------|
| 32 | Aw | 22 | Total | C | H | N | O | P | 0 | 0 |
| | | | 701 | 209 | 237 | 82 | 151 | 22 | | |

- Molecule 33 is a RNA chain called P/P-tRNA.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|----|---------|-------|
| 33 | Ax | 70 | Total | C | H | N | O | P | 0 | 0 |
| | | | 2233 | 665 | 751 | 260 | 487 | 70 | | |

- Molecule 34 is a RNA chain called mRNA.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|----|---------|-------|
| 34 | Az | 34 | Total | C | H | N | O | P | 0 | 0 |
| | | | 1079 | 324 | 360 | 123 | 238 | 34 | | |

- Molecule 35 is a RNA chain called 16S mitochondrial rRNA.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|------|-------|------|---------|-------|
| 35 | A | 1558 | Total | C | H | N | O | P | 0 | 0 |
| | | | 49871 | 14843 | 16801 | 5963 | 10706 | 1558 | | |

There are 3 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|---------------|
| A | ? | - | A | deletion | GB 1563835895 |
| A | ? | - | C | deletion | GB 1563835895 |
| A | ? | - | U | deletion | GB 1563835895 |

- Molecule 36 is a RNA chain called mitochondrial tRNA^{Val}.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|----|---------|-------|
| 36 | B | 72 | Total | C | H | N | O | P | 0 | 0 |
| | | | 2303 | 685 | 779 | 269 | 498 | 72 | | |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|----------------|
| B | 74 | C | G | conflict | GB NC_012920.1 |
| B | 76 | A | U | conflict | GB NC_012920.1 |

- Molecule 37 is a protein called 39S ribosomal protein L2, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|---------|-------|
| 37 | D | 238 | Total | C | H | N | O | S | 0 | 0 |
| | | | 3780 | 1157 | 1921 | 376 | 317 | 9 | | |

- Molecule 38 is a protein called 39S ribosomal protein L3, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|-------|
| 38 | E | 305 | Total | C | H | N | O | S | 0 | 0 |
| | | | 4822 | 1545 | 2416 | 418 | 432 | 11 | | |

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

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|---------|-------|
| 39 | F | 252 | Total | C | H | N | O | S | 0 | 0 |
| | | | 4097 | 1305 | 2066 | 370 | 350 | 6 | | |

- Molecule 40 is a protein called 39S ribosomal protein L9, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|---------|-------|
| 40 | H | 202 | Total | C | H | N | O | S | 0 | 0 |
| | | | 3397 | 1067 | 1736 | 304 | 286 | 4 | | |

- Molecule 41 is a protein called 39S ribosomal protein L10, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|-------|
| 41 | I | 212 | Total | C | H | N | O | S | 0 | 0 |
| | | | 3481 | 1088 | 1786 | 304 | 292 | 11 | | |

- Molecule 42 is a protein called 39S ribosomal protein L11, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 42 | J | 175 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2738 | 847 | 1408 | 237 | 244 | 2 | | |

- Molecule 43 is a protein called 39S ribosomal protein L13, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 43 | K | 177 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2907 | 936 | 1452 | 259 | 253 | 7 | | |

- Molecule 44 is a protein called 39S ribosomal protein L14, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 44 | L | 115 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1832 | 559 | 942 | 171 | 155 | 5 | | |

- Molecule 45 is a protein called 39S ribosomal protein L15, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|---------|-------|
| 45 | M | 291 | Total | C | H | N | O | S | 0 | 0 |
| | | | 4723 | 1483 | 2396 | 430 | 408 | 6 | | |

- Molecule 46 is a protein called 39S ribosomal protein L16, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|-------|
| 46 | N | 222 | Total | C | H | N | O | S | 0 | 0 |
| | | | 3604 | 1143 | 1818 | 326 | 307 | 10 | | |

- Molecule 47 is a protein called 39S ribosomal protein L17, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 47 | O | 154 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2554 | 792 | 1295 | 241 | 219 | 7 | | |

- Molecule 48 is a protein called 39S ribosomal protein L18, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 48 | P | 144 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2339 | 733 | 1166 | 224 | 211 | 5 | | |

- Molecule 49 is a protein called 39S ribosomal protein L19, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|---------|-------|
| 49 | Q | 239 | Total | C | H | N | O | S | 0 | 0 |
| | | | 4021 | 1277 | 2031 | 353 | 351 | 9 | | |

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

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 50 | R | 140 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2369 | 732 | 1215 | 231 | 187 | 4 | | |

- Molecule 51 is a protein called 39S ribosomal protein L21, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 51 | S | 161 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2659 | 835 | 1366 | 227 | 227 | 4 | | |

- Molecule 52 is a protein called 39S ribosomal protein L22, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 52 | T | 166 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2781 | 875 | 1412 | 254 | 233 | 7 | | |

- Molecule 53 is a protein called 39S ribosomal protein L23, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 53 | U | 152 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2483 | 788 | 1232 | 234 | 226 | 3 | | |

- Molecule 54 is a protein called 39S ribosomal protein L24, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|---------|-------|
| 54 | V | 205 | Total | C | H | N | O | S | 0 | 0 |
| | | | 3365 | 1068 | 1689 | 298 | 302 | 8 | | |

- Molecule 55 is a protein called 39S ribosomal protein L27, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 55 | W | 116 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1840 | 577 | 936 | 171 | 153 | 3 | | |

- Molecule 56 is a protein called 39S ribosomal protein L28, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|---------|-------|
| 56 | X | 244 | Total | C | H | N | O | S | 0 | 0 |
| | | | 4105 | 1322 | 2061 | 352 | 365 | 5 | | |

- Molecule 57 is a protein called 39S ribosomal protein L47, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 57 | Y | 181 | Total | C | H | N | O | S | 0 | 0 |
| | | | 3154 | 995 | 1598 | 298 | 259 | 4 | | |

- Molecule 58 is a protein called 39S ribosomal protein L30, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 58 | Z | 122 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2041 | 636 | 1045 | 186 | 171 | 3 | | |

- Molecule 59 is a protein called 39S ribosomal protein L32, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 59 | 0 | 110 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1815 | 554 | 917 | 176 | 162 | 6 | | |

- Molecule 60 is a protein called 39S ribosomal protein L33, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|----|---|---------|-------|
| 60 | 1 | 56 | Total | C | H | N | O | S | 0 | 0 |
| | | | 977 | 296 | 513 | 89 | 77 | 2 | | |

- Molecule 61 is a protein called 39S ribosomal protein L34, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|----|---|---------|-------|
| 61 | 2 | 46 | Total | C | H | N | O | S | 0 | 0 |
| | | | 784 | 233 | 407 | 83 | 60 | 1 | | |

- Molecule 62 is a protein called 39S ribosomal protein L35, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 62 | 3 | 95 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1716 | 539 | 884 | 162 | 128 | 3 | | |

- Molecule 63 is a protein called 39S ribosomal protein L36, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|----|---|---------|-------|
| 63 | 4 | 38 | Total | C | H | N | O | S | 0 | 0 |
| | | | 704 | 217 | 362 | 72 | 49 | 4 | | |

- Molecule 64 is a protein called 39S ribosomal protein L37, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|-------|
| 64 | 5 | 394 | Total | C | H | N | O | S | 0 | 0 |
| | | | 6419 | 2073 | 3209 | 560 | 566 | 11 | | |

- Molecule 65 is a protein called 39S ribosomal protein L38, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|---------|-------|
| 65 | 6 | 354 | Total | C | H | N | O | S | 0 | 0 |
| | | | 5792 | 1881 | 2844 | 525 | 533 | 9 | | |

- Molecule 66 is a protein called 39S ribosomal protein L39, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|-------|
| 66 | 7 | 294 | Total | C | H | N | O | S | 0 | 0 |
| | | | 4789 | 1529 | 2399 | 405 | 438 | 18 | | |

- Molecule 67 is a protein called 39S ribosomal protein L40, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 67 | 8 | 151 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2588 | 812 | 1310 | 226 | 238 | 2 | | |

- Molecule 68 is a protein called 39S ribosomal protein L41, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 68 | 9 | 124 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1985 | 644 | 988 | 170 | 181 | 2 | | |

- Molecule 69 is a protein called 39S ribosomal protein L42, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 69 | a | 100 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1652 | 529 | 812 | 152 | 154 | 5 | | |

- Molecule 70 is a protein called 39S ribosomal protein L43, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 70 | b | 150 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2392 | 744 | 1196 | 231 | 218 | 3 | | |

- Molecule 71 is a protein called 39S ribosomal protein L44, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|---------|-------|
| 71 | c | 286 | Total | C | H | N | O | S | 0 | 0 |
| | | | 4621 | 1470 | 2322 | 397 | 423 | 9 | | |

- Molecule 72 is a protein called 39S ribosomal protein L45, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|-------|
| 72 | d | 241 | Total | C | H | N | O | S | 0 | 0 |
| | | | 3965 | 1273 | 1980 | 340 | 359 | 13 | | |

- Molecule 73 is a protein called 39S ribosomal protein L46, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|---------|-------|
| 73 | e | 238 | Total | C | H | N | O | S | 0 | 0 |
| | | | 3848 | 1222 | 1917 | 339 | 364 | 6 | | |

- Molecule 74 is a protein called 39S ribosomal protein L48, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 74 | f | 157 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2523 | 799 | 1271 | 207 | 242 | 4 | | |

- Molecule 75 is a protein called 39S ribosomal protein L49, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 75 | g | 134 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2210 | 719 | 1097 | 193 | 199 | 2 | | |

- Molecule 76 is a protein called 39S ribosomal protein L50, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 76 | h | 110 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1778 | 568 | 883 | 156 | 168 | 3 | | |

- Molecule 77 is a protein called 39S ribosomal protein L51, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 77 | i | 97 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1687 | 532 | 859 | 165 | 127 | 4 | | |

- Molecule 78 is a protein called 39S ribosomal protein L52, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 78 | j | 94 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1492 | 463 | 747 | 144 | 136 | 2 | | |

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

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 79 | k | 101 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1559 | 479 | 785 | 148 | 142 | 5 | | |

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

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 80 | l | 82 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1363 | 437 | 675 | 120 | 128 | 3 | | |

- Molecule 81 is a protein called 39S ribosomal protein L55, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 81 | m | 92 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1551 | 488 | 760 | 159 | 142 | 2 | | |

- Molecule 82 is a protein called Ribosomal protein 63, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 82 | o | 94 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1604 | 501 | 806 | 165 | 129 | 3 | | |

- Molecule 83 is a protein called Peptidyl-tRNA hydrolase ICT1, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 83 | p | 147 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2430 | 748 | 1225 | 228 | 225 | 4 | | |

- Molecule 84 is a protein called Growth arrest and DNA damage-inducible proteins-interacting protein 1.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 84 | q | 155 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2571 | 809 | 1273 | 251 | 233 | 5 | | |

- Molecule 85 is a protein called 39S ribosomal protein S18a, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 85 | r | 162 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2671 | 839 | 1349 | 252 | 223 | 8 | | |

- Molecule 86 is a protein called 39S ribosomal protein S30, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|-------|
| 86 | s | 386 | Total | C | H | N | O | S | 0 | 0 |
| | | | 6300 | 2023 | 3145 | 559 | 559 | 14 | | |

- Molecule 87 is a protein called 39S ribosomal protein L12, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|----|--|---------|-------|
| 87 | t | 46 | Total | C | H | N | O | | 0 | 0 |
| | | | 732 | 228 | 378 | 56 | 70 | | | |
| 87 | u | 32 | Total | C | H | N | O | | 0 | 0 |
| | | | 541 | 168 | 284 | 40 | 49 | | | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|----|---------|-------|
| 87 | v | 32 | Total | C | H | N | O | 0 | 0 |
| | | | 541 | 168 | 284 | 40 | 49 | | |
| 87 | w | 31 | Total | C | H | N | O | 0 | 0 |
| | | | 520 | 159 | 275 | 39 | 47 | | |
| 87 | x | 31 | Total | C | H | N | O | 0 | 0 |
| | | | 520 | 159 | 275 | 39 | 47 | | |
| 87 | y | 31 | Total | C | H | N | O | 0 | 0 |
| | | | 520 | 159 | 275 | 39 | 47 | | |

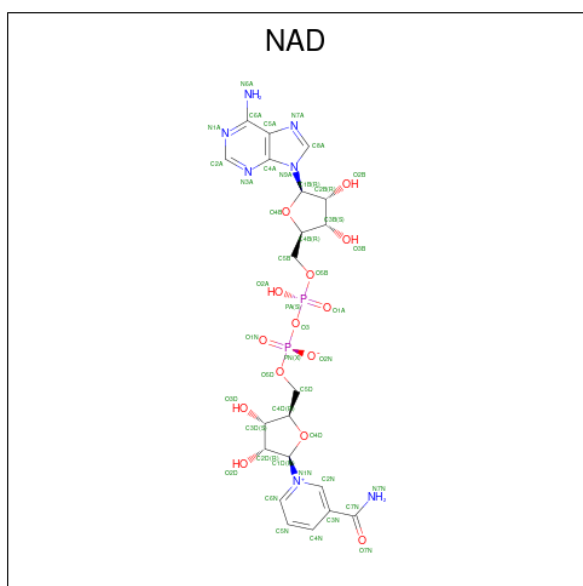
- Molecule 88 is a protein called 39S ribosomal protein L1, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---------|-------|
| 88 | z | 164 | Total | C | H | N | O | 0 | 0 |
| | | | 2682 | 856 | 1355 | 217 | 250 | | |

- Molecule 89 is a RNA chain called E/E-tRNA.

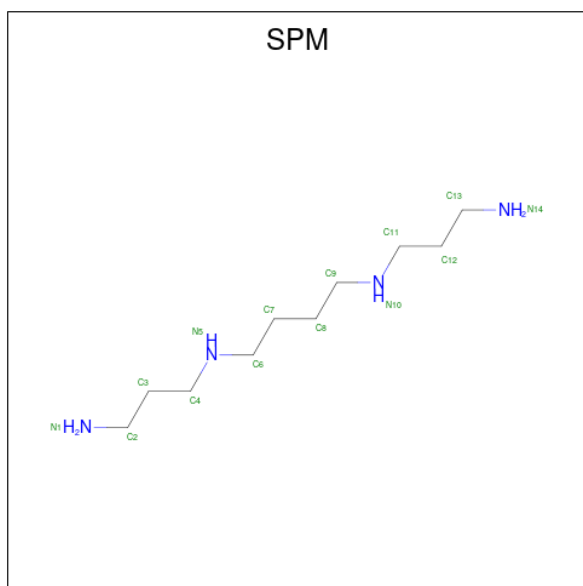
| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---------|-------|
| 89 | Ay | 52 | Total | C | H | N | O | 0 | 0 |
| | | | 1667 | 496 | 560 | 199 | 360 | | |

- Molecule 90 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).



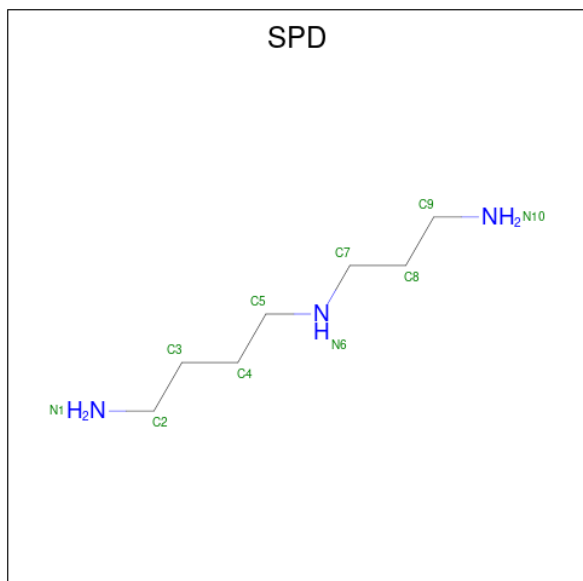
| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|----|---|----|---------|
| 90 | AA | 1 | Total | C | H | N | O | P |
| | | | 70 | 21 | 26 | 7 | 14 | 2 |
| | | | | | | | | 0 |

- Molecule 91 is SPERMINE (three-letter code: SPM) (formula: $C_{10}H_{26}N_4$) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms | | | | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 91 | AA | 1 | Total | C | H | N | |
| | | | 44 | 10 | 30 | 4 | 0 |

- Molecule 92 is SPERMIDINE (three-letter code: SPD) (formula: $C_7H_{19}N_3$) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms | | | | AltConf |
|-----|-------|----------|-------|---|----|---|---------|
| 92 | AA | 1 | Total | C | H | N | 0 |
| | | | 32 | 7 | 22 | 3 | |
| 92 | A | 1 | Total | C | H | N | 0 |
| | | | 32 | 7 | 22 | 3 | |
| 92 | A | 1 | Total | C | H | N | 0 |
| | | | 32 | 7 | 22 | 3 | |
| 92 | A | 1 | Total | C | H | N | 0 |
| | | | 32 | 7 | 22 | 3 | |

- Molecule 93 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|-----|---------|
| 93 | AA | 61 | Total | Mg | 0 |
| | | | 61 | 61 | |
| 93 | AB | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 93 | AX | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 93 | A3 | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 93 | Aw | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 93 | A | 137 | Total | Mg | 0 |
| | | | 137 | 137 | |
| 93 | D | 2 | Total | Mg | 0 |
| | | | 2 | 2 | |
| 93 | E | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 93 | g | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |

- Molecule 94 is POTASSIUM ION (three-letter code: K) (formula: K).

| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|----|---------|
| 94 | AA | 18 | Total | K | 0 |
| | | | 18 | 18 | |
| 94 | A | 29 | Total | K | 0 |
| | | | 29 | 29 | |
| 94 | D | 1 | Total | K | 0 |
| | | | 1 | 1 | |
| 94 | M | 1 | Total | K | 0 |
| | | | 1 | 1 | |
| 94 | W | 1 | Total | K | 0 |
| | | | 1 | 1 | |

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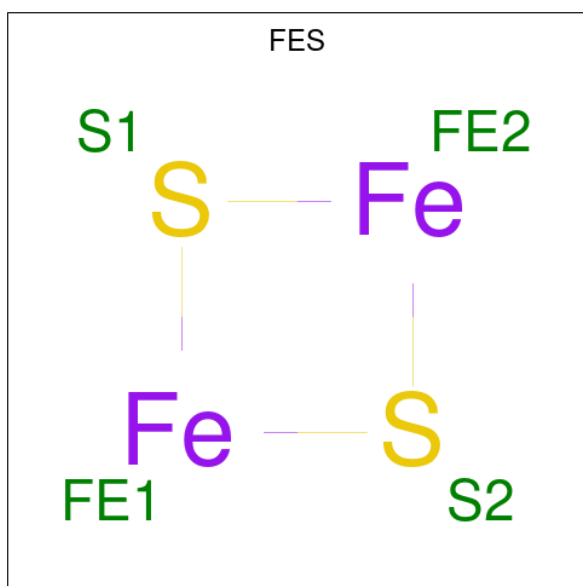
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| Mol | Chain | Residues | Atoms | AltConf |
|-----|-------|----------|----------------|---------|
| 94 | 3 | 1 | Total K 1 1 | 0 |
| 94 | 6 | 1 | Total K 1 1 | 0 |
| 94 | i | 1 | Total K 1 1 | 0 |
| 94 | o | 1 | Total K 1 1 | 0 |

- Molecule 95 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | AltConf |
|-----|-------|----------|-----------------|---------|
| 95 | AO | 1 | Total Zn 1 1 | 0 |
| 95 | 0 | 1 | Total Zn 1 1 | 0 |
| 95 | 4 | 1 | Total Zn 1 1 | 0 |

- Molecule 96 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂) (labeled as "Ligand of Interest" by depositor).



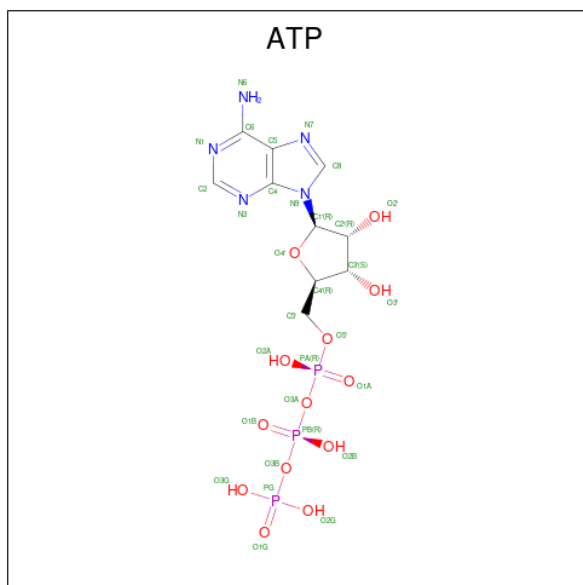
| Mol | Chain | Residues | Atoms | AltConf |
|-----|-------|----------|---------------------|---------|
| 96 | AP | 1 | Total Fe S 4 2 2 | 0 |
| 96 | AT | 1 | Total Fe S 4 2 2 | 0 |

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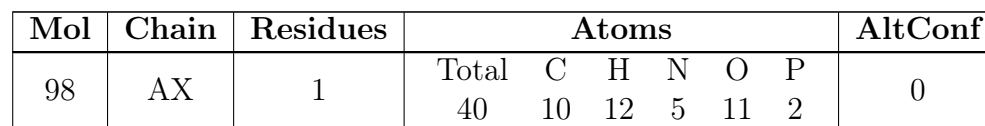
| Mol | Chain | Residues | Atoms | | | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 96 | r | 1 | Total | Fe | S | 0 |
| | | | 4 | 2 | 2 | |

- Molecule 97 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



| Mol | Chain | Residues | Atoms | | | | | | AltConf |
|-----|-------|----------|-------|----|----|---|----|---|---------|
| 97 | AX | 1 | Total | C | H | N | O | P | 0 |
| | | | 43 | 10 | 12 | 5 | 13 | 3 | |

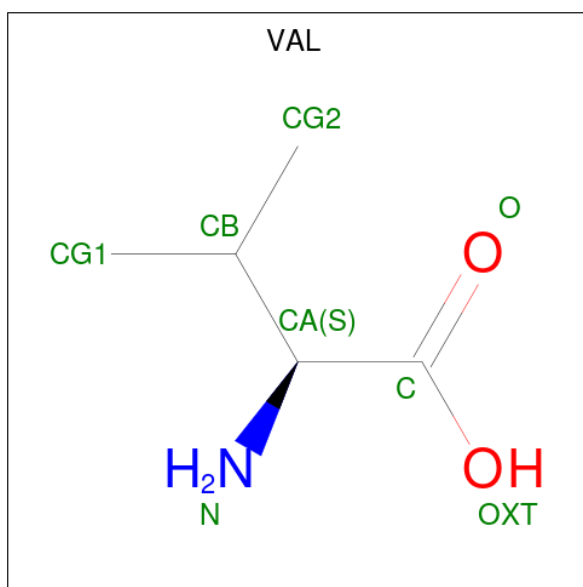
- Molecule 98 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$) (labeled as "Ligand of Interest" by depositor).



- PUT
-
- The chemical structure of Putrescine (PUT) is shown, consisting of a four-carbon chain with terminal primary amine groups. The carbons are labeled C1, C2, C3, and C4 from right to left. The terminal amine groups are labeled NH₂N1 and NH₂N2. The structure is drawn in a zig-zag conformation.

| Mol | Chain | Residues | Atoms | | | | AltConf |
|-----|-------|----------|-------|---|----|---|---------|
| 99 | A | 1 | Total | C | H | N | 0 |
| | | | 20 | 4 | 14 | 2 | |

- 
- WORLD WIDE
PDB
PROTEIN DATA BANK



| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|---|----|---|---|---------|
| 100 | B | 1 | Total | C | H | N | O | 0 |
| | | | 18 | 5 | 11 | 1 | 1 | |

- Molecule 101 is water.

| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|------|---------|
| 101 | AA | 2157 | Total | O | 0 |
| | | | 2157 | 2157 | |
| 101 | AB | 80 | Total | O | 0 |
| | | | 80 | 80 | |
| 101 | AC | 58 | Total | O | 0 |
| | | | 58 | 58 | |
| 101 | AD | 79 | Total | O | 0 |
| | | | 79 | 79 | |
| 101 | AE | 30 | Total | O | 0 |
| | | | 30 | 30 | |
| 101 | AF | 36 | Total | O | 0 |
| | | | 36 | 36 | |
| 101 | AG | 70 | Total | O | 0 |
| | | | 70 | 70 | |
| 101 | AH | 50 | Total | O | 0 |
| | | | 50 | 50 | |
| 101 | AI | 44 | Total | O | 0 |
| | | | 44 | 44 | |
| 101 | AJ | 29 | Total | O | 0 |
| | | | 29 | 29 | |
| 101 | AK | 51 | Total | O | 0 |
| | | | 51 | 51 | |

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| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------------|---------|---------|
| 101 | AL | 43 | Total 43 | O 43 | 0 |
| 101 | AM | 21 | Total 21 | O 21 | 0 |
| 101 | AN | 34 | Total 34 | O 34 | 0 |
| 101 | AO | 37 | Total 37 | O 37 | 0 |
| 101 | AP | 31 | Total 31 | O 31 | 0 |
| 101 | AQ | 68 | Total 68 | O 68 | 0 |
| 101 | AR | 12 | Total 12 | O 12 | 0 |
| 101 | AS | 23 | Total 23 | O 23 | 0 |
| 101 | AT | 43 | Total 43 | O 43 | 0 |
| 101 | AU | 8 | Total 8 | O 8 | 0 |
| 101 | AW | 15 | Total 15 | O 15 | 0 |
| 101 | AX | 61 | Total 61 | O 61 | 0 |
| 101 | AY | 20 | Total 20 | O 20 | 0 |
| 101 | AZ | 27 | Total 27 | O 27 | 0 |
| 101 | A0 | 1 | Total 1 | O 1 | 0 |
| 101 | A1 | 36 | Total 36 | O 36 | 0 |
| 101 | A2 | 35 | Total 35 | O 35 | 0 |
| 101 | A3 | 52 | Total 52 | O 52 | 0 |
| 101 | A4 | 11 | Total 11 | O 11 | 0 |
| 101 | Aw | 5 | Total 5 | O 5 | 0 |
| 101 | Ax | 5 | Total 5 | O 5 | 0 |

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| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|---------------|-----------|---------|
| 101 | Az | 15 | Total 15 | O 15 | 0 |
| 101 | A | 3056 | Total 3056 | O 3056 | 0 |
| 101 | B | 63 | Total 63 | O 63 | 0 |
| 101 | D | 73 | Total 73 | O 73 | 0 |
| 101 | E | 74 | Total 74 | O 74 | 0 |
| 101 | F | 78 | Total 78 | O 78 | 0 |
| 101 | H | 9 | Total 9 | O 9 | 0 |
| 101 | I | 23 | Total 23 | O 23 | 0 |
| 101 | J | 1 | Total 1 | O 1 | 0 |
| 101 | K | 65 | Total 65 | O 65 | 0 |
| 101 | L | 25 | Total 25 | O 25 | 0 |
| 101 | M | 66 | Total 66 | O 66 | 0 |
| 101 | N | 60 | Total 60 | O 60 | 0 |
| 101 | O | 38 | Total 38 | O 38 | 0 |
| 101 | P | 89 | Total 89 | O 89 | 0 |
| 101 | Q | 27 | Total 27 | O 27 | 0 |
| 101 | R | 57 | Total 57 | O 57 | 0 |
| 101 | S | 49 | Total 49 | O 49 | 0 |
| 101 | T | 48 | Total 48 | O 48 | 0 |
| 101 | U | 26 | Total 26 | O 26 | 0 |
| 101 | V | 5 | Total 5 | O 5 | 0 |

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| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|--------------|----------|---------|
| 101 | W | 48 | Total 48 | O 48 | 0 |
| 101 | X | 12 | Total 12 | O 12 | 0 |
| 101 | Y | 29 | Total 29 | O 29 | 0 |
| 101 | Z | 34 | Total 34 | O 34 | 0 |
| 101 | 0 | 27 | Total 27 | O 27 | 0 |
| 101 | 1 | 3 | Total 3 | O 3 | 0 |
| 101 | 2 | 34 | Total 34 | O 34 | 0 |
| 101 | 3 | 40 | Total 40 | O 40 | 0 |
| 101 | 4 | 13 | Total 13 | O 13 | 0 |
| 101 | 5 | 22 | Total 22 | O 22 | 0 |
| 101 | 6 | 100 | Total 100 | O 100 | 0 |
| 101 | 7 | 17 | Total 17 | O 17 | 0 |
| 101 | 8 | 19 | Total 19 | O 19 | 0 |
| 101 | 9 | 17 | Total 17 | O 17 | 0 |
| 101 | a | 13 | Total 13 | O 13 | 0 |
| 101 | b | 39 | Total 39 | O 39 | 0 |
| 101 | c | 20 | Total 20 | O 20 | 0 |
| 101 | d | 5 | Total 5 | O 5 | 0 |
| 101 | e | 13 | Total 13 | O 13 | 0 |
| 101 | f | 22 | Total 22 | O 22 | 0 |
| 101 | g | 13 | Total 13 | O 13 | 0 |

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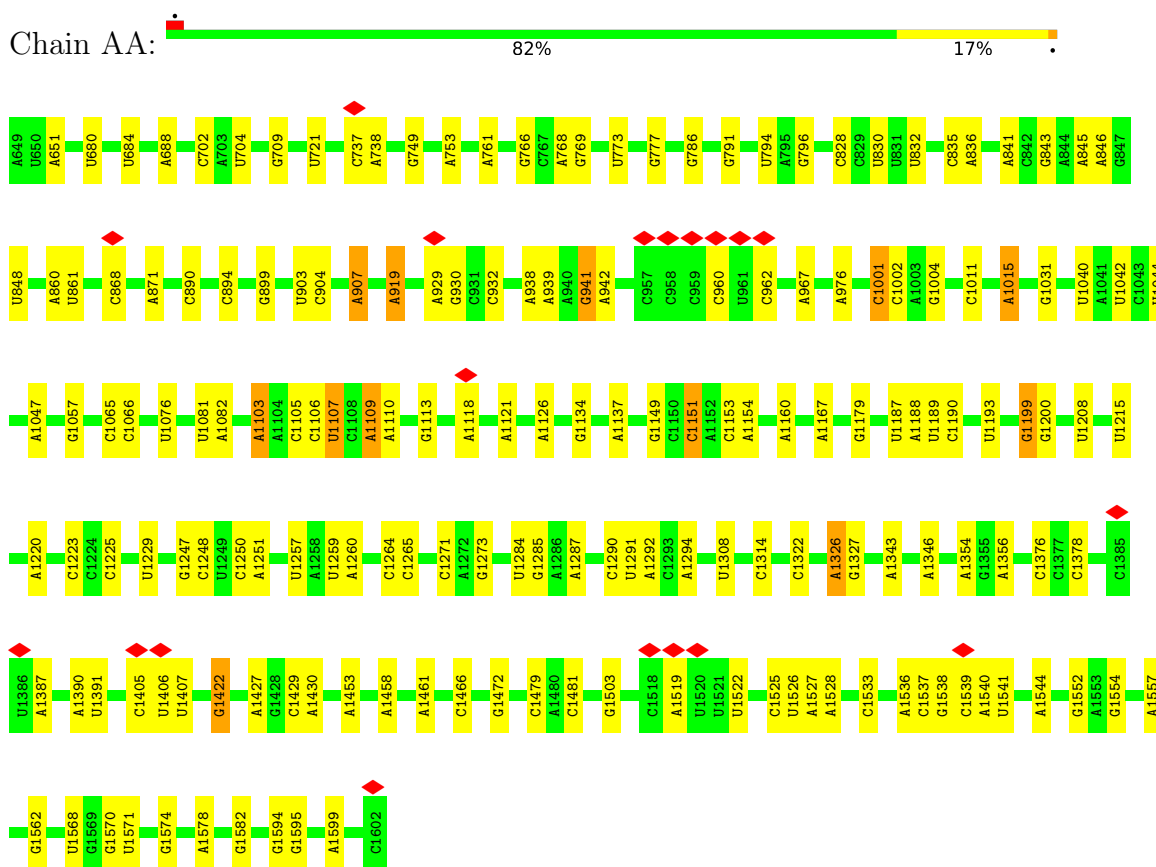
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| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------------|---------|---------|
| 101 | i | 54 | Total 54 | O 54 | 0 |
| 101 | j | 23 | Total 23 | O 23 | 0 |
| 101 | k | 6 | Total 6 | O 6 | 0 |
| 101 | l | 5 | Total 5 | O 5 | 0 |
| 101 | m | 8 | Total 8 | O 8 | 0 |
| 101 | o | 34 | Total 34 | O 34 | 0 |
| 101 | p | 10 | Total 10 | O 10 | 0 |
| 101 | r | 50 | Total 50 | O 50 | 0 |
| 101 | s | 51 | Total 51 | O 51 | 0 |
| 101 | Ay | 1 | Total 1 | O 1 | 0 |

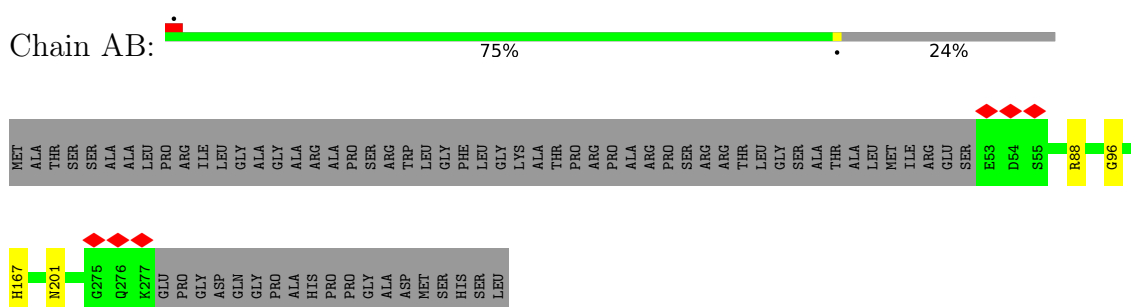
3 Residue-property plots

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 mitochondrial rRNA

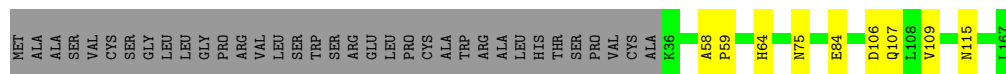


• Molecule 2: 28S ribosomal protein S2, mitochondrial




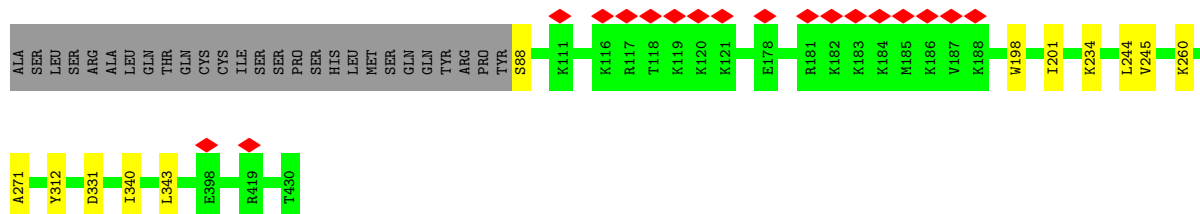
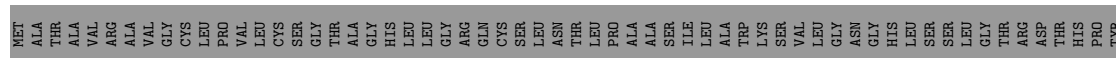
- Molecule 3: 28S ribosomal protein S24, mitochondrial

Chain AC:  74% 5% 21%



- Molecule 4: 28S ribosomal protein S5, mitochondrial

Chain AD:  77% 20%




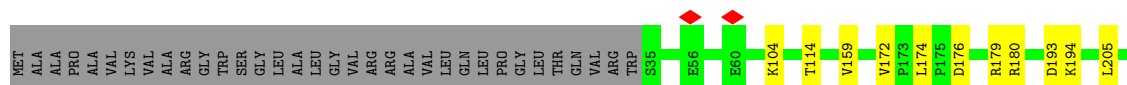
- Molecule 5: 28S ribosomal protein S6, mitochondrial

Chain AE:  94% 5% 1%




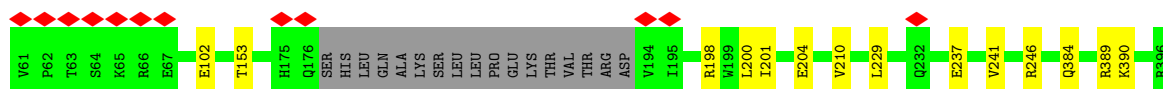
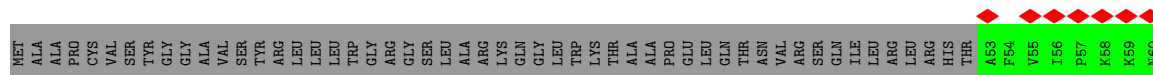
- Molecule 6: 28S ribosomal protein S7, mitochondrial

Chain AF:  81% 5% 14%



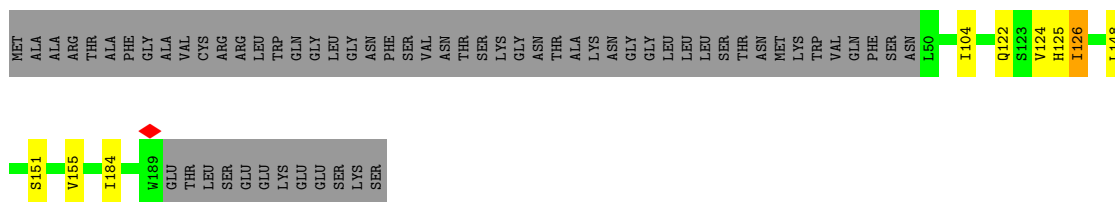
- Molecule 7: 28S ribosomal protein S9, mitochondrial

Chain AG:  5% 79% 17%



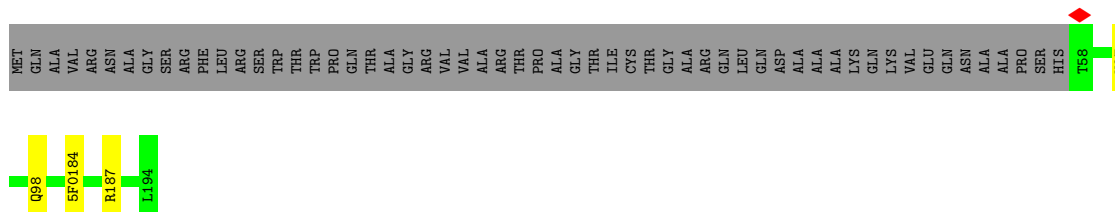
- Molecule 8: 28S ribosomal protein S10, mitochondrial

Chain AH:  65% 30%




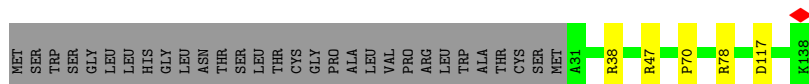
- Molecule 9: 28S ribosomal protein S11, mitochondrial

Chain AI:  69% 29%




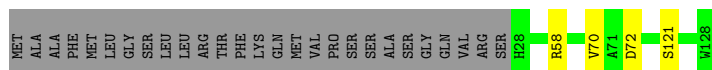
- Molecule 10: 28S ribosomal protein S12, mitochondrial

Chain AJ:  75% 22%



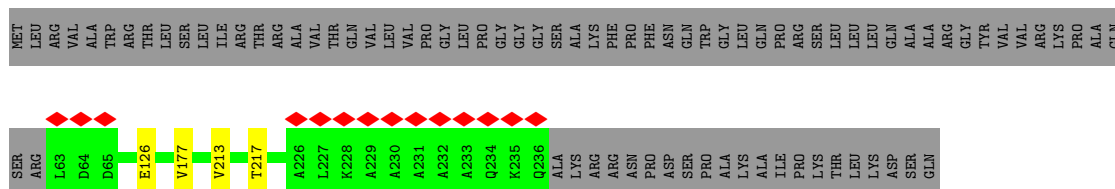
- Molecule 11: 28S ribosomal protein S14, mitochondrial

Chain AK:  76% 21%



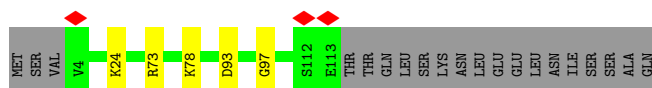
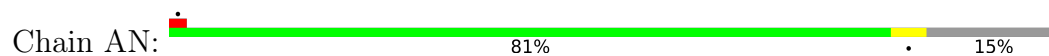
- Molecule 12: 28S ribosomal protein S15, mitochondrial

Chain AL:  5% 66% 32%

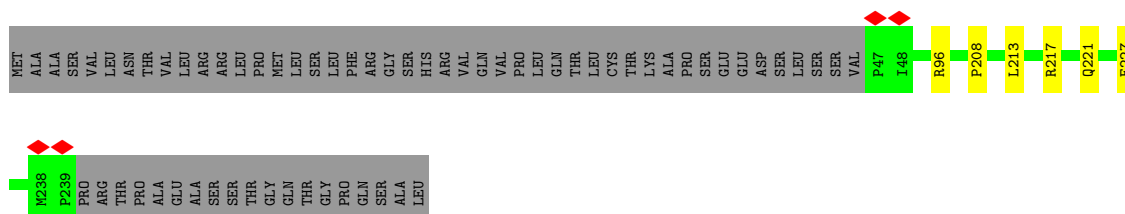




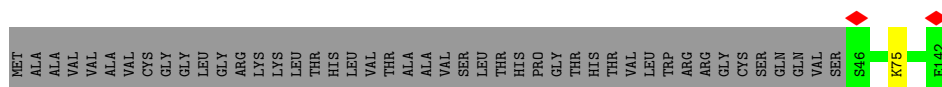
- Molecule 14: 28S ribosomal protein S17, mitochondrial



- Molecule 15: 28S ribosomal protein S18b, mitochondrial



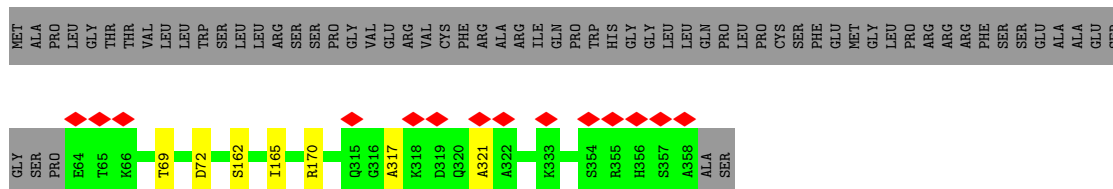
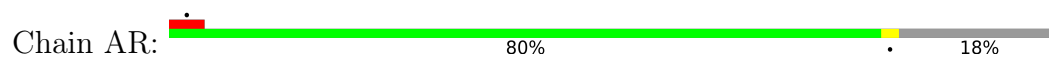
- Molecule 16: 28S ribosomal protein S18c, mitochondrial



- Molecule 17: MRPS21 isoform 1

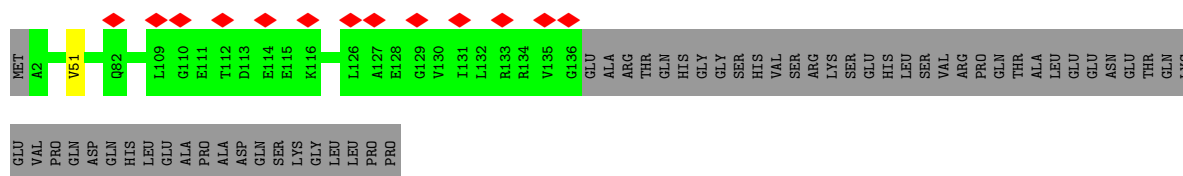


- Molecule 18: 28S ribosomal protein S22, mitochondrial

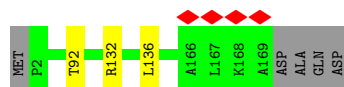


- Molecule 19: 28S ribosomal protein S23, mitochondrial

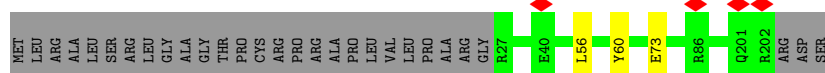
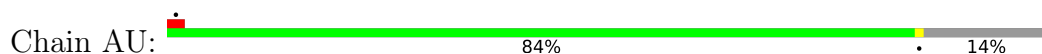




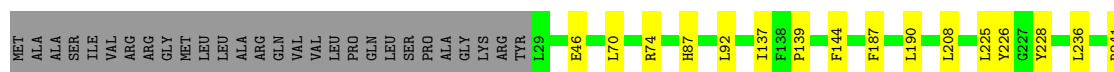
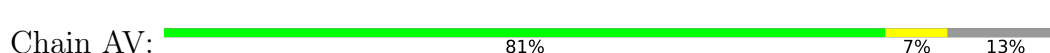
- Molecule 20: 28S ribosomal protein S25, mitochondrial



- Molecule 21: 28S ribosomal protein S26, mitochondrial



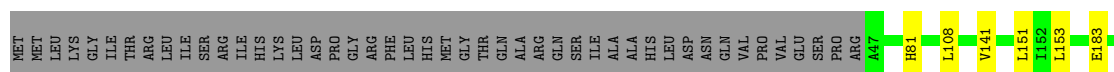
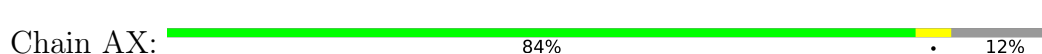
- Molecule 22: 28S ribosomal protein S27, mitochondrial

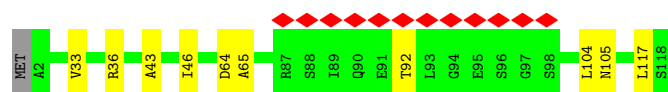


- Molecule 23: 28S ribosomal protein S28, mitochondrial



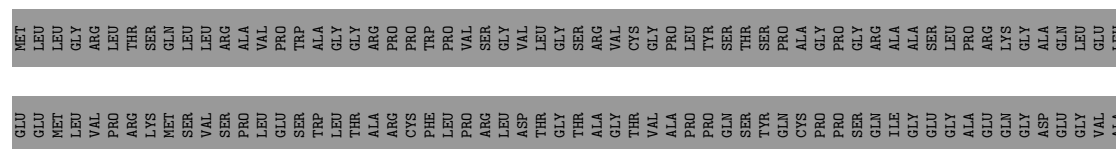
- Molecule 24: 28S ribosomal protein S29, mitochondrial





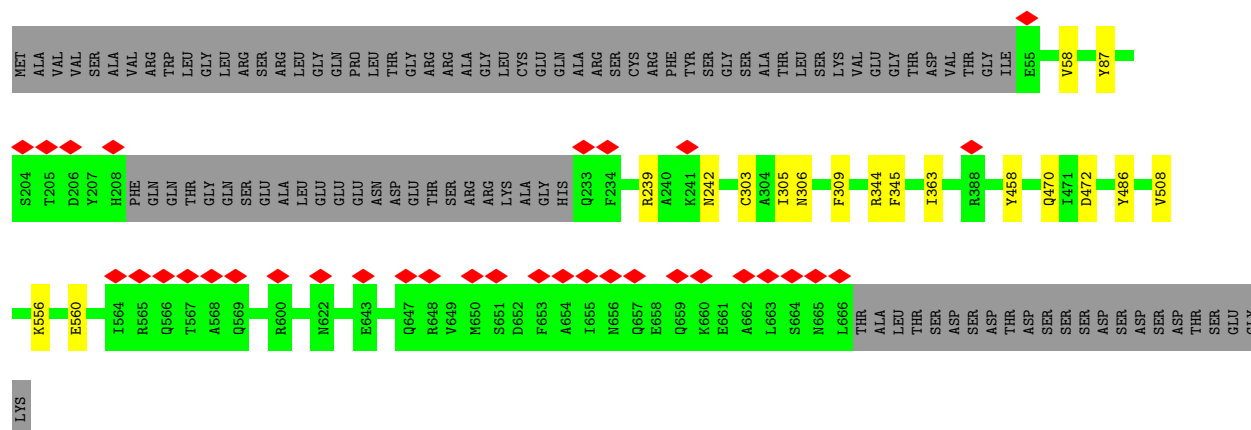
- Molecule 30: Aurora kinase A-interacting protein

Chain A3: 32% 65%



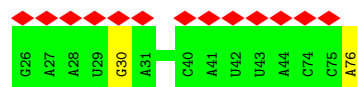
- Molecule 31: Pentatricopeptide repeat domain-containing protein 3, mitochondrial

Chain A4: 5% 83% 15%



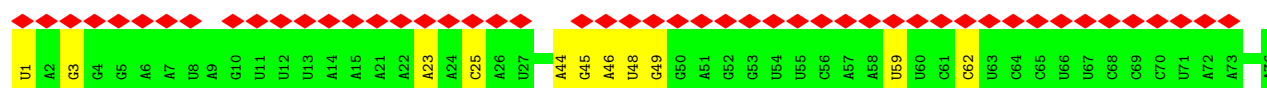
- Molecule 32: A/A-tRNA

Chain Aw: 59% 91% 9%



- Molecule 33: P/P-tRNA

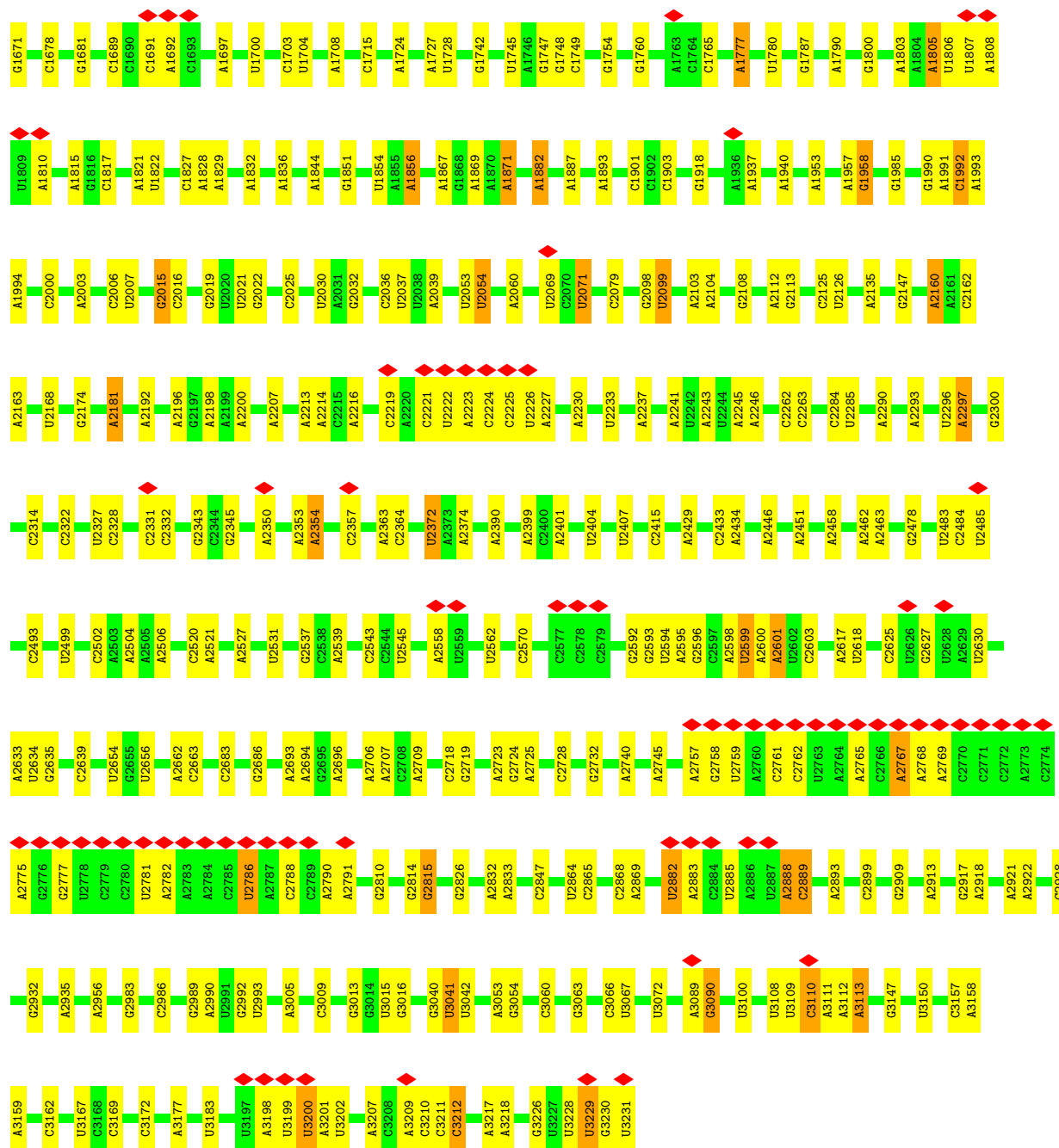
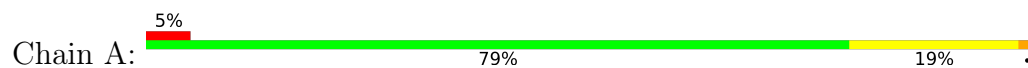
Chain Ax: 70% 84% 16%




- Molecule 34: mRNA



• Molecule 35: 16S mitochondrial rRNA




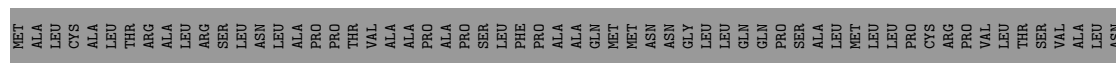
• Molecule 36: mitochondrial tRNAVal

Chain B:  75% 24%




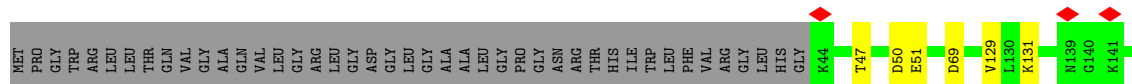
- Molecule 37: 39S ribosomal protein L2, mitochondrial

Chain D:  76% 22%




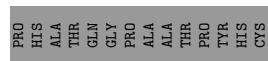
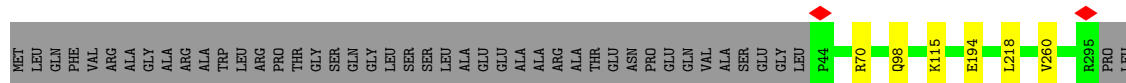
- Molecule 38: 39S ribosomal protein L3, mitochondrial

Chain E:  84% 12%




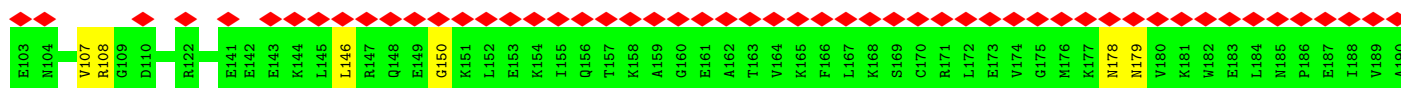
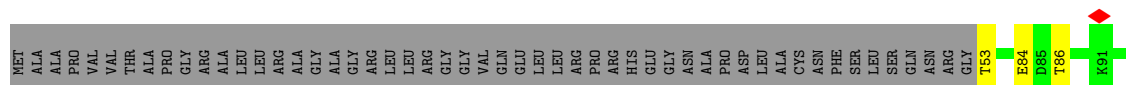
- Molecule 39: 39S ribosomal protein L4, mitochondrial

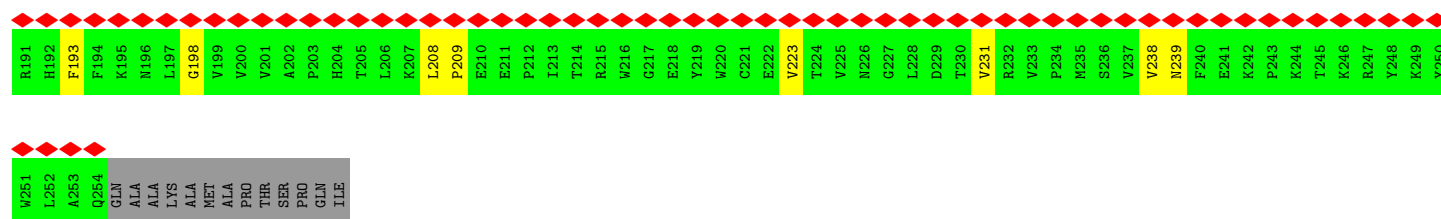
Chain F:  79% 19%



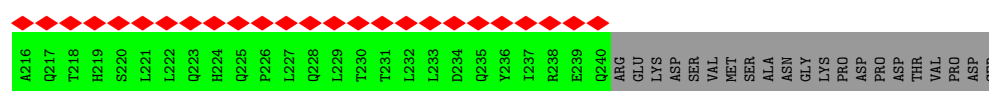
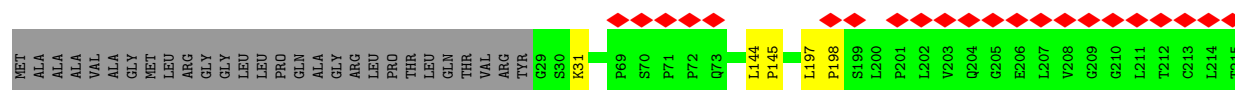
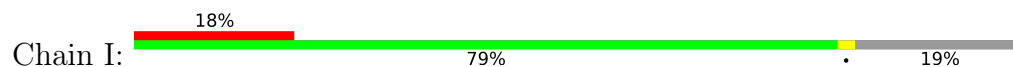
- Molecule 40: 39S ribosomal protein L9, mitochondrial

Chain H:  44% 69% 6% 24%

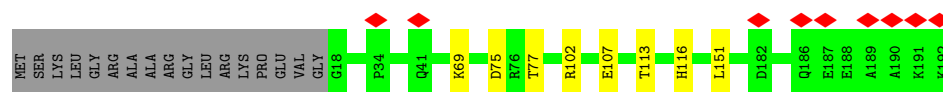
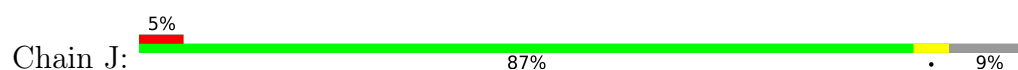




- Molecule 41: 39S ribosomal protein L10, mitochondrial



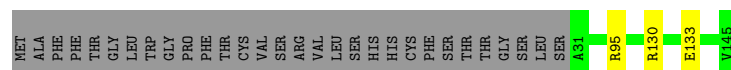
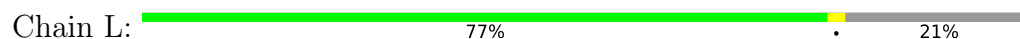
- Molecule 42: 39S ribosomal protein L11, mitochondrial



- Molecule 43: 39S ribosomal protein L13, mitochondrial




- Molecule 44: 39S ribosomal protein L14, mitochondrial

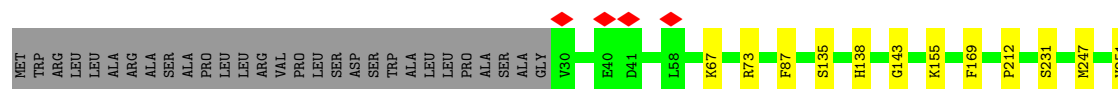


- Molecule 45: 39S ribosomal protein L15, mitochondrial




- Molecule 46: 39S ribosomal protein L16, mitochondrial

Chain N: 




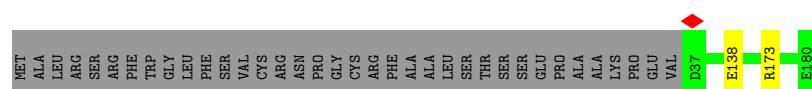
- Molecule 47: 39S ribosomal protein L17, mitochondrial

Chain O: 




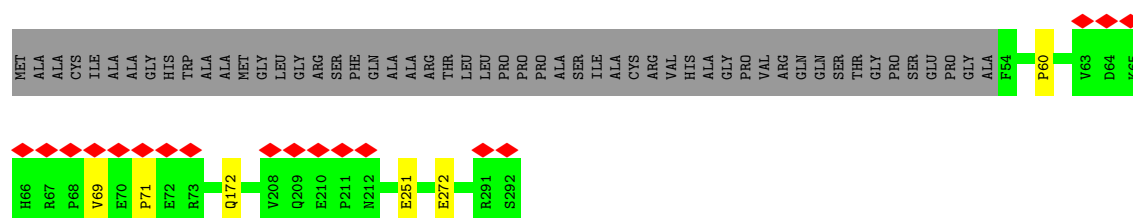
- Molecule 48: 39S ribosomal protein L18, mitochondrial

Chain P: 



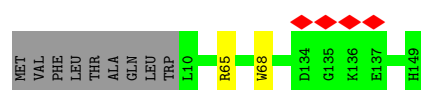
- Molecule 49: 39S ribosomal protein L19, mitochondrial

Chain Q: 



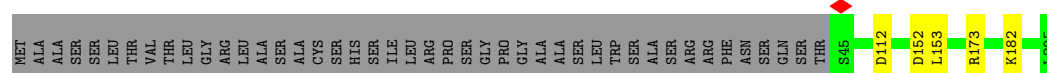
- Molecule 50: 39S ribosomal protein L20, mitochondrial

Chain R: 




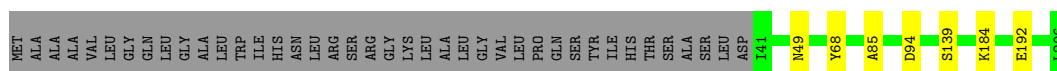
- Molecule 51: 39S ribosomal protein L21, mitochondrial

Chain S: 

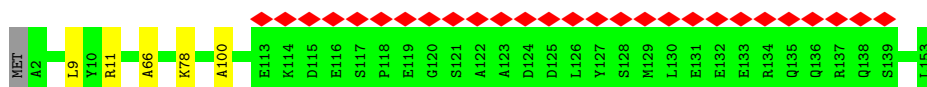


- Molecule 52: 39S ribosomal protein L22, mitochondrial

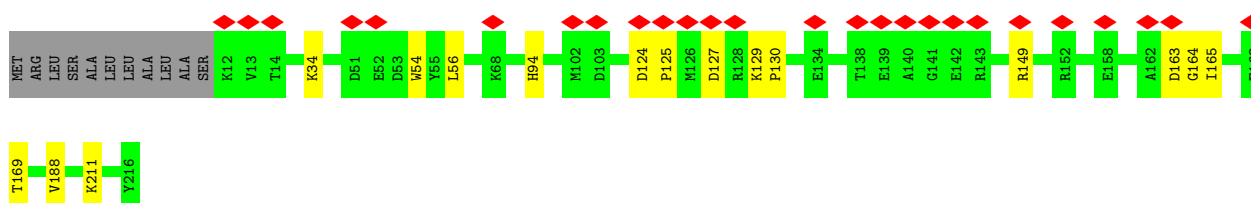
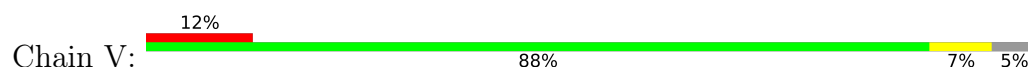
Chain T: 



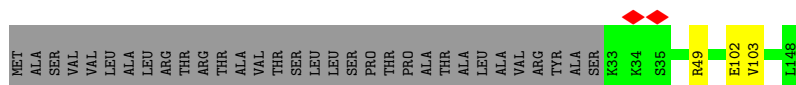
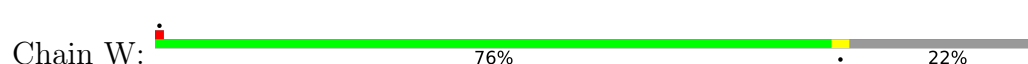
- Molecule 53: 39S ribosomal protein L23, mitochondrial



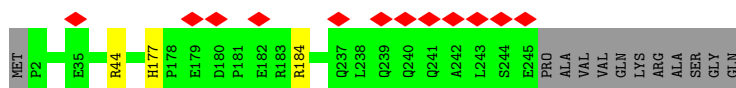
- Molecule 54: 39S ribosomal protein L24, mitochondrial



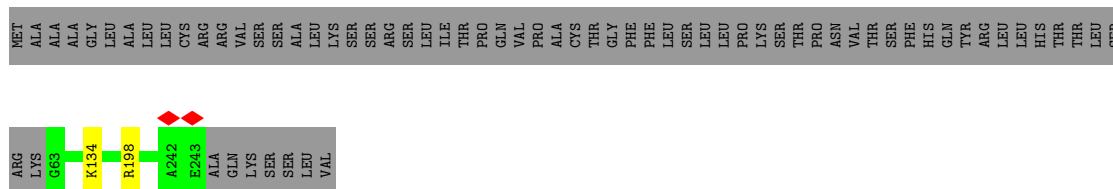
- Molecule 55: 39S ribosomal protein L27, mitochondrial



- Molecule 56: 39S ribosomal protein L28, mitochondrial

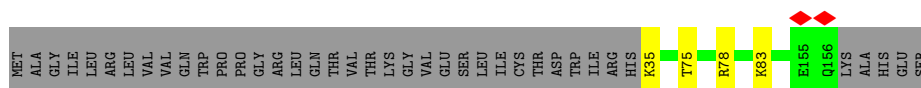


- Molecule 57: 39S ribosomal protein L47, mitochondrial

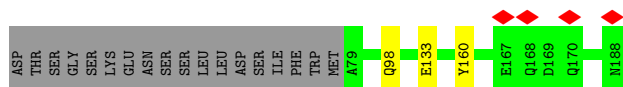
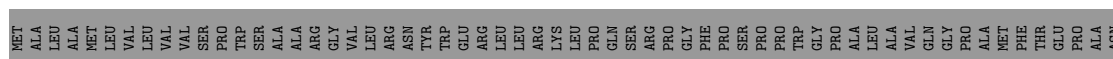


- Molecule 58: 39S ribosomal protein L30, mitochondrial

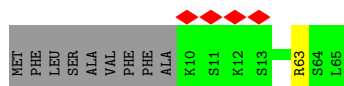
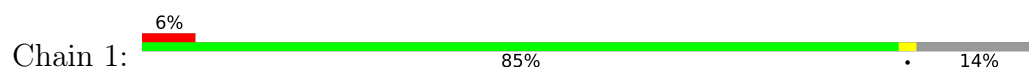




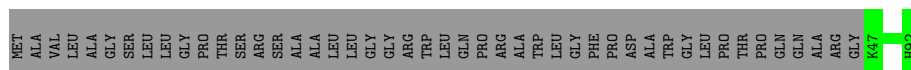
- Molecule 59: 39S ribosomal protein L32, mitochondrial



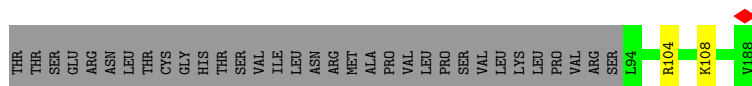
- Molecule 60: 39S ribosomal protein L33, mitochondrial



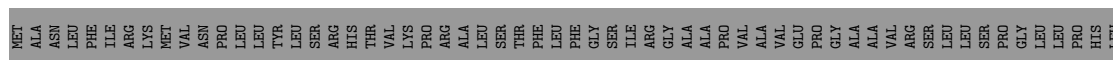
- Molecule 61: 39S ribosomal protein L34, mitochondrial



- Molecule 62: 39S ribosomal protein L35, mitochondrial

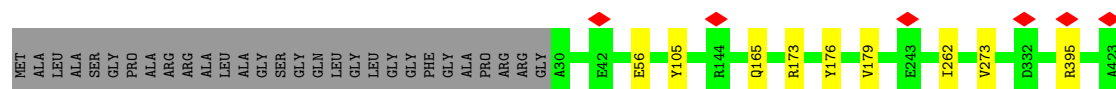


- Molecule 63: 39S ribosomal protein L36, mitochondrial




- Molecule 64: 39S ribosomal protein L37, mitochondrial

Chain 5:  91% 7%




- Molecule 65: 39S ribosomal protein L38, mitochondrial

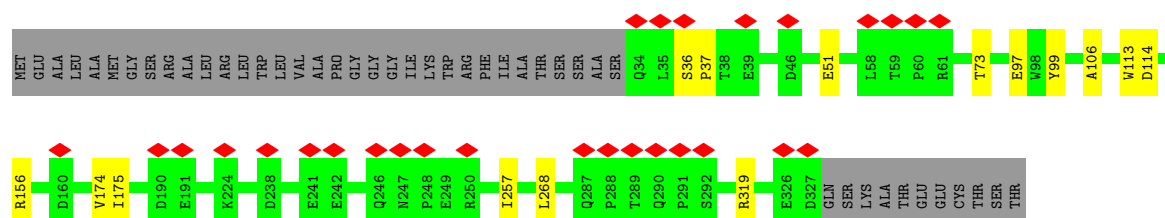
Chain 6:  89% 7%



T380

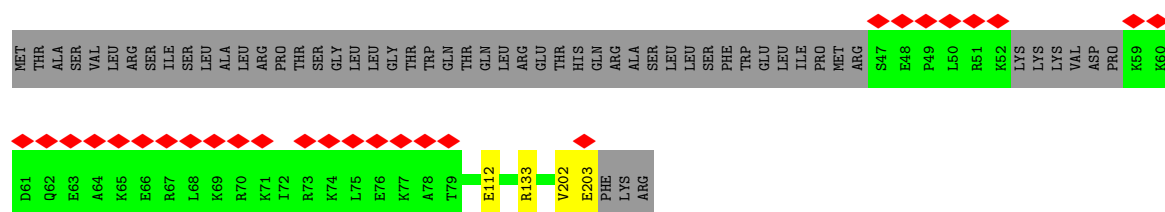
- Molecule 66: 39S ribosomal protein L39, mitochondrial

Chain 7:  8% 83% 13%




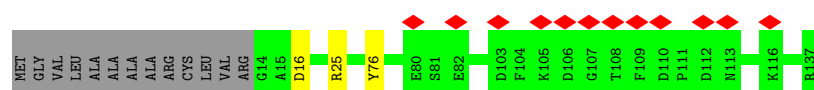
- Molecule 67: 39S ribosomal protein L40, mitochondrial

Chain 8:  13% 71% 27%



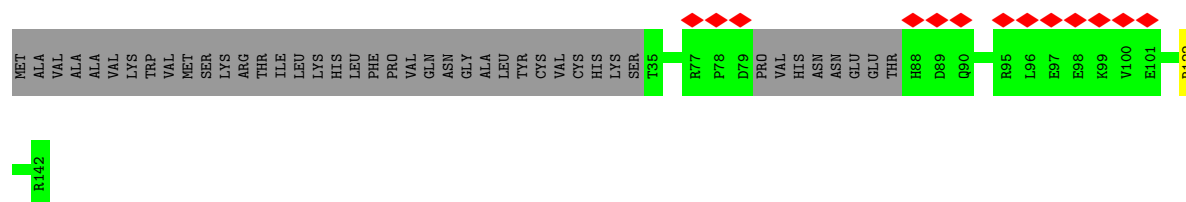
- Molecule 68: 39S ribosomal protein L41, mitochondrial

Chain 9:  9% 88% 9%

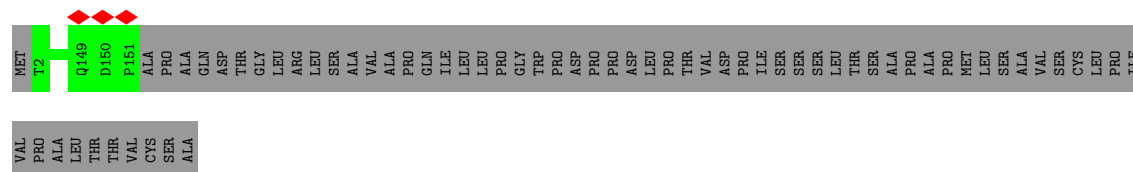


- Molecule 69: 39S ribosomal protein L42, mitochondrial

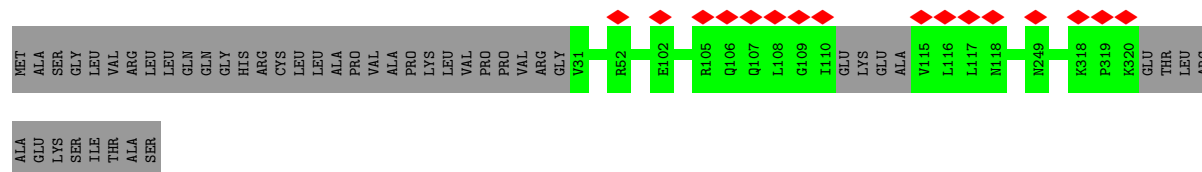
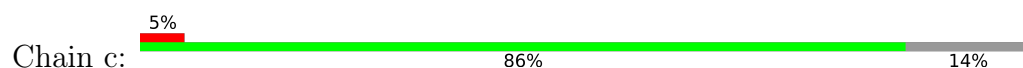
Chain a:  9% 70% 30%



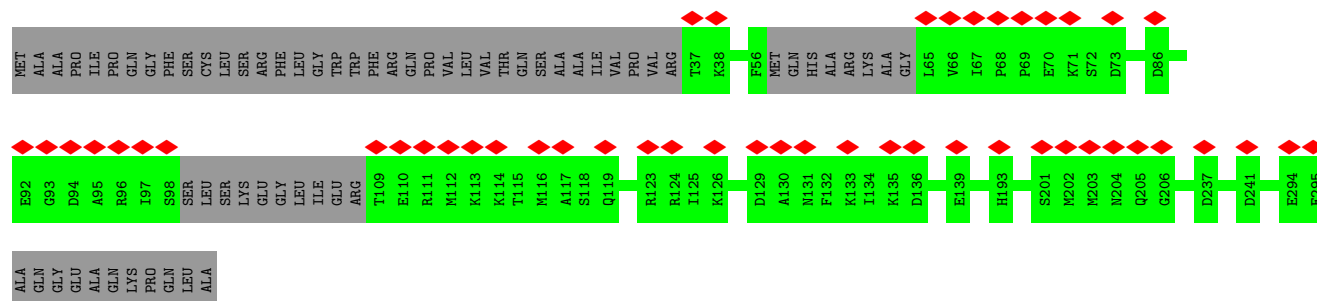
- Molecule 70: 39S ribosomal protein L43, mitochondrial



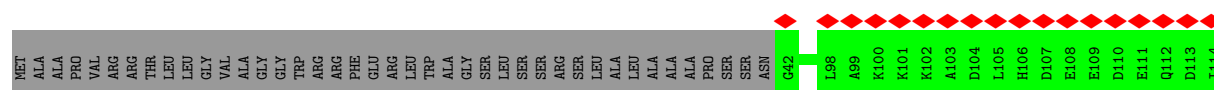
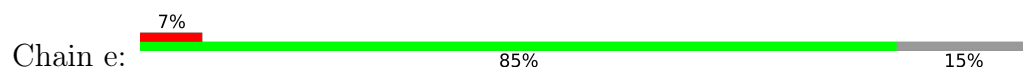
- Molecule 71: 39S ribosomal protein L44, mitochondrial

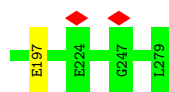


- Molecule 72: 39S ribosomal protein L45, mitochondrial

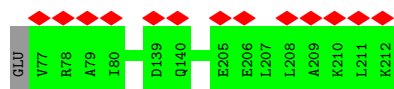
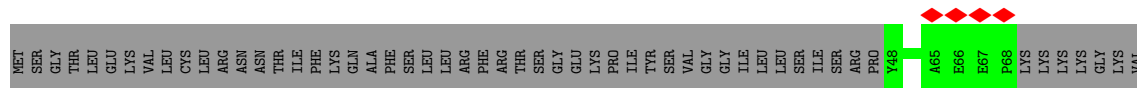
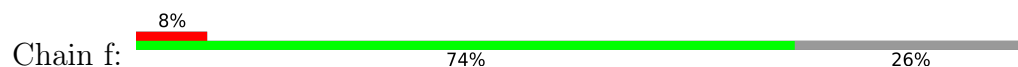


- Molecule 73: 39S ribosomal protein L46, mitochondrial

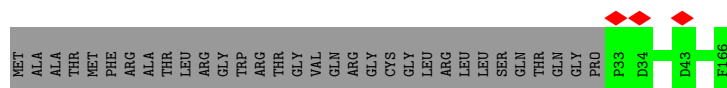
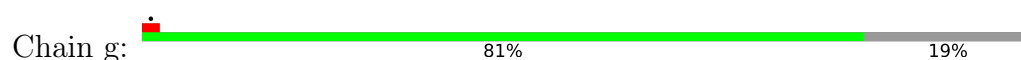




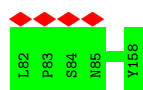
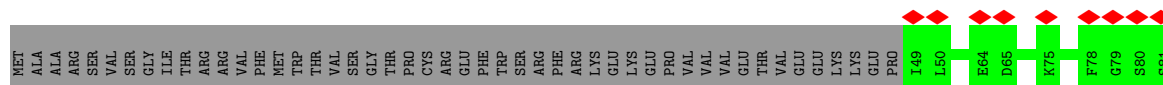
- Molecule 74: 39S ribosomal protein L48, mitochondrial



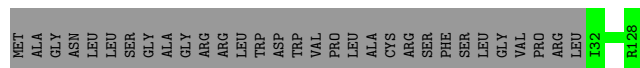
- Molecule 75: 39S ribosomal protein L49, mitochondrial



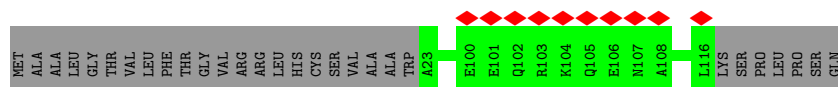
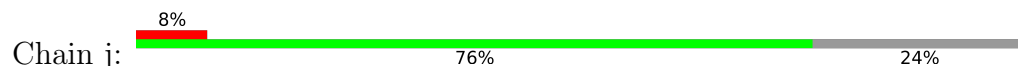
- Molecule 76: 39S ribosomal protein L50, mitochondrial




- Molecule 77: 39S ribosomal protein L51, mitochondrial

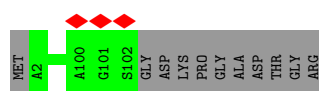


- Molecule 78: 39S ribosomal protein L52, mitochondrial



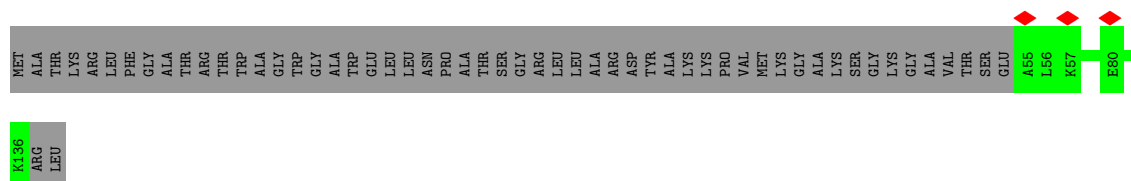
- Molecule 79: 39S ribosomal protein L53, mitochondrial

Chain k:  90% 10%




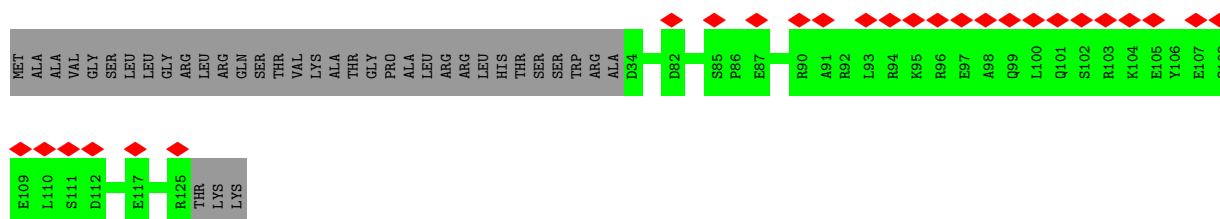
- Molecule 80: 39S ribosomal protein L54, mitochondrial

Chain l:  59% 41%




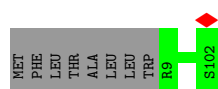
- Molecule 81: 39S ribosomal protein L55, mitochondrial

Chain m:  20% 72% 28%



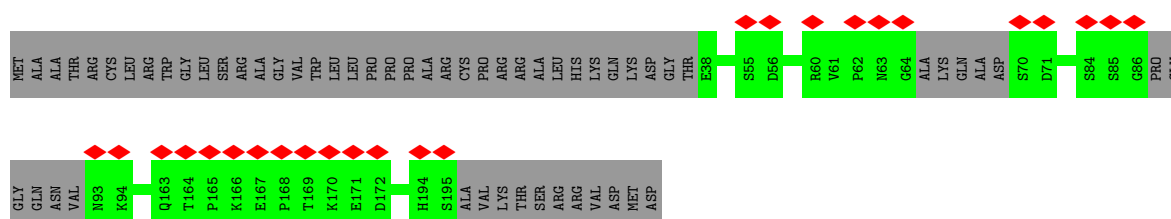
- Molecule 82: Ribosomal protein 63, mitochondrial

Chain o:  92% 8%



- Molecule 83: Peptidyl-tRNA hydrolase ICT1, mitochondrial

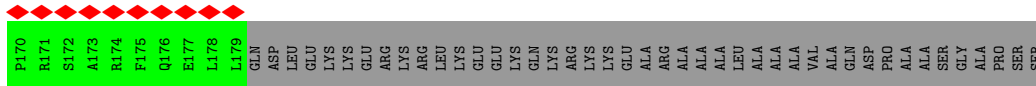
Chain p:  12% 71% 29%

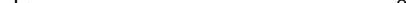


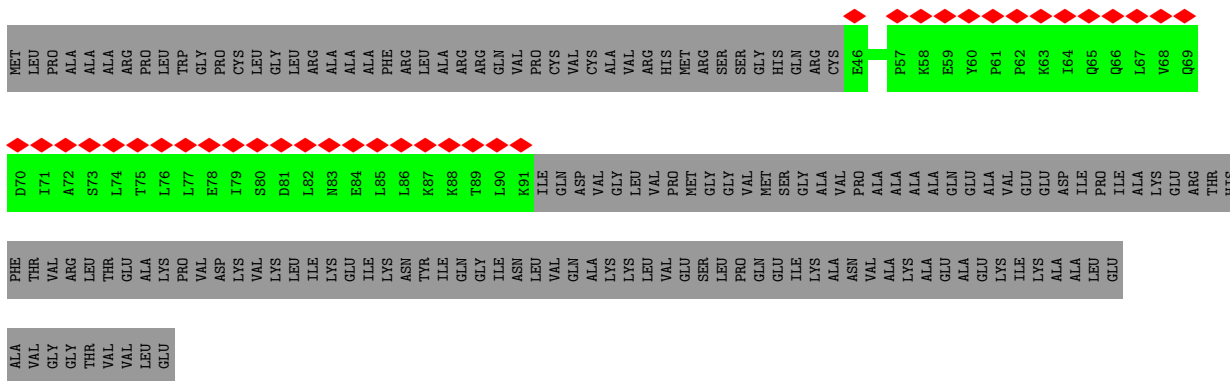
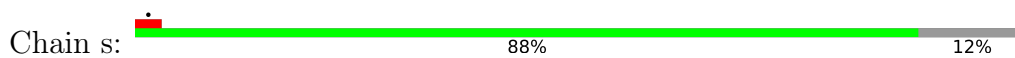
- Molecule 84: Growth arrest and DNA damage-inducible proteins-interacting protein 1

Chain q:  18% 70% 30%

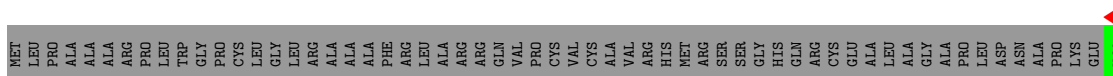


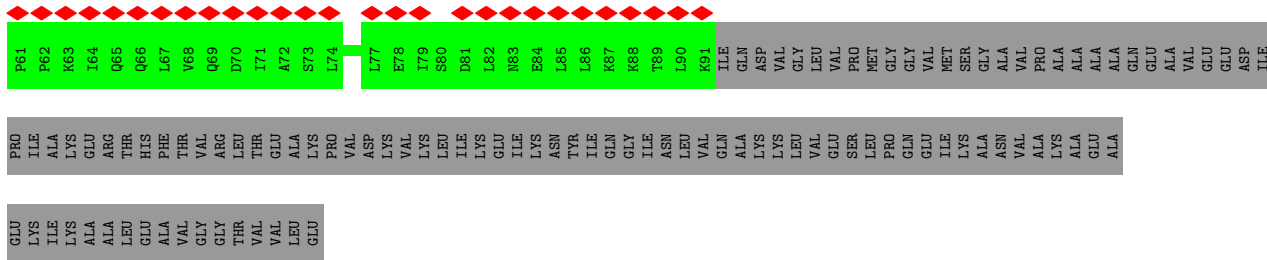


- Chain r:  83% 17%

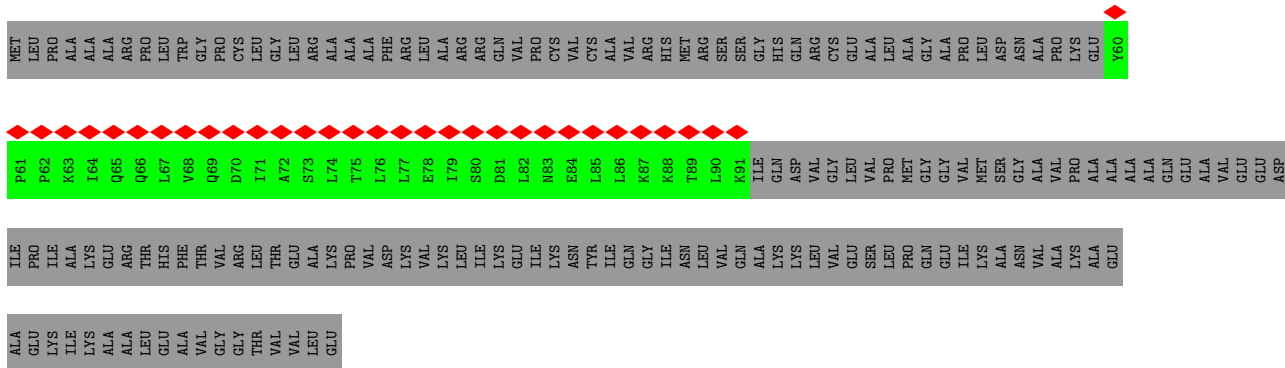


- Chain u:  15% 16% 84%

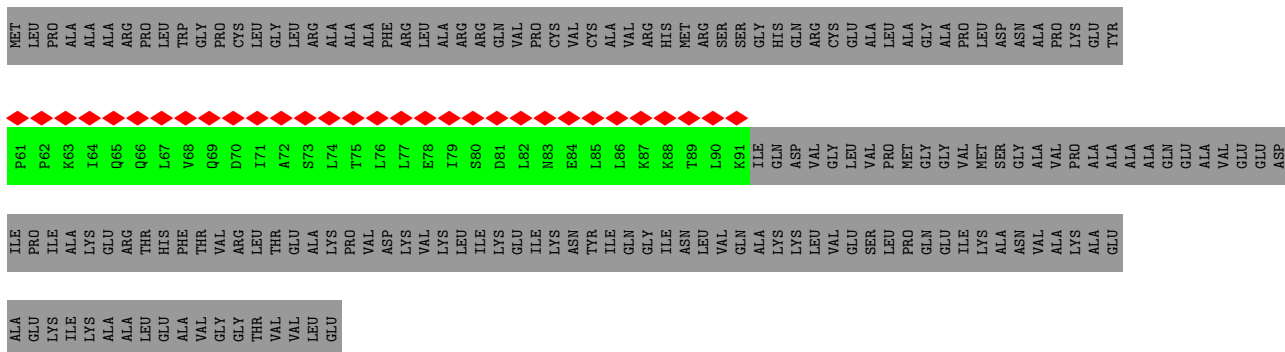




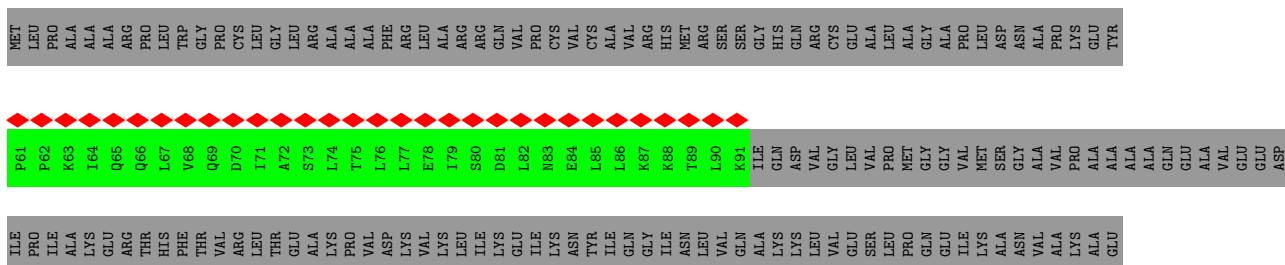
- Molecule 87: 39S ribosomal protein L12, mitochondrial



- Molecule 87: 39S ribosomal protein L12, mitochondrial



- Molecule 87: 39S ribosomal protein L12, mitochondrial



4 Experimental information

| Property | Value | Source |
|--------------------------------------|---|-----------|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 509691 | 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 ($e^-/\text{\AA}^2$) | 30 | Depositor |
| Minimum defocus (nm) | 600 | Depositor |
| Maximum defocus (nm) | 2800 | Depositor |
| Magnification | Not provided | |
| Image detector | GATAN K2 SUMMIT (4k x 4k) | Depositor |
| Maximum map value | 71.473 | Depositor |
| Minimum map value | -28.186 | Depositor |
| Average map value | 0.002 | Depositor |
| Map value standard deviation | 1.438 | Depositor |
| Recommended contour level | 4.0 | Depositor |
| Map size (Å) | 448.19998, 448.19998, 448.19998 | wwPDB |
| Map dimensions | 540, 540, 540 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 0.83, 0.83, 0.83 | Depositor |

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, AYA, FES, 5MC, ATP, MA6, OMU, SPD, 2MG, NAD, B8T, PSU, K, THC, SAC, 1MA, 5F0, PUT, 5MU, OMG, SPM, GDP

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 | 0.19 | 0/22537 | 0.67 | 0/35085 |
| 2 | AB | 0.24 | 0/1871 | 0.49 | 0/2531 |
| 3 | AC | 0.25 | 0/1113 | 0.48 | 0/1505 |
| 4 | AD | 0.24 | 0/2783 | 0.51 | 0/3724 |
| 5 | AE | 0.24 | 0/989 | 0.52 | 0/1335 |
| 6 | AF | 0.24 | 0/1767 | 0.46 | 0/2373 |
| 7 | AG | 0.24 | 0/2746 | 0.48 | 0/3681 |
| 8 | AH | 0.24 | 0/1178 | 0.47 | 0/1598 |
| 9 | AI | 0.25 | 0/1030 | 0.49 | 0/1386 |
| 10 | AJ | 0.25 | 0/855 | 0.55 | 0/1148 |
| 11 | AK | 0.22 | 0/880 | 0.57 | 0/1182 |
| 12 | AL | 0.23 | 0/1477 | 0.47 | 0/1974 |
| 13 | AM | 0.24 | 0/963 | 0.53 | 0/1295 |
| 14 | AN | 0.23 | 0/886 | 0.50 | 0/1199 |
| 15 | AO | 0.24 | 0/1648 | 0.48 | 0/2243 |
| 16 | AP | 0.24 | 0/798 | 0.44 | 0/1070 |
| 17 | AQ | 0.23 | 0/748 | 0.56 | 0/994 |
| 18 | AR | 0.23 | 0/2456 | 0.44 | 0/3317 |
| 19 | AS | 0.24 | 0/1138 | 0.50 | 0/1533 |
| 20 | AT | 0.24 | 0/1402 | 0.46 | 0/1883 |
| 21 | AU | 0.23 | 0/1510 | 0.53 | 0/2025 |
| 22 | AV | 0.26 | 0/3030 | 0.43 | 0/4093 |
| 23 | AW | 0.25 | 0/801 | 0.51 | 0/1079 |
| 24 | AX | 0.24 | 0/2921 | 0.44 | 0/3954 |
| 25 | AY | 0.24 | 0/1280 | 0.39 | 0/1725 |
| 26 | AZ | 0.25 | 0/857 | 0.50 | 0/1141 |
| 27 | A0 | 0.24 | 0/1834 | 0.54 | 0/2484 |
| 28 | A1 | 0.24 | 0/2313 | 0.45 | 0/3129 |
| 29 | A2 | 0.24 | 0/941 | 0.54 | 0/1257 |
| 30 | A3 | 0.23 | 0/636 | 0.57 | 0/839 |
| 31 | A4 | 0.24 | 0/4877 | 0.43 | 0/6598 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|----------------|-------------|---------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 32 | Aw | 0.13 | 0/517 | 0.64 | 0/799 |
| 33 | Ax | 0.29 | 1/1655 (0.1%) | 0.65 | 0/2569 |
| 34 | Az | 0.13 | 0/803 | 0.65 | 0/1244 |
| 35 | A | 0.19 | 1/36876 (0.0%) | 0.68 | 0/57402 |
| 36 | B | 0.33 | 1/1627 (0.1%) | 0.67 | 0/2527 |
| 37 | D | 0.23 | 0/1896 | 0.56 | 0/2549 |
| 38 | E | 0.24 | 0/2475 | 0.47 | 0/3355 |
| 39 | F | 0.23 | 0/2090 | 0.50 | 0/2842 |
| 40 | H | 0.23 | 0/1698 | 0.49 | 0/2292 |
| 41 | I | 0.24 | 0/1731 | 0.48 | 0/2345 |
| 42 | J | 0.25 | 0/1348 | 0.48 | 0/1813 |
| 43 | K | 0.24 | 0/1490 | 0.47 | 0/2021 |
| 44 | L | 0.23 | 0/905 | 0.54 | 0/1218 |
| 45 | M | 0.25 | 0/2381 | 0.53 | 0/3212 |
| 46 | N | 0.24 | 0/1833 | 0.51 | 0/2468 |
| 47 | O | 0.23 | 0/1283 | 0.53 | 0/1727 |
| 48 | P | 0.24 | 0/1199 | 0.53 | 0/1623 |
| 49 | Q | 0.24 | 0/2039 | 0.50 | 0/2750 |
| 50 | R | 0.23 | 0/1175 | 0.54 | 0/1572 |
| 51 | S | 0.23 | 0/1320 | 0.53 | 0/1789 |
| 52 | T | 0.25 | 0/1403 | 0.51 | 0/1886 |
| 53 | U | 0.24 | 0/1274 | 0.54 | 0/1723 |
| 54 | V | 0.24 | 0/1721 | 0.51 | 0/2333 |
| 55 | W | 0.25 | 0/926 | 0.49 | 0/1244 |
| 56 | X | 0.24 | 0/2099 | 0.47 | 0/2837 |
| 57 | Y | 0.23 | 0/1593 | 0.49 | 0/2136 |
| 58 | Z | 0.23 | 0/1021 | 0.47 | 0/1378 |
| 59 | 0 | 0.23 | 0/913 | 0.53 | 0/1224 |
| 60 | 1 | 0.25 | 0/469 | 0.55 | 0/621 |
| 61 | 2 | 0.23 | 0/383 | 0.58 | 0/507 |
| 62 | 3 | 0.23 | 0/853 | 0.53 | 0/1136 |
| 63 | 4 | 0.23 | 0/350 | 0.56 | 0/461 |
| 64 | 5 | 0.24 | 0/3305 | 0.48 | 0/4502 |
| 65 | 6 | 0.25 | 0/3043 | 0.52 | 0/4140 |
| 66 | 7 | 0.24 | 0/2447 | 0.47 | 0/3310 |
| 67 | 8 | 0.24 | 0/1303 | 0.48 | 0/1750 |
| 68 | 9 | 0.26 | 0/1025 | 0.48 | 0/1379 |
| 69 | a | 0.24 | 0/866 | 0.51 | 0/1174 |
| 70 | b | 0.23 | 0/1211 | 0.54 | 0/1639 |
| 71 | c | 0.24 | 0/2347 | 0.47 | 0/3171 |
| 72 | d | 0.24 | 0/2039 | 0.47 | 0/2759 |
| 73 | e | 0.24 | 0/1970 | 0.47 | 0/2658 |
| 74 | f | 0.24 | 0/1273 | 0.44 | 0/1716 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|-----------------|-------------|----------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 75 | g | 0.25 | 0/1151 | 0.49 | 0/1569 |
| 76 | h | 0.23 | 0/918 | 0.45 | 0/1249 |
| 77 | i | 0.23 | 0/850 | 0.53 | 0/1135 |
| 78 | j | 0.24 | 0/760 | 0.51 | 0/1023 |
| 79 | k | 0.23 | 0/777 | 0.53 | 0/1048 |
| 80 | l | 0.24 | 0/707 | 0.49 | 0/960 |
| 81 | m | 0.23 | 0/805 | 0.57 | 0/1081 |
| 82 | o | 0.23 | 0/819 | 0.57 | 0/1097 |
| 83 | p | 0.23 | 0/1223 | 0.50 | 0/1641 |
| 84 | q | 0.23 | 0/1332 | 0.50 | 0/1801 |
| 85 | r | 0.24 | 0/1362 | 0.53 | 0/1846 |
| 86 | s | 0.24 | 0/3239 | 0.51 | 0/4400 |
| 87 | t | 0.23 | 0/358 | 0.35 | 0/486 |
| 87 | u | 0.22 | 0/259 | 0.33 | 0/350 |
| 87 | v | 0.22 | 0/259 | 0.34 | 0/350 |
| 87 | w | 0.21 | 0/246 | 0.35 | 0/331 |
| 87 | x | 0.22 | 0/246 | 0.34 | 0/331 |
| 87 | y | 0.22 | 0/246 | 0.34 | 0/331 |
| 88 | z | 0.25 | 0/1354 | 0.47 | 0/1831 |
| 89 | Ay | 0.32 | 1/1235 (0.1%) | 0.66 | 0/1912 |
| All | All | 0.23 | 4/188586 (0.0%) | 0.57 | 0/267953 |

All (4) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|--------|-------------|----------|
| 35 | A | 1671 | G | OP3-P | -10.76 | 1.48 | 1.61 |
| 36 | B | 1 | C | OP3-P | -10.61 | 1.48 | 1.61 |
| 33 | Ax | 1 | U | OP3-P | -10.58 | 1.48 | 1.61 |
| 89 | Ay | 1 | U | OP3-P | -10.56 | 1.48 | 1.61 |

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | AA | 20260 | 10304 | 10285 | 56 | 0 |
| 2 | AB | 1828 | 1816 | 1815 | 4 | 0 |
| 3 | AC | 1083 | 1089 | 1088 | 8 | 0 |
| 4 | AD | 2731 | 2805 | 2804 | 8 | 0 |
| 5 | AE | 972 | 1000 | 1000 | 6 | 0 |
| 6 | AF | 1725 | 1771 | 1769 | 8 | 0 |
| 7 | AG | 2688 | 2689 | 2687 | 10 | 0 |
| 8 | AH | 1152 | 1187 | 1183 | 9 | 0 |
| 9 | AI | 1020 | 1061 | 1053 | 3 | 0 |
| 10 | AJ | 839 | 888 | 887 | 5 | 0 |
| 11 | AK | 862 | 886 | 885 | 3 | 0 |
| 12 | AL | 1453 | 1541 | 1540 | 3 | 0 |
| 13 | AM | 942 | 966 | 965 | 4 | 0 |
| 14 | AN | 868 | 929 | 928 | 4 | 0 |
| 15 | AO | 1592 | 1557 | 1557 | 4 | 0 |
| 16 | AP | 781 | 806 | 806 | 3 | 0 |
| 17 | AQ | 744 | 758 | 758 | 0 | 0 |
| 18 | AR | 2409 | 2430 | 2428 | 5 | 0 |
| 19 | AS | 1111 | 1116 | 1115 | 1 | 0 |
| 20 | AT | 1371 | 1393 | 1393 | 2 | 0 |
| 21 | AU | 1488 | 1501 | 1499 | 4 | 0 |
| 22 | AV | 2969 | 2964 | 2961 | 19 | 0 |
| 23 | AW | 789 | 804 | 802 | 2 | 0 |
| 24 | AX | 2849 | 2845 | 2843 | 12 | 0 |
| 25 | AY | 1246 | 1198 | 1197 | 6 | 0 |
| 26 | AZ | 839 | 859 | 858 | 1 | 0 |
| 27 | A0 | 1787 | 1797 | 1796 | 7 | 0 |
| 28 | A1 | 2265 | 2296 | 2294 | 9 | 0 |
| 29 | A2 | 935 | 971 | 971 | 6 | 0 |
| 30 | A3 | 625 | 701 | 699 | 6 | 0 |
| 31 | A4 | 4768 | 4770 | 4766 | 11 | 0 |
| 32 | Aw | 464 | 237 | 238 | 0 | 0 |
| 33 | Ax | 1482 | 751 | 752 | 0 | 0 |
| 34 | Az | 719 | 360 | 360 | 0 | 0 |
| 35 | A | 33070 | 16801 | 16794 | 97 | 0 |
| 36 | B | 1524 | 779 | 779 | 2 | 0 |
| 37 | D | 1859 | 1921 | 1920 | 5 | 0 |
| 38 | E | 2406 | 2416 | 2415 | 10 | 0 |
| 39 | F | 2031 | 2066 | 2065 | 4 | 0 |
| 40 | H | 1661 | 1736 | 1734 | 10 | 0 |
| 41 | I | 1695 | 1786 | 1785 | 3 | 0 |
| 42 | J | 1330 | 1408 | 1407 | 5 | 0 |
| 43 | K | 1455 | 1452 | 1452 | 3 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 44 | L | 890 | 942 | 941 | 2 | 0 |
| 45 | M | 2327 | 2396 | 2395 | 6 | 0 |
| 46 | N | 1786 | 1818 | 1817 | 10 | 0 |
| 47 | O | 1259 | 1295 | 1294 | 8 | 0 |
| 48 | P | 1173 | 1166 | 1165 | 2 | 0 |
| 49 | Q | 1990 | 2031 | 2031 | 5 | 0 |
| 50 | R | 1154 | 1215 | 1214 | 1 | 0 |
| 51 | S | 1293 | 1366 | 1365 | 4 | 0 |
| 52 | T | 1369 | 1412 | 1410 | 4 | 0 |
| 53 | U | 1251 | 1232 | 1232 | 4 | 0 |
| 54 | V | 1676 | 1689 | 1687 | 11 | 0 |
| 55 | W | 904 | 936 | 935 | 3 | 0 |
| 56 | X | 2044 | 2061 | 2060 | 2 | 0 |
| 57 | Y | 1556 | 1598 | 1597 | 1 | 0 |
| 58 | Z | 996 | 1045 | 1044 | 3 | 0 |
| 59 | 0 | 898 | 917 | 916 | 2 | 0 |
| 60 | 1 | 464 | 513 | 511 | 1 | 0 |
| 61 | 2 | 377 | 407 | 406 | 0 | 0 |
| 62 | 3 | 832 | 884 | 883 | 2 | 0 |
| 63 | 4 | 342 | 362 | 361 | 2 | 0 |
| 64 | 5 | 3210 | 3209 | 3206 | 5 | 0 |
| 65 | 6 | 2948 | 2844 | 2841 | 10 | 0 |
| 66 | 7 | 2390 | 2399 | 2397 | 10 | 0 |
| 67 | 8 | 1278 | 1310 | 1308 | 3 | 0 |
| 68 | 9 | 997 | 988 | 987 | 3 | 0 |
| 69 | a | 840 | 812 | 810 | 0 | 0 |
| 70 | b | 1196 | 1196 | 1190 | 0 | 0 |
| 71 | c | 2299 | 2322 | 2320 | 0 | 0 |
| 72 | d | 1985 | 1980 | 1976 | 0 | 0 |
| 73 | e | 1931 | 1917 | 1916 | 0 | 0 |
| 74 | f | 1252 | 1271 | 1269 | 0 | 0 |
| 75 | g | 1113 | 1097 | 1097 | 0 | 0 |
| 76 | h | 895 | 883 | 881 | 0 | 0 |
| 77 | i | 828 | 859 | 857 | 0 | 0 |
| 78 | j | 745 | 747 | 746 | 0 | 0 |
| 79 | k | 774 | 785 | 784 | 0 | 0 |
| 80 | l | 688 | 675 | 674 | 0 | 0 |
| 81 | m | 791 | 760 | 796 | 0 | 0 |
| 82 | o | 798 | 806 | 804 | 0 | 0 |
| 83 | p | 1205 | 1225 | 1223 | 0 | 0 |
| 84 | q | 1298 | 1273 | 1272 | 0 | 0 |
| 85 | r | 1322 | 1349 | 1348 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 86 | s | 3155 | 3145 | 3139 | 0 | 0 |
| 87 | t | 354 | 378 | 377 | 0 | 0 |
| 87 | u | 257 | 284 | 283 | 0 | 0 |
| 87 | v | 257 | 284 | 283 | 0 | 0 |
| 87 | w | 245 | 275 | 275 | 0 | 0 |
| 87 | x | 245 | 275 | 275 | 0 | 0 |
| 87 | y | 245 | 275 | 275 | 0 | 0 |
| 88 | z | 1327 | 1355 | 1353 | 0 | 0 |
| 89 | Ay | 1107 | 560 | 563 | 0 | 0 |
| 90 | AA | 44 | 26 | 26 | 0 | 0 |
| 91 | AA | 14 | 30 | 26 | 0 | 0 |
| 92 | A | 30 | 66 | 57 | 0 | 0 |
| 92 | AA | 10 | 22 | 19 | 0 | 0 |
| 93 | A | 137 | 0 | 0 | 0 | 0 |
| 93 | A3 | 1 | 0 | 0 | 0 | 0 |
| 93 | AA | 61 | 0 | 0 | 0 | 0 |
| 93 | AB | 1 | 0 | 0 | 0 | 0 |
| 93 | AX | 1 | 0 | 0 | 0 | 0 |
| 93 | Aw | 1 | 0 | 0 | 0 | 0 |
| 93 | D | 2 | 0 | 0 | 0 | 0 |
| 93 | E | 1 | 0 | 0 | 0 | 0 |
| 93 | g | 1 | 0 | 0 | 0 | 0 |
| 94 | 3 | 1 | 0 | 0 | 0 | 0 |
| 94 | 6 | 1 | 0 | 0 | 0 | 0 |
| 94 | A | 29 | 0 | 0 | 0 | 0 |
| 94 | AA | 18 | 0 | 0 | 0 | 0 |
| 94 | D | 1 | 0 | 0 | 0 | 0 |
| 94 | M | 1 | 0 | 0 | 0 | 0 |
| 94 | W | 1 | 0 | 0 | 0 | 0 |
| 94 | i | 1 | 0 | 0 | 0 | 0 |
| 94 | o | 1 | 0 | 0 | 0 | 0 |
| 95 | 0 | 1 | 0 | 0 | 0 | 0 |
| 95 | 4 | 1 | 0 | 0 | 0 | 0 |
| 95 | AO | 1 | 0 | 0 | 0 | 0 |
| 96 | AP | 4 | 0 | 0 | 0 | 0 |
| 96 | AT | 4 | 0 | 0 | 0 | 0 |
| 96 | r | 4 | 0 | 0 | 0 | 0 |
| 97 | AX | 31 | 12 | 12 | 1 | 0 |
| 98 | AX | 28 | 12 | 12 | 0 | 0 |
| 99 | A | 6 | 14 | 12 | 0 | 0 |
| 100 | B | 7 | 11 | 8 | 0 | 0 |
| 101 | 0 | 27 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 101 | 1 | 3 | 0 | 0 | 0 | 0 |
| 101 | 2 | 34 | 0 | 0 | 0 | 0 |
| 101 | 3 | 40 | 0 | 0 | 0 | 0 |
| 101 | 4 | 13 | 0 | 0 | 0 | 0 |
| 101 | 5 | 22 | 0 | 0 | 0 | 0 |
| 101 | 6 | 100 | 0 | 0 | 1 | 0 |
| 101 | 7 | 17 | 0 | 0 | 0 | 0 |
| 101 | 8 | 19 | 0 | 0 | 1 | 0 |
| 101 | 9 | 17 | 0 | 0 | 0 | 0 |
| 101 | A | 3056 | 0 | 0 | 22 | 0 |
| 101 | A0 | 1 | 0 | 0 | 0 | 0 |
| 101 | A1 | 36 | 0 | 0 | 0 | 0 |
| 101 | A2 | 35 | 0 | 0 | 0 | 0 |
| 101 | A3 | 52 | 0 | 0 | 1 | 0 |
| 101 | A4 | 11 | 0 | 0 | 0 | 0 |
| 101 | AA | 2157 | 0 | 0 | 23 | 0 |
| 101 | AB | 80 | 0 | 0 | 1 | 0 |
| 101 | AC | 58 | 0 | 0 | 0 | 0 |
| 101 | AD | 79 | 0 | 0 | 1 | 0 |
| 101 | AE | 30 | 0 | 0 | 0 | 0 |
| 101 | AF | 36 | 0 | 0 | 0 | 0 |
| 101 | AG | 70 | 0 | 0 | 1 | 0 |
| 101 | AH | 50 | 0 | 0 | 0 | 0 |
| 101 | AI | 44 | 0 | 0 | 1 | 0 |
| 101 | AJ | 29 | 0 | 0 | 1 | 0 |
| 101 | AK | 51 | 0 | 0 | 0 | 0 |
| 101 | AL | 43 | 0 | 0 | 0 | 0 |
| 101 | AM | 21 | 0 | 0 | 0 | 0 |
| 101 | AN | 34 | 0 | 0 | 0 | 0 |
| 101 | AO | 37 | 0 | 0 | 0 | 0 |
| 101 | AP | 31 | 0 | 0 | 0 | 0 |
| 101 | AQ | 68 | 0 | 0 | 0 | 0 |
| 101 | AR | 12 | 0 | 0 | 0 | 0 |
| 101 | AS | 23 | 0 | 0 | 0 | 0 |
| 101 | AT | 43 | 0 | 0 | 0 | 0 |
| 101 | AU | 8 | 0 | 0 | 0 | 0 |
| 101 | AW | 15 | 0 | 0 | 0 | 0 |
| 101 | AX | 61 | 0 | 0 | 1 | 0 |
| 101 | AY | 20 | 0 | 0 | 1 | 0 |
| 101 | AZ | 27 | 0 | 0 | 0 | 0 |
| 101 | Aw | 5 | 0 | 0 | 0 | 0 |
| 101 | Ax | 5 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 101 | Ay | 1 | 0 | 0 | 0 | 0 |
| 101 | Az | 15 | 0 | 0 | 0 | 0 |
| 101 | B | 63 | 0 | 0 | 0 | 0 |
| 101 | D | 73 | 0 | 0 | 0 | 0 |
| 101 | E | 74 | 0 | 0 | 1 | 0 |
| 101 | F | 78 | 0 | 0 | 2 | 0 |
| 101 | H | 9 | 0 | 0 | 0 | 0 |
| 101 | I | 23 | 0 | 0 | 1 | 0 |
| 101 | J | 1 | 0 | 0 | 0 | 0 |
| 101 | K | 65 | 0 | 0 | 1 | 0 |
| 101 | L | 25 | 0 | 0 | 1 | 0 |
| 101 | M | 66 | 0 | 0 | 1 | 0 |
| 101 | N | 60 | 0 | 0 | 4 | 0 |
| 101 | O | 38 | 0 | 0 | 0 | 0 |
| 101 | P | 89 | 0 | 0 | 1 | 0 |
| 101 | Q | 27 | 0 | 0 | 0 | 0 |
| 101 | R | 57 | 0 | 0 | 0 | 0 |
| 101 | S | 49 | 0 | 0 | 1 | 0 |
| 101 | T | 48 | 0 | 0 | 0 | 0 |
| 101 | U | 26 | 0 | 0 | 0 | 0 |
| 101 | V | 5 | 0 | 0 | 0 | 0 |
| 101 | W | 48 | 0 | 0 | 0 | 0 |
| 101 | X | 12 | 0 | 0 | 0 | 0 |
| 101 | Y | 29 | 0 | 0 | 0 | 0 |
| 101 | Z | 34 | 0 | 0 | 0 | 0 |
| 101 | a | 13 | 0 | 0 | 0 | 0 |
| 101 | b | 39 | 0 | 0 | 0 | 0 |
| 101 | c | 20 | 0 | 0 | 0 | 0 |
| 101 | d | 5 | 0 | 0 | 0 | 0 |
| 101 | e | 13 | 0 | 0 | 0 | 0 |
| 101 | f | 22 | 0 | 0 | 0 | 0 |
| 101 | g | 13 | 0 | 0 | 0 | 0 |
| 101 | i | 54 | 0 | 0 | 0 | 0 |
| 101 | j | 23 | 0 | 0 | 0 | 0 |
| 101 | k | 6 | 0 | 0 | 0 | 0 |
| 101 | l | 5 | 0 | 0 | 0 | 0 |
| 101 | m | 8 | 0 | 0 | 0 | 0 |
| 101 | o | 34 | 0 | 0 | 0 | 0 |
| 101 | p | 10 | 0 | 0 | 0 | 0 |
| 101 | r | 50 | 0 | 0 | 0 | 0 |
| 101 | s | 51 | 0 | 0 | 0 | 0 |
| All | All | 187689 | 152427 | 152294 | 391 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

All (391) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:A:2103:A:HO2' | 58:Z:35:LYS:N | 1.72 | 0.86 |
| 22:AV:226:TYR:HE1 | 22:AV:282:VAL:HG21 | 1.42 | 0.83 |
| 7:AG:389:ARG:NH1 | 7:AG:390:LYS:O | 2.12 | 0.83 |
| 6:AF:159:VAL:HG23 | 6:AF:172:VAL:HG21 | 1.63 | 0.80 |
| 35:A:3063:G:O2' | 35:A:3066:C:OP2 | 2.00 | 0.79 |
| 35:A:3042:U:OP2 | 101:A:3501:HOH:O | 2.00 | 0.79 |
| 35:A:3198:A:O2' | 35:A:3200:U:O2' | 2.01 | 0.78 |
| 53:U:9:LEU:O | 53:U:11:ARG:NH1 | 2.16 | 0.78 |
| 1:AA:1472:G:O6 | 101:AA:1801:HOH:O | 2.01 | 0.78 |
| 65:6:121:ARG:NH1 | 67:8:112:GLU:OE2 | 2.19 | 0.76 |
| 35:A:3147:G:OP1 | 101:A:3502:HOH:O | 2.04 | 0.75 |
| 35:A:2098:G:O2' | 35:A:2099:U:OP2 | 2.04 | 0.75 |
| 22:AV:92:LEU:HD21 | 22:AV:137:ILE:HD11 | 1.69 | 0.74 |
| 35:A:3226:G:O2' | 35:A:3229:U:O4 | 2.04 | 0.74 |
| 31:A4:303:CYS:SG | 31:A4:344:ARG:NH2 | 2.60 | 0.74 |
| 35:A:3041:U:OP1 | 101:A:3504:HOH:O | 2.05 | 0.74 |
| 35:A:3113:A:OP1 | 35:A:3167:U:O2' | 2.04 | 0.73 |
| 24:AX:108:LEU:HD23 | 24:AX:141:VAL:HG21 | 1.71 | 0.73 |
| 39:F:115:LYS:NZ | 101:F:401:HOH:O | 2.21 | 0.72 |
| 1:AA:1287:A:OP2 | 4:AD:260:LYS:NZ | 2.21 | 0.72 |
| 53:U:11:ARG:NH2 | 54:V:211:LYS:O | 2.22 | 0.72 |
| 1:AA:941:G:OP1 | 101:AA:1802:HOH:O | 2.07 | 0.72 |
| 22:AV:208:LEU:HD13 | 22:AV:226:TYR:HD2 | 1.56 | 0.71 |
| 22:AV:46:GLU:OE2 | 22:AV:74:ARG:NE | 2.21 | 0.70 |
| 1:AA:1047:A:OP2 | 101:AA:1804:HOH:O | 2.09 | 0.70 |
| 22:AV:226:TYR:CE1 | 22:AV:282:VAL:HG21 | 2.27 | 0.69 |
| 1:AA:1570:G:O6 | 101:AA:1803:HOH:O | 2.09 | 0.69 |
| 65:6:217:LEU:HD11 | 65:6:271:LEU:HD12 | 1.74 | 0.69 |
| 35:A:1777:A:N6 | 35:A:1780:U:OP2 | 2.25 | 0.69 |
| 35:A:3015:U:OP1 | 101:A:3506:HOH:O | 2.10 | 0.69 |
| 35:A:2290:A:N7 | 101:A:3533:HOH:O | 2.26 | 0.69 |
| 25:AY:318:GLU:OE1 | 101:AY:401:HOH:O | 2.11 | 0.68 |
| 24:AX:272:THR:OG1 | 24:AX:282:ILE:O | 2.10 | 0.68 |
| 31:A4:556:LYS:NZ | 31:A4:560:GLU:OE2 | 2.27 | 0.68 |
| 1:AA:976:A:N7 | 101:AA:1832:HOH:O | 2.25 | 0.68 |
| 1:AA:1578:A:OP2 | 101:AA:1806:HOH:O | 2.11 | 0.68 |
| 35:A:2181:A:OP1 | 101:A:3509:HOH:O | 2.12 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AA:1314:C:OP2 | 101:AA:1805:HOH:O | 2.11 | 0.68 |
| 44:L:95:ARG:NH2 | 101:L:201:HOH:O | 2.28 | 0.67 |
| 51:S:112:ASP:OD2 | 101:S:301:HOH:O | 2.13 | 0.67 |
| 46:N:73:ARG:O | 46:N:155:LYS:NZ | 2.27 | 0.67 |
| 1:AA:1040:U:OP2 | 101:AA:1807:HOH:O | 2.14 | 0.66 |
| 46:N:212:PRO:O | 101:N:301:HOH:O | 2.13 | 0.66 |
| 35:A:2543:C:OP1 | 101:A:3508:HOH:O | 2.11 | 0.66 |
| 1:AA:1154:A:OP2 | 30:A3:155:ARG:NH2 | 2.29 | 0.66 |
| 1:AA:684:U:OP1 | 101:AA:1808:HOH:O | 2.14 | 0.66 |
| 37:D:281:TRP:O | 37:D:285:LYS:NZ | 2.29 | 0.66 |
| 1:AA:1151:C:N3 | 101:AA:1843:HOH:O | 2.29 | 0.66 |
| 40:H:178:ASN:OD1 | 40:H:179:ASN:N | 2.28 | 0.66 |
| 46:N:143:GLY:O | 101:N:302:HOH:O | 2.14 | 0.66 |
| 64:5:165:GLN:NE2 | 64:5:179:VAL:HG21 | 2.11 | 0.66 |
| 35:A:2372:U:OP2 | 101:A:3511:HOH:O | 2.14 | 0.66 |
| 97:AX:501:ATP:O1G | 101:AX:601:HOH:O | 2.15 | 0.65 |
| 35:A:1957:A:OP1 | 101:A:3510:HOH:O | 2.13 | 0.65 |
| 35:A:2314:C:OP2 | 101:A:3512:HOH:O | 2.14 | 0.65 |
| 1:AA:894:C:OP1 | 101:AA:1809:HOH:O | 2.14 | 0.65 |
| 35:A:2160:A:OP2 | 63:4:88:TRP:NE1 | 2.29 | 0.65 |
| 65:6:322:ARG:NH1 | 101:6:502:HOH:O | 2.29 | 0.65 |
| 1:AA:930:G:O6 | 10:AJ:47:ARG:NH2 | 2.29 | 0.65 |
| 67:8:133:ARG:NH1 | 101:8:301:HOH:O | 2.24 | 0.65 |
| 35:A:1990:G:OP1 | 37:D:269:ARG:NH2 | 2.28 | 0.64 |
| 35:A:2826:G:OP1 | 55:W:49:ARG:NH1 | 2.31 | 0.64 |
| 35:A:2562:U:O2' | 37:D:284:ARG:O | 2.09 | 0.64 |
| 35:A:1882:A:N7 | 101:A:3546:HOH:O | 2.29 | 0.64 |
| 1:AA:828:C:OP2 | 101:AA:1810:HOH:O | 2.15 | 0.64 |
| 35:A:2216:A:O2' | 101:A:3505:HOH:O | 2.09 | 0.64 |
| 35:A:3013:G:HO2' | 63:4:66:PHE:N | 1.96 | 0.64 |
| 35:A:2539:A:OP1 | 101:A:3515:HOH:O | 2.15 | 0.64 |
| 35:A:1856:A:OP2 | 35:A:2986:C:O2' | 2.16 | 0.64 |
| 35:A:2531:U:O4 | 37:D:246:ARG:NH2 | 2.31 | 0.64 |
| 35:A:1745:U:O4 | 62:3:108:LYS:NZ | 2.30 | 0.63 |
| 4:AD:244:LEU:HD22 | 4:AD:343:LEU:HD23 | 1.81 | 0.63 |
| 7:AG:210:VAL:HG12 | 7:AG:210:VAL:O | 1.98 | 0.63 |
| 25:AY:322:ASP:O | 25:AY:324:ASP:N | 2.32 | 0.62 |
| 3:AC:109:VAL:HG23 | 28:A1:103:LEU:HD11 | 1.82 | 0.61 |
| 35:A:1871:A:N3 | 62:3:104:ARG:NH2 | 2.48 | 0.61 |
| 38:E:129:VAL:CG1 | 38:E:145:LEU:HD11 | 2.30 | 0.61 |
| 6:AF:174:LEU:O | 6:AF:179:ARG:NH1 | 2.33 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:A:2767:A:O2' | 35:A:2769:A:N7 | 2.33 | 0.61 |
| 47:O:62:TYR:OH | 49:Q:272:GLU:OE2 | 2.18 | 0.61 |
| 57:Y:134:LYS:NZ | 68:9:76:TYR:OH | 2.32 | 0.61 |
| 58:Z:78:ARG:O | 58:Z:83:LYS:NZ | 2.34 | 0.60 |
| 8:AH:104:ILE:HG23 | 8:AH:148:LEU:HD21 | 1.84 | 0.60 |
| 1:AA:1554:G:OP2 | 101:AA:1814:HOH:O | 2.17 | 0.60 |
| 35:A:1747:G:OP2 | 35:A:1749:C:N4 | 2.34 | 0.59 |
| 42:J:113:THR:OG1 | 42:J:116:HIS:ND1 | 2.26 | 0.59 |
| 66:7:175:ILE:O | 66:7:319:ARG:NH2 | 2.35 | 0.59 |
| 29:A2:64:ASP:OD1 | 29:A2:65:ALA:N | 2.36 | 0.59 |
| 41:I:31:LYS:NZ | 101:I:301:HOH:O | 2.35 | 0.59 |
| 68:9:16:ASP:OD1 | 68:9:25:ARG:NH2 | 2.35 | 0.59 |
| 35:A:1958:G:OP1 | 101:A:3516:HOH:O | 2.17 | 0.58 |
| 35:A:2108:G:O6 | 46:N:67:LYS:NZ | 2.36 | 0.58 |
| 1:AA:1188:A:OP2 | 1:AA:1429:C:O2' | 2.15 | 0.58 |
| 1:AA:1294:A:OP1 | 2:AB:201:ASN:ND2 | 2.36 | 0.58 |
| 35:A:2196:A:O2' | 35:A:2213:A:N1 | 2.35 | 0.58 |
| 38:E:129:VAL:HG11 | 38:E:145:LEU:HD11 | 1.86 | 0.58 |
| 1:AA:769:G:OP2 | 14:AN:73:ARG:NH2 | 2.35 | 0.58 |
| 44:L:130:ARG:NH1 | 44:L:133:GLU:OE2 | 2.36 | 0.58 |
| 22:AV:208:LEU:HD13 | 22:AV:226:TYR:CD2 | 2.36 | 0.58 |
| 1:AA:1208:U:OP1 | 101:AA:1813:HOH:O | 2.16 | 0.57 |
| 101:AA:1827:HOH:O | 5:AE:123:ARG:NH2 | 2.36 | 0.57 |
| 35:A:2021:U:OP1 | 101:A:3517:HOH:O | 2.17 | 0.57 |
| 35:A:2740:A:N3 | 35:A:2921:A:O2' | 2.32 | 0.57 |
| 38:E:50:ASP:O | 47:O:138:ARG:NH2 | 2.37 | 0.57 |
| 39:F:70:ARG:NH2 | 39:F:194:GLU:OE1 | 2.37 | 0.57 |
| 11:AK:58:ARG:NE | 11:AK:72:ASP:OD1 | 2.36 | 0.57 |
| 35:A:3089:A:H3' | 35:A:3090:G:C5' | 2.34 | 0.57 |
| 28:A1:152:ASP:OD2 | 28:A1:174:ARG:NH1 | 2.31 | 0.57 |
| 35:A:3110:C:O2' | 38:E:266:ARG:NH1 | 2.38 | 0.57 |
| 1:AA:1015:A:OP2 | 101:AA:1816:HOH:O | 2.18 | 0.56 |
| 18:AR:69:THR:N | 18:AR:72:ASP:OD2 | 2.38 | 0.56 |
| 1:AA:1109:A:OP2 | 101:AA:1815:HOH:O | 2.17 | 0.56 |
| 2:AB:88:ARG:NH1 | 101:AB:403:HOH:O | 2.38 | 0.56 |
| 4:AD:245:VAL:HG22 | 4:AD:271:ALA:HB1 | 1.86 | 0.56 |
| 6:AF:172:VAL:HG12 | 6:AF:240:ARG:HD3 | 1.86 | 0.56 |
| 35:A:2545:U:O2' | 101:A:3514:HOH:O | 2.15 | 0.56 |
| 29:A2:43:ALA:HB1 | 29:A2:46:ILE:HD11 | 1.88 | 0.56 |
| 35:A:2364:C:OP2 | 53:U:78:LYS:NZ | 2.38 | 0.56 |
| 22:AV:236:LEU:CD1 | 22:AV:290:LEU:HD13 | 2.36 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:1308:U:O2' | 3:AC:64:HIS:ND1 | 2.36 | 0.55 |
| 48:P:138:GLU:OE2 | 101:P:201:HOH:O | 2.18 | 0.55 |
| 4:AD:340:ILE:HG22 | 4:AD:340:ILE:O | 2.07 | 0.55 |
| 35:A:1760:G:OP1 | 45:M:196:ARG:NE | 2.40 | 0.55 |
| 1:AA:1257:U:O2' | 1:AA:1260:A:OP2 | 2.14 | 0.55 |
| 29:A2:33:VAL:HG21 | 29:A2:104:LEU:HD23 | 1.87 | 0.55 |
| 35:A:1805:A:OP2 | 54:V:94:HIS:NE2 | 2.36 | 0.55 |
| 1:AA:1346:A:OP2 | 101:AA:1818:HOH:O | 2.18 | 0.54 |
| 1:AA:845:A:H4' | 21:AU:60:TYR:CE2 | 2.43 | 0.54 |
| 22:AV:228:TYR:HB3 | 22:AV:259:ALA:HB2 | 1.89 | 0.54 |
| 1:AA:843:G:N2 | 1:AA:846:A:OP2 | 2.35 | 0.54 |
| 1:AA:1044:U:OP1 | 1:AA:1110:A:O2' | 2.22 | 0.54 |
| 22:AV:236:LEU:HD12 | 22:AV:290:LEU:HD13 | 1.89 | 0.54 |
| 24:AX:151:LEU:CD2 | 24:AX:247:LEU:HD22 | 2.38 | 0.54 |
| 35:A:2016:C:OP2 | 45:M:59:ARG:NH1 | 2.41 | 0.54 |
| 1:AA:1264:C:H1' | 8:AH:124:VAL:HG13 | 1.90 | 0.53 |
| 10:AJ:117:ASP:OD1 | 101:AJ:201:HOH:O | 2.17 | 0.53 |
| 35:A:2761:C:O2 | 35:A:2786:U:N3 | 2.42 | 0.53 |
| 8:AH:184:ILE:O | 8:AH:184:ILE:HG22 | 2.08 | 0.53 |
| 24:AX:108:LEU:HD21 | 24:AX:307:VAL:HG11 | 1.90 | 0.53 |
| 35:A:1953:A:O2' | 35:A:2463:A:OP1 | 2.26 | 0.53 |
| 35:A:2462:A:N3 | 101:A:3569:HOH:O | 2.34 | 0.53 |
| 1:AA:1458:A:OP1 | 6:AF:104:LYS:NZ | 2.29 | 0.53 |
| 35:A:2071:U:O2' | 65:6:28:ARG:NH2 | 2.42 | 0.52 |
| 35:A:2354:A:O2' | 101:A:3503:HOH:O | 2.05 | 0.52 |
| 29:A2:36:ARG:NH2 | 29:A2:92:THR:HG23 | 2.25 | 0.52 |
| 7:AG:229:LEU:HD21 | 7:AG:241:VAL:HG11 | 1.91 | 0.52 |
| 1:AA:702:C:OP1 | 1:AA:848:U:O2' | 2.26 | 0.52 |
| 7:AG:200:LEU:HD11 | 7:AG:204:GLU:HB3 | 1.91 | 0.52 |
| 65:6:161:LEU:HD13 | 65:6:271:LEU:HD11 | 1.91 | 0.52 |
| 64:5:173:ARG:HA | 64:5:176:TYR:CE1 | 2.45 | 0.52 |
| 9:AI:87:HIS:NE2 | 101:AI:201:HOH:O | 2.25 | 0.51 |
| 30:A3:144:ARG:NH2 | 101:A3:301:HOH:O | 2.43 | 0.51 |
| 35:A:1742:G:O2' | 35:A:1754:G:O6 | 2.23 | 0.51 |
| 54:V:163:ASP:OD1 | 54:V:164:GLY:N | 2.44 | 0.51 |
| 1:AA:1134:G:OP2 | 10:AJ:38:ARG:NH2 | 2.43 | 0.51 |
| 22:AV:187:PHE:CE1 | 22:AV:352:LEU:HD13 | 2.46 | 0.51 |
| 5:AE:65:LEU:HD11 | 16:AP:75:LYS:CD | 2.41 | 0.51 |
| 46:N:247:MET:SD | 101:N:331:HOH:O | 2.60 | 0.50 |
| 52:T:184:LYS:NZ | 52:T:192:GLU:OE1 | 2.38 | 0.50 |
| 35:A:1749:C:OP2 | 35:A:2899:C:O2' | 2.28 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 46:N:251:VAL:OXT | 101:N:303:HOH:O | 2.19 | 0.50 |
| 40:H:53:THR:N | 40:H:86:THR:HG1 | 2.10 | 0.50 |
| 54:V:188:VAL:O | 54:V:188:VAL:HG23 | 2.11 | 0.50 |
| 1:AA:841:A:OP1 | 13:AM:39:ASN:ND2 | 2.42 | 0.50 |
| 22:AV:225:LEU:HD11 | 22:AV:283:LEU:HD22 | 1.94 | 0.50 |
| 24:AX:108:LEU:HD21 | 24:AX:307:VAL:CG1 | 2.42 | 0.50 |
| 24:AX:183:GLU:N | 24:AX:183:GLU:OE1 | 2.42 | 0.50 |
| 28:A1:250:GLU:OE2 | 28:A1:301:ASN:ND2 | 2.45 | 0.50 |
| 56:X:177:HIS:O | 56:X:184:ARG:NH1 | 2.44 | 0.50 |
| 35:A:2162:C:OP2 | 101:A:3519:HOH:O | 2.19 | 0.49 |
| 35:A:2537:G:O2' | 35:A:2634:U:OP2 | 2.26 | 0.49 |
| 28:A1:46:ARG:HB2 | 28:A1:47:PRO:HD3 | 1.93 | 0.49 |
| 1:AA:768:A:O2' | 14:AN:24:LYS:NZ | 2.45 | 0.49 |
| 1:AA:1004:G:O2' | 9:AI:98:GLN:NE2 | 2.45 | 0.49 |
| 51:S:173:ARG:HB2 | 51:S:182:LYS:HG2 | 1.92 | 0.49 |
| 40:H:146:LEU:O | 40:H:150:GLY:N | 2.42 | 0.49 |
| 1:AA:1215:U:O4 | 101:AA:1819:HOH:O | 2.18 | 0.49 |
| 43:K:52:ASP:OD1 | 101:K:201:HOH:O | 2.19 | 0.49 |
| 29:A2:33:VAL:HG22 | 29:A2:105:ASN:OD1 | 2.13 | 0.49 |
| 35:A:2483:U:H2' | 35:A:2484:C:O4' | 2.13 | 0.49 |
| 15:AO:208:PRO:HG2 | 15:AO:213:LEU:HD21 | 1.94 | 0.48 |
| 28:A1:46:ARG:HB2 | 28:A1:47:PRO:CD | 2.43 | 0.48 |
| 1:AA:899:G:O2' | 1:AA:907:A:N1 | 2.33 | 0.48 |
| 24:AX:268:LEU:HD21 | 24:AX:293:LEU:HD23 | 1.96 | 0.48 |
| 54:V:169:THR:HG22 | 54:V:169:THR:O | 2.12 | 0.48 |
| 3:AC:106:ASP:OD1 | 3:AC:107:GLN:N | 2.43 | 0.48 |
| 6:AF:159:VAL:CG2 | 6:AF:172:VAL:HG21 | 2.40 | 0.48 |
| 7:AG:384:GLN:NE2 | 101:AG:404:HOH:O | 2.47 | 0.48 |
| 31:A4:239:ARG:O | 31:A4:242:ASN:ND2 | 2.44 | 0.48 |
| 35:A:2909:G:OP1 | 60:1:63:ARG:NH1 | 2.42 | 0.48 |
| 10:AJ:78:ARG:NH2 | 10:AJ:117:ASP:OD2 | 2.47 | 0.48 |
| 55:W:102:GLU:OE2 | 65:6:74:TYR:N | 2.45 | 0.48 |
| 8:AH:155:VAL:HG21 | 28:A1:129:PHE:CB | 2.43 | 0.48 |
| 24:AX:297:MET:HE3 | 24:AX:306:ILE:HG21 | 1.95 | 0.48 |
| 35:A:2104:A:OP1 | 46:N:231:SER:OG | 2.21 | 0.48 |
| 35:A:2888:A:H3' | 35:A:2889:C:C5' | 2.44 | 0.48 |
| 47:O:64:LYS:NZ | 47:O:100:GLN:O | 2.47 | 0.48 |
| 35:A:2499:U:OP2 | 35:A:2504:A:N6 | 2.36 | 0.48 |
| 1:AA:1427:A:N7 | 101:AA:1873:HOH:O | 2.35 | 0.48 |
| 66:7:156:ARG:HG3 | 66:7:156:ARG:HH11 | 1.78 | 0.48 |
| 1:AA:749:G:O3' | 14:AN:78:LYS:NZ | 2.40 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 15:AO:217:ARG:NH1 | 15:AO:227:GLU:OE2 | 2.46 | 0.47 |
| 22:AV:360:VAL:HG13 | 22:AV:364:LEU:HD22 | 1.96 | 0.47 |
| 1:AA:1479:C:OP1 | 101:AA:1820:HOH:O | 2.20 | 0.47 |
| 22:AV:190:LEU:HD13 | 22:AV:226:TYR:CE2 | 2.49 | 0.47 |
| 35:A:1851:G:H2' | 35:A:2693:A:N7 | 2.29 | 0.47 |
| 47:O:144:LEU:HD12 | 66:7:174:VAL:HG11 | 1.97 | 0.47 |
| 3:AC:115:ASN:ND2 | 25:AY:309:LYS:O | 2.48 | 0.47 |
| 35:A:3201:A:H2' | 35:A:3202:U:O4' | 2.15 | 0.47 |
| 3:AC:109:VAL:CG2 | 28:A1:103:LEU:HD11 | 2.45 | 0.47 |
| 4:AD:88:SER:N | 101:AD:504:HOH:O | 2.47 | 0.47 |
| 12:AL:126:GLU:HG2 | 12:AL:177:VAL:HG11 | 1.97 | 0.47 |
| 41:I:197:LEU:HD12 | 41:I:198:PRO:HD2 | 1.97 | 0.47 |
| 20:AT:132:ARG:NH1 | 20:AT:136:LEU:O | 2.48 | 0.47 |
| 1:AA:1453:A:OP1 | 101:AA:1822:HOH:O | 2.21 | 0.47 |
| 8:AH:125:HIS:CE1 | 8:AH:126:ILE:HG23 | 2.49 | 0.47 |
| 15:AO:221:GLN:NE2 | 22:AV:314:VAL:O | 2.39 | 0.47 |
| 42:J:75:ASP:OD1 | 42:J:77:THR:HG22 | 2.15 | 0.47 |
| 66:7:257:ILE:O | 66:7:257:ILE:HG13 | 2.15 | 0.47 |
| 35:A:1958:G:O2' | 101:A:3518:HOH:O | 2.18 | 0.47 |
| 35:A:2663:C:OP1 | 47:O:13:ARG:NH2 | 2.47 | 0.47 |
| 6:AF:176:ASP:OD2 | 6:AF:180:ARG:NH1 | 2.48 | 0.47 |
| 66:7:106:ALA:O | 66:7:113:TRP:N | 2.47 | 0.47 |
| 52:T:85:ALA:O | 52:T:139:SER:OG | 2.33 | 0.46 |
| 8:AH:155:VAL:HG21 | 28:A1:129:PHE:HB2 | 1.97 | 0.46 |
| 24:AX:153:LEU:HD21 | 24:AX:244:LEU:CD2 | 2.46 | 0.46 |
| 53:U:66:ALA:HB2 | 53:U:100:ALA:HA | 1.98 | 0.46 |
| 54:V:127:ASP:O | 54:V:129:LYS:N | 2.49 | 0.46 |
| 59:O:133:GLU:OE2 | 59:O:160:TYR:OH | 2.26 | 0.46 |
| 38:E:47:THR:OG1 | 38:E:51:GLU:OE1 | 2.22 | 0.46 |
| 22:AV:225:LEU:HD21 | 22:AV:280:LEU:HD23 | 1.97 | 0.46 |
| 40:H:107:VAL:HG12 | 40:H:108:ARG:N | 2.30 | 0.46 |
| 22:AV:87:HIS:ND1 | 49:Q:60:PRO:HB2 | 2.30 | 0.46 |
| 35:A:2458:A:O2' | 38:E:215:PHE:O | 2.29 | 0.46 |
| 8:AH:184:ILE:O | 8:AH:184:ILE:CG2 | 2.63 | 0.46 |
| 39:F:218:LEU:HD23 | 39:F:260:VAL:HB | 1.98 | 0.46 |
| 7:AG:102:GLU:OE1 | 7:AG:102:GLU:N | 2.44 | 0.46 |
| 27:A0:54:ALA:O | 27:A0:58:VAL:HG23 | 2.16 | 0.46 |
| 35:A:2777:G:N3 | 40:H:179:ASN:ND2 | 2.63 | 0.46 |
| 36:B:12:U:HO2' | 36:B:14:A:P | 2.39 | 0.46 |
| 8:AH:151:SER:O | 8:AH:155:VAL:HG23 | 2.16 | 0.46 |
| 24:AX:81:HIS:ND1 | 24:AX:190:ASN:HB3 | 2.31 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:A4:305:ILE:HG22 | 31:A4:306:ASN:N | 2.31 | 0.46 |
| 35:A:2506:A:H1' | 35:A:2601:A:N6 | 2.31 | 0.46 |
| 6:AF:193:ASP:OD1 | 6:AF:194:LYS:N | 2.49 | 0.45 |
| 20:AT:92:THR:O | 20:AT:92:THR:HG22 | 2.16 | 0.45 |
| 21:AU:56:LEU:HD11 | 21:AU:60:TYR:CZ | 2.52 | 0.45 |
| 65:6:215:THR:OG1 | 65:6:275:GLN:OE1 | 2.31 | 0.45 |
| 27:A0:41:LEU:HD13 | 27:A0:55:TRP:CG | 2.52 | 0.45 |
| 43:K:67:PHE:HB3 | 43:K:71:LYS:HB2 | 1.99 | 0.45 |
| 45:M:43:ARG:NH2 | 101:M:404:HOH:O | 2.50 | 0.45 |
| 1:AA:1057:G:H4' | 1:AA:1578:A:H4' | 1.98 | 0.45 |
| 4:AD:312:TYR:N | 4:AD:331:ASP:OD2 | 2.49 | 0.45 |
| 35:A:3211:C:HO2' | 35:A:3212:C:H5 | 1.58 | 0.45 |
| 65:6:224:HIS:HA | 65:6:232:TYR:CE2 | 2.51 | 0.45 |
| 7:AG:198:ARG:NH1 | 7:AG:201:ILE:HG23 | 2.32 | 0.45 |
| 11:AK:70:VAL:HG11 | 25:AY:383:LYS:HE3 | 1.99 | 0.45 |
| 23:AW:92:MET:O | 23:AW:98:LYS:NZ | 2.49 | 0.45 |
| 31:A4:309:PHE:HB2 | 31:A4:345:PHE:CD1 | 2.52 | 0.45 |
| 18:AR:317:ALA:O | 18:AR:321:ALA:N | 2.49 | 0.45 |
| 38:E:131:LYS:O | 38:E:145:LEU:HD12 | 2.16 | 0.45 |
| 49:Q:251:GLU:OE1 | 49:Q:251:GLU:HA | 2.16 | 0.45 |
| 58:Z:75:THR:HB | 58:Z:83:LYS:HG2 | 1.99 | 0.45 |
| 45:M:177:ALA:HA | 45:M:222:TYR:CD1 | 2.52 | 0.45 |
| 18:AR:162:SER:O | 18:AR:170:ARG:NH1 | 2.48 | 0.44 |
| 40:H:84:GLU:OE1 | 56:X:44:ARG:NH2 | 2.50 | 0.44 |
| 19:AS:51:VAL:HG13 | 29:A2:117:LEU:HD11 | 1.99 | 0.44 |
| 35:A:1867:A:N1 | 35:A:2019:G:O2' | 2.36 | 0.44 |
| 46:N:135:SER:HG | 46:N:138:HIS:CE1 | 2.36 | 0.44 |
| 64:5:105:TYR:CE1 | 64:5:262:ILE:HD12 | 2.53 | 0.44 |
| 39:F:98:GLN:NE2 | 101:F:406:HOH:O | 2.51 | 0.44 |
| 65:6:257:PRO:HB3 | 65:6:268:LEU:HD21 | 2.00 | 0.44 |
| 35:A:1822:U:O2 | 35:A:2707:A:O2' | 2.33 | 0.44 |
| 1:AA:1259:U:H6 | 1:AA:1326:A:HO2' | 1.58 | 0.44 |
| 36:B:44:A:H2' | 36:B:45:G:O4' | 2.18 | 0.44 |
| 37:D:207:ILE:HG22 | 37:D:207:ILE:O | 2.19 | 0.43 |
| 7:AG:237:GLU:OE1 | 7:AG:237:GLU:N | 2.50 | 0.43 |
| 35:A:2598:A:H3' | 35:A:2625:C:H42 | 1.83 | 0.43 |
| 5:AE:65:LEU:HD11 | 16:AP:75:LYS:HD2 | 2.00 | 0.43 |
| 1:AA:1461:A:N6 | 101:AA:1898:HOH:O | 2.41 | 0.43 |
| 5:AE:109:VAL:HG23 | 5:AE:109:VAL:O | 2.19 | 0.43 |
| 40:H:223:VAL:N | 40:H:231:VAL:O | 2.46 | 0.43 |
| 7:AG:200:LEU:HD13 | 7:AG:246:ARG:CZ | 2.49 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 21:AU:73:GLU:OE2 | 27:A0:166:TYR:OH | 2.37 | 0.43 |
| 35:A:2135:A:N3 | 35:A:2135:A:H2' | 2.34 | 0.43 |
| 66:7:51:GLU:OE1 | 66:7:51:GLU:HA | 2.19 | 0.43 |
| 31:A4:58:VAL:O | 31:A4:58:VAL:HG23 | 2.18 | 0.43 |
| 35:A:1697:A:N3 | 35:A:1703:C:O2' | 2.48 | 0.43 |
| 35:A:2293:A:N1 | 101:A:3603:HOH:O | 2.37 | 0.43 |
| 35:A:2868:C:H2' | 35:A:2869:A:O4' | 2.19 | 0.43 |
| 5:AE:55:SER:O | 5:AE:56:GLN:NE2 | 2.51 | 0.43 |
| 13:AM:101:PRO:HB2 | 21:AU:60:TYR:CE1 | 2.53 | 0.43 |
| 35:A:1991:A:H5'' | 35:A:1992:C:OP1 | 2.18 | 0.43 |
| 35:A:2053:U:HO2' | 35:A:2054:U:H6 | 1.65 | 0.43 |
| 35:A:2429:A:N1 | 35:A:2433:C:O2' | 2.45 | 0.43 |
| 35:A:2296:U:H5'' | 35:A:2297:A:OP1 | 2.19 | 0.42 |
| 49:Q:69:VAL:HG12 | 49:Q:71:PRO:HD3 | 2.00 | 0.42 |
| 31:A4:470:GLN:NE2 | 31:A4:472:ASP:OD2 | 2.52 | 0.42 |
| 35:A:3089:A:H3' | 35:A:3090:G:H5' | 2.01 | 0.42 |
| 46:N:135:SER:OG | 46:N:138:HIS:CE1 | 2.72 | 0.42 |
| 35:A:2882:U:O4' | 48:P:173:ARG:NH2 | 2.52 | 0.42 |
| 51:S:152:ASP:OD1 | 51:S:153:LEU:N | 2.53 | 0.42 |
| 31:A4:458:TYR:HB3 | 31:A4:486:TYR:CD1 | 2.54 | 0.42 |
| 35:A:1800:G:N1 | 35:A:1803:A:OP2 | 2.51 | 0.42 |
| 24:AX:151:LEU:HD23 | 24:AX:247:LEU:HD22 | 2.00 | 0.42 |
| 54:V:165:ILE:HG21 | 68:9:76:TYR:CD2 | 2.54 | 0.42 |
| 50:R:65:ARG:HA | 50:R:68:TRP:CE3 | 2.55 | 0.42 |
| 67:8:202:VAL:O | 67:8:203:GLU:HB3 | 2.19 | 0.42 |
| 1:AA:1199:G:N1 | 1:AA:1422:G:OP2 | 2.49 | 0.42 |
| 1:AA:1322:C:N3 | 4:AD:234:LYS:NZ | 2.64 | 0.42 |
| 12:AL:213:VAL:O | 12:AL:217:THR:HG23 | 2.20 | 0.42 |
| 35:A:2728:C:H4' | 35:A:2815:OMG:HM22 | 2.01 | 0.42 |
| 3:AC:84:GLU:OE1 | 3:AC:84:GLU:N | 2.44 | 0.42 |
| 28:A1:86:ARG:NH1 | 28:A1:96:PRO:O | 2.50 | 0.42 |
| 1:AA:1528:A:OP1 | 27:A0:101:ARG:NH2 | 2.51 | 0.42 |
| 4:AD:198:TRP:HA | 4:AD:201:ILE:HD12 | 2.02 | 0.42 |
| 6:AF:114:THR:HG21 | 6:AF:205:LEU:HG | 2.02 | 0.42 |
| 22:AV:241:ARG:HA | 22:AV:244:TYR:CE2 | 2.55 | 0.42 |
| 27:A0:158:GLU:O | 27:A0:158:GLU:HG2 | 2.20 | 0.42 |
| 1:AA:1265:C:H4' | 8:AH:122:GLN:HG3 | 2.02 | 0.42 |
| 27:A0:110:ASP:OD1 | 27:A0:110:ASP:N | 2.50 | 0.42 |
| 66:7:73:THR:HG1 | 66:7:99:TYR:HH | 1.62 | 0.42 |
| 3:AC:58:ALA:HB1 | 3:AC:59:PRO:CD | 2.50 | 0.41 |
| 27:A0:13:GLU:OE2 | 27:A0:16:ARG:NH1 | 2.53 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:A:1787:G:N2 | 35:A:1790:A:OP2 | 2.51 | 0.41 |
| 35:A:2174:G:H4' | 42:J:151:LEU:HD23 | 2.00 | 0.41 |
| 54:V:124:ASP:OD1 | 54:V:125:PRO:HD2 | 2.20 | 0.41 |
| 1:AA:1103:A:N7 | 1:AA:1574:G:O2' | 2.46 | 0.41 |
| 40:H:238:VAL:HG12 | 40:H:239:ASN:N | 2.35 | 0.41 |
| 47:O:140:SER:O | 47:O:146:ASN:ND2 | 2.50 | 0.41 |
| 64:5:56:GLU:O | 64:5:56:GLU:HG3 | 2.19 | 0.41 |
| 66:7:114:ASP:OD1 | 66:7:268:LEU:N | 2.53 | 0.41 |
| 12:AL:126:GLU:OE1 | 12:AL:126:GLU:N | 2.41 | 0.41 |
| 22:AV:139:PRO:HD2 | 22:AV:144:PHE:CZ | 2.55 | 0.41 |
| 35:A:1800:G:O6 | 54:V:34:LYS:NZ | 2.52 | 0.41 |
| 35:A:2025:C:OP1 | 51:S:182:LYS:HD3 | 2.20 | 0.41 |
| 64:5:273:VAL:HG12 | 64:5:273:VAL:O | 2.20 | 0.41 |
| 1:AA:1065:C:H2' | 1:AA:1066:C:O4' | 2.21 | 0.41 |
| 30:A3:173:LEU:HD12 | 30:A3:191:THR:HG23 | 2.02 | 0.41 |
| 35:A:1815:A:N1 | 101:A:3599:HOH:O | 2.37 | 0.41 |
| 3:AC:75:ASN:ND2 | 11:AK:121:SER:O | 2.53 | 0.41 |
| 18:AR:162:SER:O | 18:AR:170:ARG:NH2 | 2.53 | 0.41 |
| 38:E:247:ASP:O | 101:E:501:HOH:O | 2.22 | 0.41 |
| 42:J:102:ARG:N | 42:J:107:GLU:OE2 | 2.51 | 0.41 |
| 43:K:7:ALA:HB3 | 43:K:8:PRO:HD3 | 2.02 | 0.41 |
| 24:AX:265:ILE:HD11 | 24:AX:297:MET:HE2 | 2.02 | 0.41 |
| 30:A3:159:GLU:OE2 | 35:A:2639:C:H5'' | 2.21 | 0.41 |
| 35:A:2015:G:O4' | 45:M:56:GLU:HG3 | 2.21 | 0.41 |
| 35:A:2662:A:OP1 | 35:A:3159:A:O2' | 2.33 | 0.41 |
| 38:E:69:ASP:OD1 | 38:E:154:ARG:NH1 | 2.54 | 0.41 |
| 52:T:49:ASN:ND2 | 52:T:68:TYR:O | 2.53 | 0.41 |
| 1:AA:1149:G:OP2 | 30:A3:165:LYS:NZ | 2.50 | 0.41 |
| 2:AB:96:GLY:HA3 | 23:AW:159:ASP:OD2 | 2.21 | 0.41 |
| 2:AB:167:HIS:CD2 | 7:AG:153:THR:HA | 2.56 | 0.41 |
| 18:AR:162:SER:HB2 | 18:AR:165:ILE:HD12 | 2.02 | 0.41 |
| 25:AY:259:PHE:HB2 | 31:A4:363:ILE:HD11 | 2.03 | 0.41 |
| 35:A:2598:A:O2' | 35:A:2599:U:H5' | 2.21 | 0.41 |
| 52:T:94:ASP:OD2 | 66:7:97:GLU:N | 2.38 | 0.41 |
| 1:AA:709:G:OP1 | 13:AM:13:ARG:NH2 | 2.53 | 0.41 |
| 1:AA:1001:C:N4 | 35:A:2558:A:O4' | 2.54 | 0.41 |
| 14:AN:93:ASP:O | 14:AN:97:GLY:N | 2.48 | 0.41 |
| 25:AY:300:GLU:OE1 | 31:A4:87:TYR:OH | 2.31 | 0.41 |
| 26:AZ:46:LYS:HA | 26:AZ:49:TYR:CE1 | 2.55 | 0.41 |
| 35:A:2595:A:H2' | 35:A:2596:G:O4' | 2.21 | 0.41 |
| 46:N:87:PHE:HE1 | 46:N:169:PHE:HB2 | 1.85 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AA:1107:U:O4 | 30:A3:128:LYS:NZ | 2.47 | 0.41 |
| 10:AJ:70:PRO:HB3 | 10:AJ:117:ASP:HB3 | 2.03 | 0.41 |
| 35:A:2343:G:H3' | 35:A:2343:G:N3 | 2.36 | 0.41 |
| 45:M:14:ASP:OD1 | 45:M:15:LEU:N | 2.54 | 0.41 |
| 55:W:103:VAL:HG11 | 65:6:61:ALA:HB1 | 2.03 | 0.41 |
| 1:AA:1066:C:O2' | 9:AI:187:ARG:O | 2.39 | 0.40 |
| 13:AM:19:ILE:HB | 13:AM:83:LEU:HD23 | 2.03 | 0.40 |
| 31:A4:508:VAL:O | 31:A4:508:VAL:HG12 | 2.20 | 0.40 |
| 35:A:2709:A:N3 | 59:0:98:GLN:OE1 | 2.53 | 0.40 |
| 40:H:193:PHE:O | 40:H:198:GLY:N | 2.54 | 0.40 |
| 54:V:130:PRO:O | 54:V:149:ARG:NH1 | 2.54 | 0.40 |
| 66:7:36:SER:HB2 | 66:7:37:PRO:HD2 | 2.02 | 0.40 |
| 5:AE:65:LEU:HD11 | 16:AP:75:LYS:HD3 | 2.03 | 0.40 |
| 22:AV:70:LEU:HD23 | 22:AV:393:GLU:OE1 | 2.22 | 0.40 |
| 35:A:2814:G:O2' | 35:A:2983:G:OP1 | 2.39 | 0.40 |
| 41:I:144:LEU:N | 41:I:145:PRO:HD2 | 2.37 | 0.40 |
| 47:O:36:LEU:O | 47:O:40:GLU:N | 2.50 | 0.40 |
| 1:AA:919:A:OP2 | 15:AO:96:ARG:NH2 | 2.49 | 0.40 |
| 35:A:2327:U:H2' | 35:A:2328:C:O4' | 2.20 | 0.40 |
| 35:A:3009:C:O2 | 35:A:3009:C:O5' | 2.38 | 0.40 |
| 38:E:345:ILE:O | 49:Q:172:GLN:NE2 | 2.51 | 0.40 |
| 42:J:69:LYS:HE3 | 42:J:69:LYS:HB2 | 1.96 | 0.40 |
| 47:O:86:ILE:HB | 47:O:87:PRO:HD3 | 2.03 | 0.40 |
| 35:A:2006:C:H2' | 35:A:2007:U:C6 | 2.57 | 0.40 |
| 40:H:208:LEU:HB3 | 40:H:209:PRO:HD2 | 2.04 | 0.40 |
| 54:V:54:TRP:NE1 | 54:V:56:LEU:O | 2.53 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|------------|---------|----------|-------------|-----|
| 2 | AB | 223/296 (75%) | 221 (99%) | 2 (1%) | 0 | 100 | 100 |
| 3 | AC | 130/167 (78%) | 126 (97%) | 4 (3%) | 0 | 100 | 100 |
| 4 | AD | 341/430 (79%) | 331 (97%) | 10 (3%) | 0 | 100 | 100 |
| 5 | AE | 120/125 (96%) | 119 (99%) | 1 (1%) | 0 | 100 | 100 |
| 6 | AF | 206/242 (85%) | 204 (99%) | 2 (1%) | 0 | 100 | 100 |
| 7 | AG | 323/396 (82%) | 319 (99%) | 4 (1%) | 0 | 100 | 100 |
| 8 | AH | 138/201 (69%) | 136 (99%) | 1 (1%) | 1 (1%) | 22 | 21 |
| 9 | AI | 134/194 (69%) | 132 (98%) | 2 (2%) | 0 | 100 | 100 |
| 10 | AJ | 106/138 (77%) | 104 (98%) | 2 (2%) | 0 | 100 | 100 |
| 11 | AK | 99/128 (77%) | 98 (99%) | 1 (1%) | 0 | 100 | 100 |
| 12 | AL | 172/257 (67%) | 171 (99%) | 1 (1%) | 0 | 100 | 100 |
| 13 | AM | 117/137 (85%) | 117 (100%) | 0 | 0 | 100 | 100 |
| 14 | AN | 108/130 (83%) | 107 (99%) | 1 (1%) | 0 | 100 | 100 |
| 15 | AO | 191/258 (74%) | 188 (98%) | 3 (2%) | 0 | 100 | 100 |
| 16 | AP | 95/142 (67%) | 94 (99%) | 1 (1%) | 0 | 100 | 100 |
| 17 | AQ | 84/87 (97%) | 82 (98%) | 2 (2%) | 0 | 100 | 100 |
| 18 | AR | 293/360 (81%) | 284 (97%) | 9 (3%) | 0 | 100 | 100 |
| 19 | AS | 133/190 (70%) | 131 (98%) | 2 (2%) | 0 | 100 | 100 |
| 20 | AT | 166/173 (96%) | 164 (99%) | 2 (1%) | 0 | 100 | 100 |
| 21 | AU | 174/205 (85%) | 174 (100%) | 0 | 0 | 100 | 100 |
| 22 | AV | 358/414 (86%) | 353 (99%) | 5 (1%) | 0 | 100 | 100 |
| 23 | AW | 98/187 (52%) | 96 (98%) | 2 (2%) | 0 | 100 | 100 |
| 24 | AX | 350/398 (88%) | 345 (99%) | 5 (1%) | 0 | 100 | 100 |
| 25 | AY | 147/395 (37%) | 146 (99%) | 0 | 1 (1%) | 22 | 21 |
| 26 | AZ | 98/106 (92%) | 97 (99%) | 1 (1%) | 0 | 100 | 100 |
| 27 | A0 | 213/217 (98%) | 209 (98%) | 4 (2%) | 0 | 100 | 100 |
| 28 | A1 | 277/323 (86%) | 273 (99%) | 4 (1%) | 0 | 100 | 100 |
| 29 | A2 | 115/118 (98%) | 113 (98%) | 2 (2%) | 0 | 100 | 100 |
| 30 | A3 | 68/199 (34%) | 67 (98%) | 1 (2%) | 0 | 100 | 100 |
| 31 | A4 | 584/689 (85%) | 577 (99%) | 7 (1%) | 0 | 100 | 100 |
| 37 | D | 236/305 (77%) | 232 (98%) | 4 (2%) | 0 | 100 | 100 |
| 38 | E | 303/348 (87%) | 296 (98%) | 6 (2%) | 1 (0%) | 41 | 45 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|------------|---------|----------|-------------|-----|
| 39 | F | 250/311 (80%) | 247 (99%) | 3 (1%) | 0 | 100 | 100 |
| 40 | H | 200/267 (75%) | 195 (98%) | 5 (2%) | 0 | 100 | 100 |
| 41 | I | 210/261 (80%) | 203 (97%) | 7 (3%) | 0 | 100 | 100 |
| 42 | J | 173/192 (90%) | 173 (100%) | 0 | 0 | 100 | 100 |
| 43 | K | 175/178 (98%) | 174 (99%) | 1 (1%) | 0 | 100 | 100 |
| 44 | L | 113/145 (78%) | 112 (99%) | 1 (1%) | 0 | 100 | 100 |
| 45 | M | 289/296 (98%) | 283 (98%) | 6 (2%) | 0 | 100 | 100 |
| 46 | N | 220/251 (88%) | 218 (99%) | 2 (1%) | 0 | 100 | 100 |
| 47 | O | 152/175 (87%) | 149 (98%) | 3 (2%) | 0 | 100 | 100 |
| 48 | P | 142/180 (79%) | 142 (100%) | 0 | 0 | 100 | 100 |
| 49 | Q | 237/292 (81%) | 237 (100%) | 0 | 0 | 100 | 100 |
| 50 | R | 138/149 (93%) | 137 (99%) | 1 (1%) | 0 | 100 | 100 |
| 51 | S | 159/205 (78%) | 156 (98%) | 3 (2%) | 0 | 100 | 100 |
| 52 | T | 164/206 (80%) | 163 (99%) | 1 (1%) | 0 | 100 | 100 |
| 53 | U | 150/153 (98%) | 147 (98%) | 3 (2%) | 0 | 100 | 100 |
| 54 | V | 203/216 (94%) | 199 (98%) | 4 (2%) | 0 | 100 | 100 |
| 55 | W | 114/148 (77%) | 113 (99%) | 1 (1%) | 0 | 100 | 100 |
| 56 | X | 242/256 (94%) | 240 (99%) | 2 (1%) | 0 | 100 | 100 |
| 57 | Y | 179/250 (72%) | 177 (99%) | 2 (1%) | 0 | 100 | 100 |
| 58 | Z | 120/161 (74%) | 120 (100%) | 0 | 0 | 100 | 100 |
| 59 | 0 | 108/188 (57%) | 108 (100%) | 0 | 0 | 100 | 100 |
| 60 | 1 | 54/65 (83%) | 53 (98%) | 1 (2%) | 0 | 100 | 100 |
| 61 | 2 | 44/92 (48%) | 43 (98%) | 1 (2%) | 0 | 100 | 100 |
| 62 | 3 | 93/188 (50%) | 92 (99%) | 1 (1%) | 0 | 100 | 100 |
| 63 | 4 | 36/103 (35%) | 36 (100%) | 0 | 0 | 100 | 100 |
| 64 | 5 | 392/423 (93%) | 382 (97%) | 10 (3%) | 0 | 100 | 100 |
| 65 | 6 | 352/380 (93%) | 344 (98%) | 8 (2%) | 0 | 100 | 100 |
| 66 | 7 | 292/338 (86%) | 286 (98%) | 6 (2%) | 0 | 100 | 100 |
| 67 | 8 | 147/206 (71%) | 144 (98%) | 3 (2%) | 0 | 100 | 100 |
| 68 | 9 | 122/137 (89%) | 121 (99%) | 1 (1%) | 0 | 100 | 100 |
| 69 | a | 96/142 (68%) | 94 (98%) | 2 (2%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-------------------|-------------|----------|----------|-------------|-----|
| 70 | b | 148/215 (69%) | 146 (99%) | 2 (1%) | 0 | 100 | 100 |
| 71 | c | 282/332 (85%) | 279 (99%) | 3 (1%) | 0 | 100 | 100 |
| 72 | d | 235/306 (77%) | 231 (98%) | 4 (2%) | 0 | 100 | 100 |
| 73 | e | 236/279 (85%) | 229 (97%) | 6 (2%) | 1 (0%) | 34 | 37 |
| 74 | f | 153/212 (72%) | 152 (99%) | 1 (1%) | 0 | 100 | 100 |
| 75 | g | 132/166 (80%) | 129 (98%) | 3 (2%) | 0 | 100 | 100 |
| 76 | h | 108/158 (68%) | 107 (99%) | 1 (1%) | 0 | 100 | 100 |
| 77 | i | 95/128 (74%) | 94 (99%) | 1 (1%) | 0 | 100 | 100 |
| 78 | j | 92/123 (75%) | 90 (98%) | 2 (2%) | 0 | 100 | 100 |
| 79 | k | 99/112 (88%) | 99 (100%) | 0 | 0 | 100 | 100 |
| 80 | l | 80/138 (58%) | 80 (100%) | 0 | 0 | 100 | 100 |
| 81 | m | 90/128 (70%) | 89 (99%) | 1 (1%) | 0 | 100 | 100 |
| 82 | o | 92/102 (90%) | 92 (100%) | 0 | 0 | 100 | 100 |
| 83 | p | 141/206 (68%) | 140 (99%) | 1 (1%) | 0 | 100 | 100 |
| 84 | q | 153/222 (69%) | 153 (100%) | 0 | 0 | 100 | 100 |
| 85 | r | 160/196 (82%) | 159 (99%) | 1 (1%) | 0 | 100 | 100 |
| 86 | s | 382/439 (87%) | 374 (98%) | 8 (2%) | 0 | 100 | 100 |
| 87 | t | 44/198 (22%) | 44 (100%) | 0 | 0 | 100 | 100 |
| 87 | u | 30/198 (15%) | 30 (100%) | 0 | 0 | 100 | 100 |
| 87 | v | 30/198 (15%) | 30 (100%) | 0 | 0 | 100 | 100 |
| 87 | w | 29/198 (15%) | 29 (100%) | 0 | 0 | 100 | 100 |
| 87 | x | 29/198 (15%) | 29 (100%) | 0 | 0 | 100 | 100 |
| 87 | y | 29/198 (15%) | 29 (100%) | 0 | 0 | 100 | 100 |
| 88 | z | 160/325 (49%) | 151 (94%) | 8 (5%) | 1 (1%) | 25 | 25 |
| All | All | 14595/19484 (75%) | 14379 (98%) | 211 (1%) | 5 (0%) | 100 | 100 |

All (5) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8 | AH | 126 | ILE |
| 25 | AY | 323 | ASP |
| 88 | z | 128 | ASP |
| 38 | E | 150 | LYS |
| 73 | e | 197 | GLU |

5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|------------|----------|-------------|-----|
| 2 | AB | 198/249 (80%) | 198 (100%) | 0 | 100 | 100 |
| 3 | AC | 115/143 (80%) | 115 (100%) | 0 | 100 | 100 |
| 4 | AD | 286/357 (80%) | 286 (100%) | 0 | 100 | 100 |
| 5 | AE | 104/107 (97%) | 104 (100%) | 0 | 100 | 100 |
| 6 | AF | 185/209 (88%) | 185 (100%) | 0 | 100 | 100 |
| 7 | AG | 285/342 (83%) | 285 (100%) | 0 | 100 | 100 |
| 8 | AH | 130/180 (72%) | 130 (100%) | 0 | 100 | 100 |
| 9 | AI | 104/146 (71%) | 104 (100%) | 0 | 100 | 100 |
| 10 | AJ | 93/118 (79%) | 93 (100%) | 0 | 100 | 100 |
| 11 | AK | 91/113 (80%) | 91 (100%) | 0 | 100 | 100 |
| 12 | AL | 158/226 (70%) | 158 (100%) | 0 | 100 | 100 |
| 13 | AM | 97/113 (86%) | 97 (100%) | 0 | 100 | 100 |
| 14 | AN | 96/115 (84%) | 96 (100%) | 0 | 100 | 100 |
| 15 | AO | 174/230 (76%) | 174 (100%) | 0 | 100 | 100 |
| 16 | AP | 88/123 (72%) | 88 (100%) | 0 | 100 | 100 |
| 17 | AQ | 78/79 (99%) | 78 (100%) | 0 | 100 | 100 |
| 18 | AR | 264/318 (83%) | 264 (100%) | 0 | 100 | 100 |
| 19 | AS | 116/164 (71%) | 116 (100%) | 0 | 100 | 100 |
| 20 | AT | 153/157 (98%) | 153 (100%) | 0 | 100 | 100 |
| 21 | AU | 152/174 (87%) | 152 (100%) | 0 | 100 | 100 |
| 22 | AV | 325/364 (89%) | 325 (100%) | 0 | 100 | 100 |
| 23 | AW | 87/158 (55%) | 87 (100%) | 0 | 100 | 100 |
| 24 | AX | 311/351 (89%) | 311 (100%) | 0 | 100 | 100 |
| 25 | AY | 137/357 (38%) | 137 (100%) | 0 | 100 | 100 |
| 26 | AZ | 90/95 (95%) | 90 (100%) | 0 | 100 | 100 |
| 27 | A0 | 188/189 (100%) | 188 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|---------------|------------|----------|-------------|-----|
| 28 | A1 | 257/291 (88%) | 257 (100%) | 0 | 100 | 100 |
| 29 | A2 | 100/101 (99%) | 100 (100%) | 0 | 100 | 100 |
| 30 | A3 | 65/166 (39%) | 65 (100%) | 0 | 100 | 100 |
| 31 | A4 | 526/609 (86%) | 526 (100%) | 0 | 100 | 100 |
| 37 | D | 192/245 (78%) | 192 (100%) | 0 | 100 | 100 |
| 38 | E | 260/290 (90%) | 259 (100%) | 1 (0%) | 91 | 95 |
| 39 | F | 219/262 (84%) | 219 (100%) | 0 | 100 | 100 |
| 40 | H | 182/228 (80%) | 182 (100%) | 0 | 100 | 100 |
| 41 | I | 194/232 (84%) | 194 (100%) | 0 | 100 | 100 |
| 42 | J | 138/150 (92%) | 138 (100%) | 0 | 100 | 100 |
| 43 | K | 154/155 (99%) | 154 (100%) | 0 | 100 | 100 |
| 44 | L | 98/124 (79%) | 98 (100%) | 0 | 100 | 100 |
| 45 | M | 246/249 (99%) | 246 (100%) | 0 | 100 | 100 |
| 46 | N | 189/211 (90%) | 189 (100%) | 0 | 100 | 100 |
| 47 | O | 134/150 (89%) | 134 (100%) | 0 | 100 | 100 |
| 48 | P | 126/155 (81%) | 126 (100%) | 0 | 100 | 100 |
| 49 | Q | 221/256 (86%) | 221 (100%) | 0 | 100 | 100 |
| 50 | R | 118/126 (94%) | 118 (100%) | 0 | 100 | 100 |
| 51 | S | 146/180 (81%) | 146 (100%) | 0 | 100 | 100 |
| 52 | T | 146/176 (83%) | 146 (100%) | 0 | 100 | 100 |
| 53 | U | 134/135 (99%) | 134 (100%) | 0 | 100 | 100 |
| 54 | V | 183/191 (96%) | 183 (100%) | 0 | 100 | 100 |
| 55 | W | 94/119 (79%) | 94 (100%) | 0 | 100 | 100 |
| 56 | X | 220/229 (96%) | 220 (100%) | 0 | 100 | 100 |
| 57 | Y | 163/223 (73%) | 162 (99%) | 1 (1%) | 86 | 92 |
| 58 | Z | 113/147 (77%) | 113 (100%) | 0 | 100 | 100 |
| 59 | 0 | 99/164 (60%) | 99 (100%) | 0 | 100 | 100 |
| 60 | 1 | 53/60 (88%) | 53 (100%) | 0 | 100 | 100 |
| 61 | 2 | 40/72 (56%) | 40 (100%) | 0 | 100 | 100 |
| 62 | 3 | 88/166 (53%) | 88 (100%) | 0 | 100 | 100 |
| 63 | 4 | 37/89 (42%) | 37 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-------------------|--------------|----------|-------------|-----|
| 64 | 5 | 353/368 (96%) | 352 (100%) | 1 (0%) | 92 | 96 |
| 65 | 6 | 313/332 (94%) | 313 (100%) | 0 | 100 | 100 |
| 66 | 7 | 270/303 (89%) | 270 (100%) | 0 | 100 | 100 |
| 67 | 8 | 140/190 (74%) | 140 (100%) | 0 | 100 | 100 |
| 68 | 9 | 104/112 (93%) | 104 (100%) | 0 | 100 | 100 |
| 69 | a | 96/133 (72%) | 95 (99%) | 1 (1%) | 76 | 85 |
| 70 | b | 131/185 (71%) | 131 (100%) | 0 | 100 | 100 |
| 71 | c | 251/288 (87%) | 251 (100%) | 0 | 100 | 100 |
| 72 | d | 223/274 (81%) | 223 (100%) | 0 | 100 | 100 |
| 73 | e | 207/236 (88%) | 207 (100%) | 0 | 100 | 100 |
| 74 | f | 139/188 (74%) | 139 (100%) | 0 | 100 | 100 |
| 75 | g | 124/148 (84%) | 124 (100%) | 0 | 100 | 100 |
| 76 | h | 104/148 (70%) | 104 (100%) | 0 | 100 | 100 |
| 77 | i | 86/110 (78%) | 86 (100%) | 0 | 100 | 100 |
| 78 | j | 74/97 (76%) | 74 (100%) | 0 | 100 | 100 |
| 79 | k | 83/90 (92%) | 83 (100%) | 0 | 100 | 100 |
| 80 | l | 76/116 (66%) | 76 (100%) | 0 | 100 | 100 |
| 81 | m | 85/113 (75%) | 85 (100%) | 0 | 100 | 100 |
| 82 | o | 80/87 (92%) | 80 (100%) | 0 | 100 | 100 |
| 83 | p | 135/181 (75%) | 135 (100%) | 0 | 100 | 100 |
| 84 | q | 132/178 (74%) | 132 (100%) | 0 | 100 | 100 |
| 85 | r | 147/169 (87%) | 147 (100%) | 0 | 100 | 100 |
| 86 | s | 340/381 (89%) | 340 (100%) | 0 | 100 | 100 |
| 87 | t | 40/158 (25%) | 40 (100%) | 0 | 100 | 100 |
| 87 | u | 31/158 (20%) | 31 (100%) | 0 | 100 | 100 |
| 87 | v | 31/158 (20%) | 31 (100%) | 0 | 100 | 100 |
| 87 | w | 30/158 (19%) | 30 (100%) | 0 | 100 | 100 |
| 87 | x | 30/158 (19%) | 30 (100%) | 0 | 100 | 100 |
| 87 | y | 30/158 (19%) | 30 (100%) | 0 | 100 | 100 |
| 88 | z | 150/287 (52%) | 150 (100%) | 0 | 100 | 100 |
| All | All | 13075/16790 (78%) | 13071 (100%) | 4 (0%) | 100 | 100 |

All (4) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 38 | E | 303 | LYS |
| 57 | Y | 198 | ARG |
| 64 | 5 | 395 | ARG |
| 69 | a | 122 | ARG |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | AD | 356 | GLN |
| 6 | AF | 113 | GLN |
| 6 | AF | 238 | HIS |
| 7 | AG | 384 | GLN |
| 9 | AI | 96 | GLN |
| 9 | AI | 98 | GLN |
| 12 | AL | 162 | GLN |
| 13 | AM | 50 | GLN |
| 17 | AQ | 41 | HIS |
| 21 | AU | 188 | ASN |
| 22 | AV | 380 | GLN |
| 23 | AW | 106 | HIS |
| 24 | AX | 159 | HIS |
| 24 | AX | 250 | GLN |
| 26 | AZ | 63 | GLN |
| 28 | A1 | 185 | HIS |
| 31 | A4 | 257 | HIS |
| 31 | A4 | 306 | ASN |
| 37 | D | 221 | ASN |
| 38 | E | 125 | GLN |
| 38 | E | 281 | ASN |
| 39 | F | 98 | GLN |
| 41 | I | 36 | HIS |
| 41 | I | 150 | HIS |
| 47 | O | 100 | GLN |
| 51 | S | 118 | ASN |
| 55 | W | 62 | HIS |
| 58 | Z | 150 | HIS |
| 59 | 0 | 118 | GLN |
| 59 | 0 | 120 | HIS |
| 60 | 1 | 52 | GLN |
| 64 | 5 | 109 | HIS |
| 64 | 5 | 331 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 64 | 5 | 367 | ASN |
| 65 | 6 | 320 | GLN |
| 66 | 7 | 298 | GLN |
| 69 | a | 126 | HIS |
| 70 | b | 58 | ASN |
| 73 | e | 212 | HIS |
| 73 | e | 252 | HIS |
| 77 | i | 124 | HIS |
| 82 | o | 21 | HIS |
| 82 | o | 94 | HIS |
| 84 | q | 107 | GLN |
| 84 | q | 142 | ASN |
| 85 | r | 96 | HIS |
| 88 | z | 104 | HIS |
| 88 | z | 241 | HIS |
| 88 | z | 266 | GLN |

5.3.3 RNA ⓘ

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1 | AA | 950/954 (99%) | 122 (12%) | 0 |
| 32 | Aw | 20/22 (90%) | 2 (10%) | 0 |
| 33 | Ax | 68/70 (97%) | 10 (14%) | 0 |
| 34 | Az | 32/34 (94%) | 12 (37%) | 0 |
| 35 | A | 1556/1558 (99%) | 220 (14%) | 3 (0%) |
| 36 | B | 71/72 (98%) | 11 (15%) | 0 |
| 89 | Ay | 48/52 (92%) | 14 (29%) | 0 |
| All | All | 2745/2762 (99%) | 391 (14%) | 3 (0%) |

All (391) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | AA | 651 | A |
| 1 | AA | 680 | U |
| 1 | AA | 688 | A |
| 1 | AA | 704 | U |
| 1 | AA | 721 | U |
| 1 | AA | 737 | C |
| 1 | AA | 738 | A |
| 1 | AA | 753 | A |
| 1 | AA | 761 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | AA | 766 | G |
| 1 | AA | 773 | U |
| 1 | AA | 777 | G |
| 1 | AA | 786 | G |
| 1 | AA | 791 | G |
| 1 | AA | 794 | U |
| 1 | AA | 796 | G |
| 1 | AA | 830 | U |
| 1 | AA | 832 | U |
| 1 | AA | 835 | C |
| 1 | AA | 836 | A |
| 1 | AA | 860 | A |
| 1 | AA | 861 | U |
| 1 | AA | 868 | C |
| 1 | AA | 871 | A |
| 1 | AA | 890 | C |
| 1 | AA | 903 | U |
| 1 | AA | 904 | C |
| 1 | AA | 907 | A |
| 1 | AA | 919 | A |
| 1 | AA | 929 | A |
| 1 | AA | 932 | C |
| 1 | AA | 938 | A |
| 1 | AA | 939 | A |
| 1 | AA | 941 | G |
| 1 | AA | 942 | A |
| 1 | AA | 960 | C |
| 1 | AA | 962 | C |
| 1 | AA | 967 | A |
| 1 | AA | 1001 | C |
| 1 | AA | 1002 | C |
| 1 | AA | 1011 | C |
| 1 | AA | 1015 | A |
| 1 | AA | 1031 | G |
| 1 | AA | 1042 | U |
| 1 | AA | 1081 | U |
| 1 | AA | 1082 | A |
| 1 | AA | 1103 | A |
| 1 | AA | 1105 | C |
| 1 | AA | 1106 | C |
| 1 | AA | 1107 | U |
| 1 | AA | 1109 | A |

Continued on next page...

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | AA | 1113 | G |
| 1 | AA | 1118 | A |
| 1 | AA | 1121 | A |
| 1 | AA | 1126 | A |
| 1 | AA | 1137 | A |
| 1 | AA | 1151 | C |
| 1 | AA | 1153 | C |
| 1 | AA | 1160 | A |
| 1 | AA | 1167 | A |
| 1 | AA | 1179 | G |
| 1 | AA | 1187 | U |
| 1 | AA | 1189 | U |
| 1 | AA | 1190 | C |
| 1 | AA | 1193 | U |
| 1 | AA | 1199 | G |
| 1 | AA | 1200 | G |
| 1 | AA | 1220 | A |
| 1 | AA | 1223 | C |
| 1 | AA | 1225 | C |
| 1 | AA | 1229 | U |
| 1 | AA | 1247 | G |
| 1 | AA | 1248 | C |
| 1 | AA | 1250 | C |
| 1 | AA | 1251 | A |
| 1 | AA | 1271 | C |
| 1 | AA | 1273 | G |
| 1 | AA | 1284 | U |
| 1 | AA | 1285 | G |
| 1 | AA | 1290 | C |
| 1 | AA | 1291 | U |
| 1 | AA | 1292 | A |
| 1 | AA | 1326 | A |
| 1 | AA | 1327 | G |
| 1 | AA | 1343 | A |
| 1 | AA | 1354 | A |
| 1 | AA | 1356 | A |
| 1 | AA | 1376 | C |
| 1 | AA | 1378 | C |
| 1 | AA | 1387 | A |
| 1 | AA | 1390 | A |
| 1 | AA | 1391 | U |
| 1 | AA | 1405 | C |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | AA | 1406 | U |
| 1 | AA | 1407 | U |
| 1 | AA | 1422 | G |
| 1 | AA | 1430 | A |
| 1 | AA | 1466 | C |
| 1 | AA | 1481 | C |
| 1 | AA | 1503 | G |
| 1 | AA | 1519 | A |
| 1 | AA | 1522 | U |
| 1 | AA | 1525 | C |
| 1 | AA | 1526 | U |
| 1 | AA | 1527 | A |
| 1 | AA | 1533 | C |
| 1 | AA | 1536 | A |
| 1 | AA | 1537 | C |
| 1 | AA | 1538 | G |
| 1 | AA | 1539 | C |
| 1 | AA | 1540 | A |
| 1 | AA | 1541 | U |
| 1 | AA | 1544 | A |
| 1 | AA | 1552 | G |
| 1 | AA | 1557 | A |
| 1 | AA | 1562 | G |
| 1 | AA | 1568 | U |
| 1 | AA | 1571 | U |
| 1 | AA | 1582 | G |
| 1 | AA | 1594 | G |
| 1 | AA | 1595 | G |
| 1 | AA | 1599 | A |
| 32 | Aw | 30 | G |
| 32 | Aw | 76 | A |
| 33 | Ax | 3 | G |
| 33 | Ax | 23 | A |
| 33 | Ax | 25 | C |
| 33 | Ax | 44 | A |
| 33 | Ax | 45 | G |
| 33 | Ax | 46 | A |
| 33 | Ax | 48 | U |
| 33 | Ax | 49 | G |
| 33 | Ax | 59 | U |
| 33 | Ax | 62 | C |
| 34 | Az | 0 | U |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 34 | Az | 12 | U |
| 34 | Az | 13 | U |
| 34 | Az | 18 | A |
| 34 | Az | 21 | A |
| 34 | Az | 22 | A |
| 34 | Az | 23 | U |
| 34 | Az | 24 | U |
| 34 | Az | 25 | U |
| 34 | Az | 26 | A |
| 34 | Az | 27 | C |
| 34 | Az | 32 | A |
| 35 | A | 1678 | C |
| 35 | A | 1681 | G |
| 35 | A | 1689 | C |
| 35 | A | 1692 | A |
| 35 | A | 1700 | U |
| 35 | A | 1704 | U |
| 35 | A | 1708 | A |
| 35 | A | 1715 | C |
| 35 | A | 1724 | A |
| 35 | A | 1727 | A |
| 35 | A | 1728 | U |
| 35 | A | 1748 | G |
| 35 | A | 1765 | C |
| 35 | A | 1777 | A |
| 35 | A | 1805 | A |
| 35 | A | 1806 | U |
| 35 | A | 1807 | U |
| 35 | A | 1808 | A |
| 35 | A | 1810 | A |
| 35 | A | 1817 | C |
| 35 | A | 1821 | A |
| 35 | A | 1827 | C |
| 35 | A | 1828 | A |
| 35 | A | 1829 | A |
| 35 | A | 1832 | A |
| 35 | A | 1836 | A |
| 35 | A | 1844 | A |
| 35 | A | 1854 | U |
| 35 | A | 1856 | A |
| 35 | A | 1869 | A |
| 35 | A | 1871 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 35 | A | 1882 | A |
| 35 | A | 1887 | A |
| 35 | A | 1893 | A |
| 35 | A | 1901 | C |
| 35 | A | 1903 | C |
| 35 | A | 1918 | G |
| 35 | A | 1937 | A |
| 35 | A | 1940 | A |
| 35 | A | 1958 | G |
| 35 | A | 1985 | G |
| 35 | A | 1992 | C |
| 35 | A | 1993 | A |
| 35 | A | 1994 | A |
| 35 | A | 2000 | C |
| 35 | A | 2003 | A |
| 35 | A | 2015 | G |
| 35 | A | 2022 | G |
| 35 | A | 2030 | U |
| 35 | A | 2032 | G |
| 35 | A | 2036 | C |
| 35 | A | 2037 | U |
| 35 | A | 2039 | A |
| 35 | A | 2054 | U |
| 35 | A | 2060 | A |
| 35 | A | 2069 | U |
| 35 | A | 2071 | U |
| 35 | A | 2079 | C |
| 35 | A | 2099 | U |
| 35 | A | 2113 | G |
| 35 | A | 2125 | C |
| 35 | A | 2126 | U |
| 35 | A | 2147 | G |
| 35 | A | 2160 | A |
| 35 | A | 2163 | A |
| 35 | A | 2168 | U |
| 35 | A | 2181 | A |
| 35 | A | 2192 | A |
| 35 | A | 2198 | A |
| 35 | A | 2200 | A |
| 35 | A | 2207 | A |
| 35 | A | 2214 | A |
| 35 | A | 2219 | C |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 35 | A | 2221 | C |
| 35 | A | 2222 | U |
| 35 | A | 2223 | A |
| 35 | A | 2224 | C |
| 35 | A | 2225 | C |
| 35 | A | 2226 | U |
| 35 | A | 2227 | A |
| 35 | A | 2230 | A |
| 35 | A | 2233 | U |
| 35 | A | 2237 | A |
| 35 | A | 2241 | A |
| 35 | A | 2243 | A |
| 35 | A | 2245 | A |
| 35 | A | 2246 | A |
| 35 | A | 2262 | C |
| 35 | A | 2263 | C |
| 35 | A | 2284 | C |
| 35 | A | 2285 | U |
| 35 | A | 2297 | A |
| 35 | A | 2300 | G |
| 35 | A | 2322 | C |
| 35 | A | 2331 | C |
| 35 | A | 2332 | C |
| 35 | A | 2345 | G |
| 35 | A | 2350 | A |
| 35 | A | 2353 | A |
| 35 | A | 2354 | A |
| 35 | A | 2357 | C |
| 35 | A | 2363 | A |
| 35 | A | 2372 | U |
| 35 | A | 2374 | A |
| 35 | A | 2390 | A |
| 35 | A | 2399 | A |
| 35 | A | 2401 | A |
| 35 | A | 2404 | U |
| 35 | A | 2407 | U |
| 35 | A | 2415 | C |
| 35 | A | 2434 | A |
| 35 | A | 2446 | A |
| 35 | A | 2451 | A |
| 35 | A | 2478 | G |
| 35 | A | 2485 | U |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 35 | A | 2493 | C |
| 35 | A | 2502 | C |
| 35 | A | 2520 | C |
| 35 | A | 2521 | A |
| 35 | A | 2527 | A |
| 35 | A | 2570 | C |
| 35 | A | 2592 | G |
| 35 | A | 2593 | G |
| 35 | A | 2594 | U |
| 35 | A | 2599 | U |
| 35 | A | 2600 | A |
| 35 | A | 2601 | A |
| 35 | A | 2603 | C |
| 35 | A | 2618 | U |
| 35 | A | 2627 | G |
| 35 | A | 2630 | U |
| 35 | A | 2633 | A |
| 35 | A | 2635 | G |
| 35 | A | 2654 | U |
| 35 | A | 2656 | U |
| 35 | A | 2683 | C |
| 35 | A | 2686 | G |
| 35 | A | 2694 | A |
| 35 | A | 2696 | A |
| 35 | A | 2706 | A |
| 35 | A | 2718 | C |
| 35 | A | 2719 | G |
| 35 | A | 2723 | A |
| 35 | A | 2724 | G |
| 35 | A | 2725 | A |
| 35 | A | 2732 | G |
| 35 | A | 2745 | A |
| 35 | A | 2757 | A |
| 35 | A | 2758 | G |
| 35 | A | 2759 | U |
| 35 | A | 2762 | C |
| 35 | A | 2765 | A |
| 35 | A | 2767 | A |
| 35 | A | 2768 | A |
| 35 | A | 2775 | A |
| 35 | A | 2781 | U |
| 35 | A | 2782 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 35 | A | 2786 | U |
| 35 | A | 2788 | C |
| 35 | A | 2790 | A |
| 35 | A | 2791 | A |
| 35 | A | 2810 | G |
| 35 | A | 2832 | A |
| 35 | A | 2833 | A |
| 35 | A | 2847 | C |
| 35 | A | 2864 | U |
| 35 | A | 2865 | C |
| 35 | A | 2882 | U |
| 35 | A | 2883 | A |
| 35 | A | 2885 | U |
| 35 | A | 2888 | A |
| 35 | A | 2889 | C |
| 35 | A | 2893 | A |
| 35 | A | 2913 | A |
| 35 | A | 2917 | G |
| 35 | A | 2918 | A |
| 35 | A | 2922 | A |
| 35 | A | 2928 | C |
| 35 | A | 2932 | G |
| 35 | A | 2935 | A |
| 35 | A | 2956 | A |
| 35 | A | 2989 | G |
| 35 | A | 2990 | A |
| 35 | A | 2992 | G |
| 35 | A | 2993 | U |
| 35 | A | 3005 | A |
| 35 | A | 3016 | G |
| 35 | A | 3041 | U |
| 35 | A | 3053 | A |
| 35 | A | 3054 | G |
| 35 | A | 3060 | C |
| 35 | A | 3072 | U |
| 35 | A | 3090 | G |
| 35 | A | 3100 | U |
| 35 | A | 3108 | U |
| 35 | A | 3109 | U |
| 35 | A | 3110 | C |
| 35 | A | 3111 | A |
| 35 | A | 3112 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 35 | A | 3113 | A |
| 35 | A | 3150 | U |
| 35 | A | 3157 | C |
| 35 | A | 3158 | A |
| 35 | A | 3162 | C |
| 35 | A | 3169 | C |
| 35 | A | 3172 | C |
| 35 | A | 3177 | A |
| 35 | A | 3183 | U |
| 35 | A | 3199 | U |
| 35 | A | 3200 | U |
| 35 | A | 3207 | A |
| 35 | A | 3209 | A |
| 35 | A | 3210 | C |
| 35 | A | 3212 | C |
| 35 | A | 3217 | A |
| 35 | A | 3218 | A |
| 35 | A | 3228 | U |
| 35 | A | 3229 | U |
| 35 | A | 3230 | G |
| 35 | A | 3231 | U |
| 36 | B | 8 | U |
| 36 | B | 16 | C |
| 36 | B | 21 | A |
| 36 | B | 45 | G |
| 36 | B | 48 | U |
| 36 | B | 54 | C |
| 36 | B | 55 | U |
| 36 | B | 56 | U |
| 36 | B | 64 | A |
| 36 | B | 69 | U |
| 36 | B | 76 | A |
| 89 | Ay | 3 | G |
| 89 | Ay | 4 | G |
| 89 | Ay | 9 | A |
| 89 | Ay | 23 | A |
| 89 | Ay | 25 | C |
| 89 | Ay | 44 | A |
| 89 | Ay | 45 | G |
| 89 | Ay | 46 | A |
| 89 | Ay | 48 | U |
| 89 | Ay | 49 | G |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 89 | Ay | 59 | U |
| 89 | Ay | 72 | A |
| 89 | Ay | 75 | C |
| 89 | Ay | 76 | A |

All (3) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 35 | A | 1691 | C |
| 35 | A | 2112 | A |
| 35 | A | 2245 | A |

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

20 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 |
| 1 | 5MC | AA | 1488 | 1 | 18,22,23 | 0.32 | 0 | 26,32,35 | 0.42 | 0 |
| 36 | 2MG | B | 10 | 36 | 18,26,27 | 1.16 | 2 (11%) | 16,38,41 | 0.87 | 1 (6%) |
| 53 | AYA | U | 2 | 53 | 6,7,8 | 0.80 | 0 | 5,8,10 | 0.58 | 0 |
| 1 | 5MU | AA | 1076 | 1 | 19,22,23 | 0.62 | 0 | 28,32,35 | 1.21 | 3 (10%) |
| 79 | AYA | k | 2 | 79 | 6,7,8 | 0.81 | 0 | 5,8,10 | 0.46 | 0 |
| 35 | 1MA | A | 2617 | 35 | 16,25,26 | 1.15 | 3 (18%) | 18,37,40 | 0.92 | 1 (5%) |
| 1 | MA6 | AA | 1583 | 1 | 18,26,27 | 0.74 | 0 | 19,38,41 | 0.57 | 0 |
| 1 | MA6 | AA | 1584 | 1 | 18,26,27 | 0.75 | 0 | 19,38,41 | 0.56 | 0 |
| 35 | OMG | A | 3040 | 32,35 | 18,26,27 | 0.91 | 2 (11%) | 19,38,41 | 0.60 | 0 |
| 36 | 1MA | B | 9 | 36 | 16,25,26 | 1.16 | 3 (18%) | 18,37,40 | 0.88 | 1 (5%) |
| 9 | 5F0 | AI | 184 | 9 | 8,8,9 | 0.58 | 0 | 7,9,11 | 1.16 | 1 (14%) |
| 17 | AYA | AQ | 2 | 17 | 6,7,8 | 0.80 | 0 | 5,8,10 | 0.81 | 0 |
| 1 | B8T | AA | 1486 | 93,1 | 19,22,23 | 0.29 | 0 | 26,31,34 | 0.34 | 0 |
| 29 | AYA | A2 | 2 | 29 | 6,7,8 | 0.81 | 0 | 5,8,10 | 0.45 | 0 |
| 35 | OMU | A | 3039 | 35,94 | 19,22,23 | 0.27 | 0 | 26,31,34 | 0.44 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|----------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 43 | SAC | K | 2 | 43 | 7,8,9 | 0.22 | 0 | 8,9,11 | 0.61 | 0 |
| 35 | OMG | A | 2815 | 35,33,94 | 18,26,27 | 0.94 | 2 (11%) | 19,38,41 | 0.63 | 0 |
| 35 | PSU | A | 3067 | 35 | 18,21,22 | 0.78 | 0 | 22,30,33 | 2.56 | 5 (22%) |
| 70 | THC | b | 2 | 70 | 8,9,10 | 0.28 | 0 | 9,11,13 | 0.48 | 0 |
| 36 | PSU | B | 39 | 36 | 18,21,22 | 0.76 | 0 | 22,30,33 | 2.54 | 4 (18%) |

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 |
|-----|------|-------|------|----------|---------|-----------|---------|
| 1 | 5MC | AA | 1488 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 36 | 2MG | B | 10 | 36 | - | 0/5/27/28 | 0/3/3/3 |
| 53 | AYA | U | 2 | 53 | - | 1/4/6/8 | - |
| 1 | 5MU | AA | 1076 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 79 | AYA | k | 2 | 79 | - | 0/4/6/8 | - |
| 35 | 1MA | A | 2617 | 35 | - | 0/3/25/26 | 0/3/3/3 |
| 1 | MA6 | AA | 1583 | 1 | - | 0/7/29/30 | 0/3/3/3 |
| 1 | MA6 | AA | 1584 | 1 | - | 2/7/29/30 | 0/3/3/3 |
| 35 | OMG | A | 3040 | 32,35 | - | 0/5/27/28 | 0/3/3/3 |
| 36 | 1MA | B | 9 | 36 | - | 0/3/25/26 | 0/3/3/3 |
| 9 | 5F0 | AI | 184 | 9 | - | 0/9/9/10 | - |
| 17 | AYA | AQ | 2 | 17 | - | 1/4/6/8 | - |
| 1 | B8T | AA | 1486 | 93,1 | - | 0/7/27/28 | 0/2/2/2 |
| 29 | AYA | A2 | 2 | 29 | - | 0/4/6/8 | - |
| 35 | OMU | A | 3039 | 35,94 | - | 0/9/27/28 | 0/2/2/2 |
| 43 | SAC | K | 2 | 43 | - | 0/7/8/10 | - |
| 35 | OMG | A | 2815 | 35,33,94 | - | 0/5/27/28 | 0/3/3/3 |
| 35 | PSU | A | 3067 | 35 | - | 0/7/25/26 | 0/2/2/2 |
| 70 | THC | b | 2 | 70 | - | 0/8/10/12 | - |
| 36 | PSU | B | 39 | 36 | - | 0/7/25/26 | 0/2/2/2 |

All (12) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 36 | B | 10 | 2MG | C8-N7 | -3.11 | 1.29 | 1.35 |
| 35 | A | 2617 | 1MA | C6-N6 | 3.11 | 1.35 | 1.27 |
| 36 | B | 9 | 1MA | C6-N6 | 3.08 | 1.35 | 1.27 |
| 36 | B | 10 | 2MG | C5-C6 | -2.38 | 1.42 | 1.47 |
| 35 | A | 2815 | OMG | C5-C6 | -2.32 | 1.42 | 1.47 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 35 | A | 3040 | OMG | C5-C6 | -2.21 | 1.42 | 1.47 |
| 36 | B | 9 | 1MA | C5-C4 | -2.13 | 1.37 | 1.43 |
| 35 | A | 2617 | 1MA | C5-C4 | -2.10 | 1.37 | 1.43 |
| 35 | A | 2815 | OMG | C8-N7 | -2.04 | 1.31 | 1.35 |
| 36 | B | 9 | 1MA | C8-N7 | -2.02 | 1.31 | 1.35 |
| 35 | A | 2617 | 1MA | C8-N7 | -2.01 | 1.31 | 1.35 |
| 35 | A | 3040 | OMG | C8-N7 | -2.01 | 1.31 | 1.35 |

All (16) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 36 | B | 39 | PSU | N1-C2-N3 | 8.06 | 124.26 | 115.13 |
| 35 | A | 3067 | PSU | N1-C2-N3 | 8.06 | 124.26 | 115.13 |
| 35 | A | 3067 | PSU | C4-N3-C2 | -6.55 | 116.90 | 126.34 |
| 36 | B | 39 | PSU | C4-N3-C2 | -6.50 | 116.97 | 126.34 |
| 1 | AA | 1076 | 5MU | C4-N3-C2 | -4.77 | 121.18 | 127.35 |
| 36 | B | 39 | PSU | O2-C2-N1 | -3.68 | 118.74 | 122.79 |
| 35 | A | 3067 | PSU | O2-C2-N1 | -3.64 | 118.78 | 122.79 |
| 9 | AI | 184 | 5F0 | O-C-CB | -2.69 | 117.58 | 125.43 |
| 1 | AA | 1076 | 5MU | C5-C4-N3 | 2.63 | 117.56 | 115.31 |
| 35 | A | 3067 | PSU | O2-C2-N3 | -2.58 | 116.96 | 121.82 |
| 36 | B | 39 | PSU | O2-C2-N3 | -2.56 | 117.00 | 121.82 |
| 1 | AA | 1076 | 5MU | N3-C2-N1 | 2.23 | 117.84 | 114.89 |
| 35 | A | 2617 | 1MA | N1-C6-N6 | 2.21 | 125.39 | 119.77 |
| 35 | A | 3067 | PSU | O4'-C1'-C2' | 2.15 | 108.17 | 105.14 |
| 36 | B | 10 | 2MG | O6-C6-C5 | 2.12 | 128.52 | 124.37 |
| 36 | B | 9 | 1MA | N1-C6-N6 | 2.10 | 125.11 | 119.77 |

There are no chirality outliers.

All (4) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|---------------|
| 17 | AQ | 2 | AYA | C-CA-N-CT |
| 1 | AA | 1584 | MA6 | C5-C6-N6-C9 |
| 53 | U | 2 | AYA | C-CA-N-CT |
| 1 | AA | 1584 | MA6 | C4'-C5'-O5'-P |

There are no ring outliers.

1 monomer is involved in 1 short contact:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 35 | A | 2815 | OMG | 1 | 0 |

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 276 ligands modelled in this entry, 263 are monoatomic - leaving 13 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 | SPD | AA | 1703 | - | 9,9,9 | 0.28 | 0 | 8,8,8 | 1.31 | 2 (25%) |
| 90 | NAD | AA | 1701 | 93 | 42,48,48 | 0.57 | 0 | 50,73,73 | 0.59 | 1 (2%) |
| 96 | FES | AP | 201 | 16,5 | 0,4,4 | - | - | - | | |
| 100 | VAL | B | 101 | 36 | 4,6,7 | 0.51 | 0 | 6,7,9 | 0.95 | 0 |
| 96 | FES | AT | 201 | 13,20 | 0,4,4 | - | - | - | | |
| 97 | ATP | AX | 501 | 93 | 26,33,33 | 0.75 | 0 | 31,52,52 | 0.64 | 0 |
| 99 | PUT | A | 3304 | - | 5,5,5 | 0.25 | 0 | 4,4,4 | 0.53 | 0 |
| 92 | SPD | A | 3303 | - | 9,9,9 | 0.38 | 0 | 8,8,8 | 1.14 | 0 |
| 96 | FES | r | 201 | 41,85 | 0,4,4 | - | - | - | | |
| 98 | GDP | AX | 503 | - | 24,30,30 | 0.88 | 1 (4%) | 30,47,47 | 0.61 | 0 |
| 92 | SPD | A | 3301 | - | 9,9,9 | 0.42 | 0 | 8,8,8 | 1.07 | 0 |
| 92 | SPD | A | 3302 | - | 9,9,9 | 0.33 | 0 | 8,8,8 | 1.22 | 0 |
| 91 | SPM | AA | 1702 | - | 13,13,13 | 0.28 | 0 | 12,12,12 | 0.98 | 0 |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|------------|---------|
| 92 | SPD | AA | 1703 | - | - | 0/7/7/7 | - |
| 90 | NAD | AA | 1701 | 93 | - | 0/26/62/62 | 0/5/5/5 |

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Continued from previous page...

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|-------|---------|------------|---------|
| 100 | VAL | B | 101 | 36 | - | 1/5/6/8 | - |
| 96 | FES | AP | 201 | 16,5 | - | - | 0/1/1/1 |
| 96 | FES | AT | 201 | 13,20 | - | - | 0/1/1/1 |
| 97 | ATP | AX | 501 | 93 | - | 0/18/38/38 | 0/3/3/3 |
| 99 | PUT | A | 3304 | - | - | 0/3/3/3 | - |
| 92 | SPD | A | 3303 | - | - | 2/7/7/7 | - |
| 96 | FES | r | 201 | 41,85 | - | - | 0/1/1/1 |
| 98 | GDP | AX | 503 | - | - | 0/12/32/32 | 0/3/3/3 |
| 92 | SPD | A | 3301 | - | - | 2/7/7/7 | - |
| 92 | SPD | A | 3302 | - | - | 0/7/7/7 | - |
| 91 | SPM | AA | 1702 | - | - | 1/11/11/11 | - |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 98 | AX | 503 | GDP | C5-C6 | -2.22 | 1.42 | 1.47 |

All (3) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 90 | AA | 1701 | NAD | C5A-C6A-N6A | 2.32 | 123.88 | 120.35 |
| 92 | AA | 1703 | SPD | C4-C5-N6 | -2.24 | 106.09 | 112.14 |
| 92 | AA | 1703 | SPD | C8-C7-N6 | -2.13 | 106.38 | 112.14 |

There are no chirality outliers.

All (6) torsion outliers are listed below:

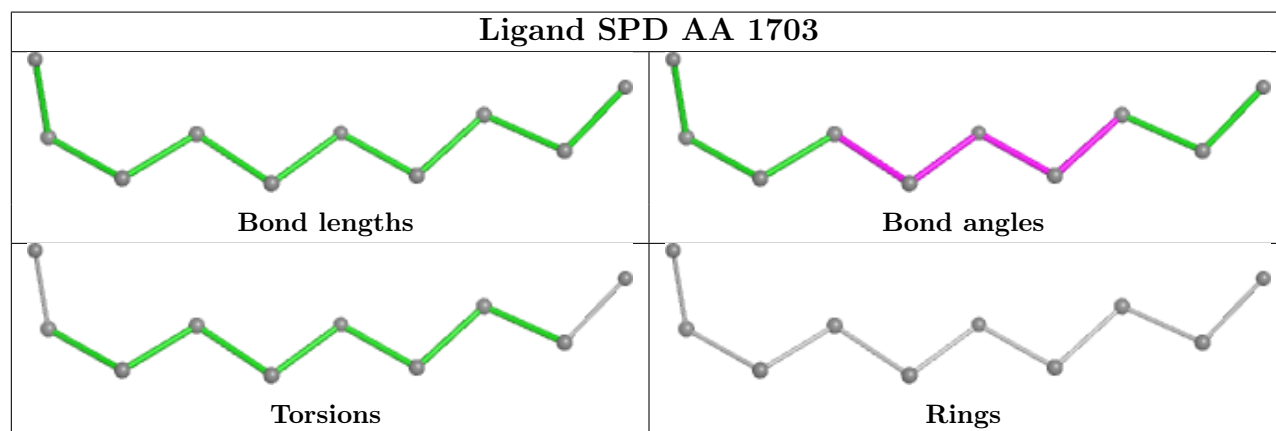
| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|----------------|
| 92 | A | 3301 | SPD | N6-C7-C8-C9 |
| 92 | A | 3301 | SPD | C3-C4-C5-N6 |
| 92 | A | 3303 | SPD | C4-C5-N6-C7 |
| 91 | AA | 1702 | SPM | C12-C11-N10-C9 |
| 92 | A | 3303 | SPD | C8-C7-N6-C5 |
| 100 | B | 101 | VAL | O-C-CA-CB |

There are no ring outliers.

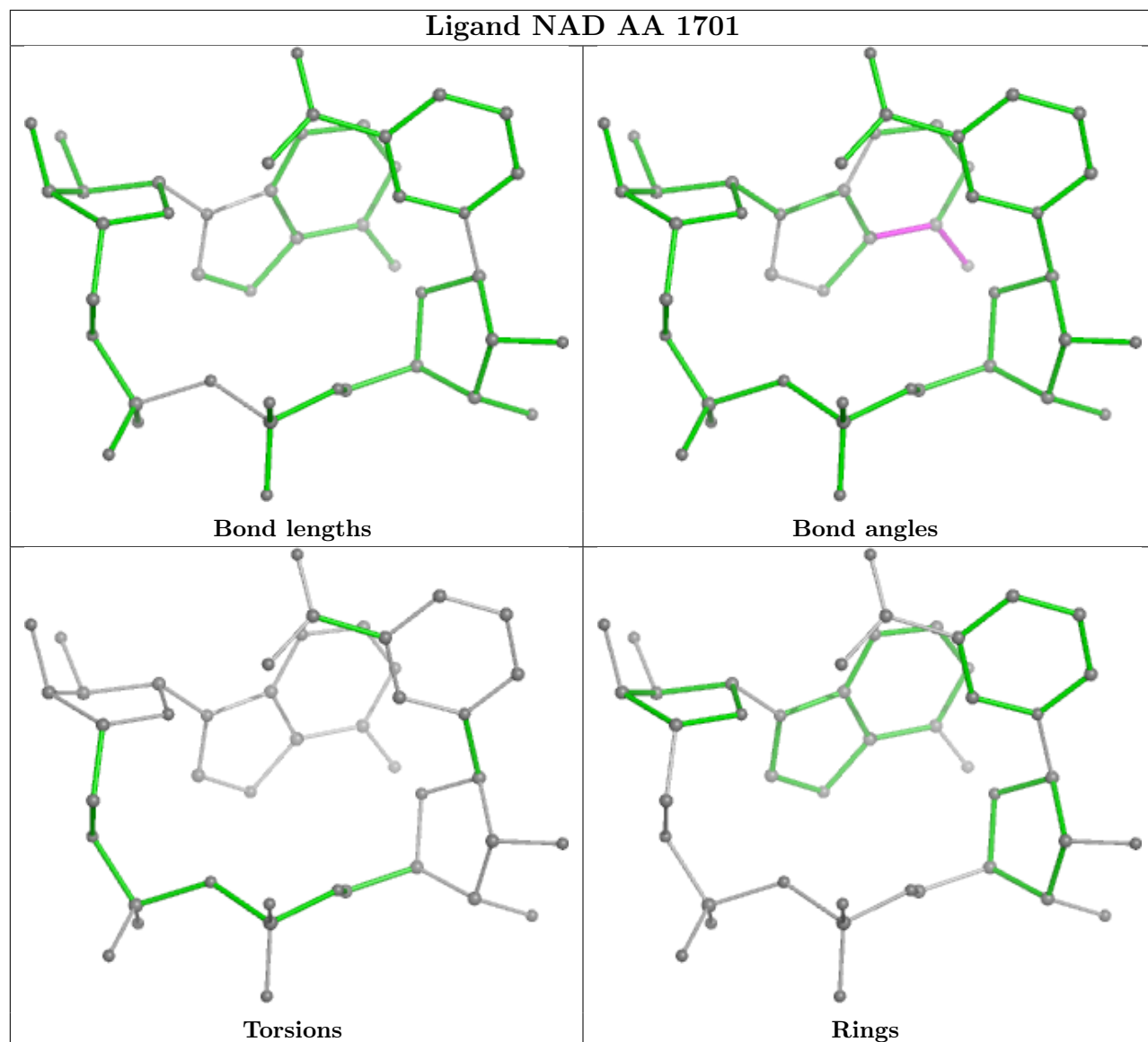
1 monomer is involved in 1 short contact:

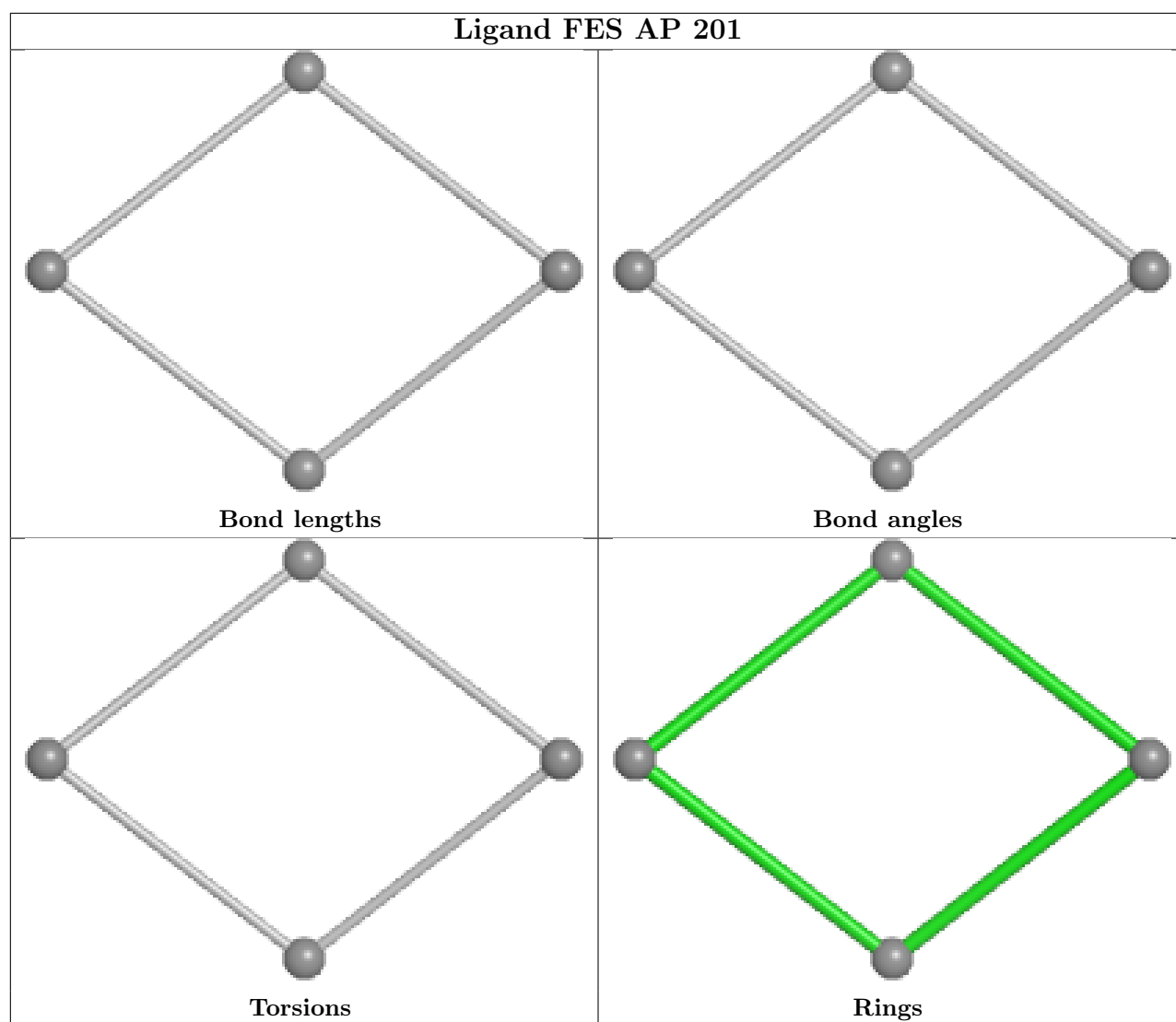
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 97 | AX | 501 | ATP | 1 | 0 |

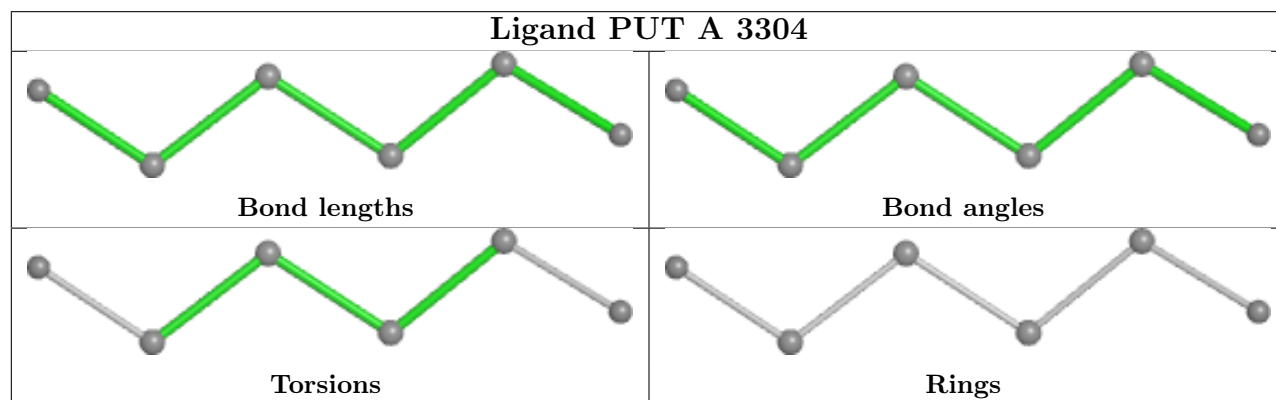
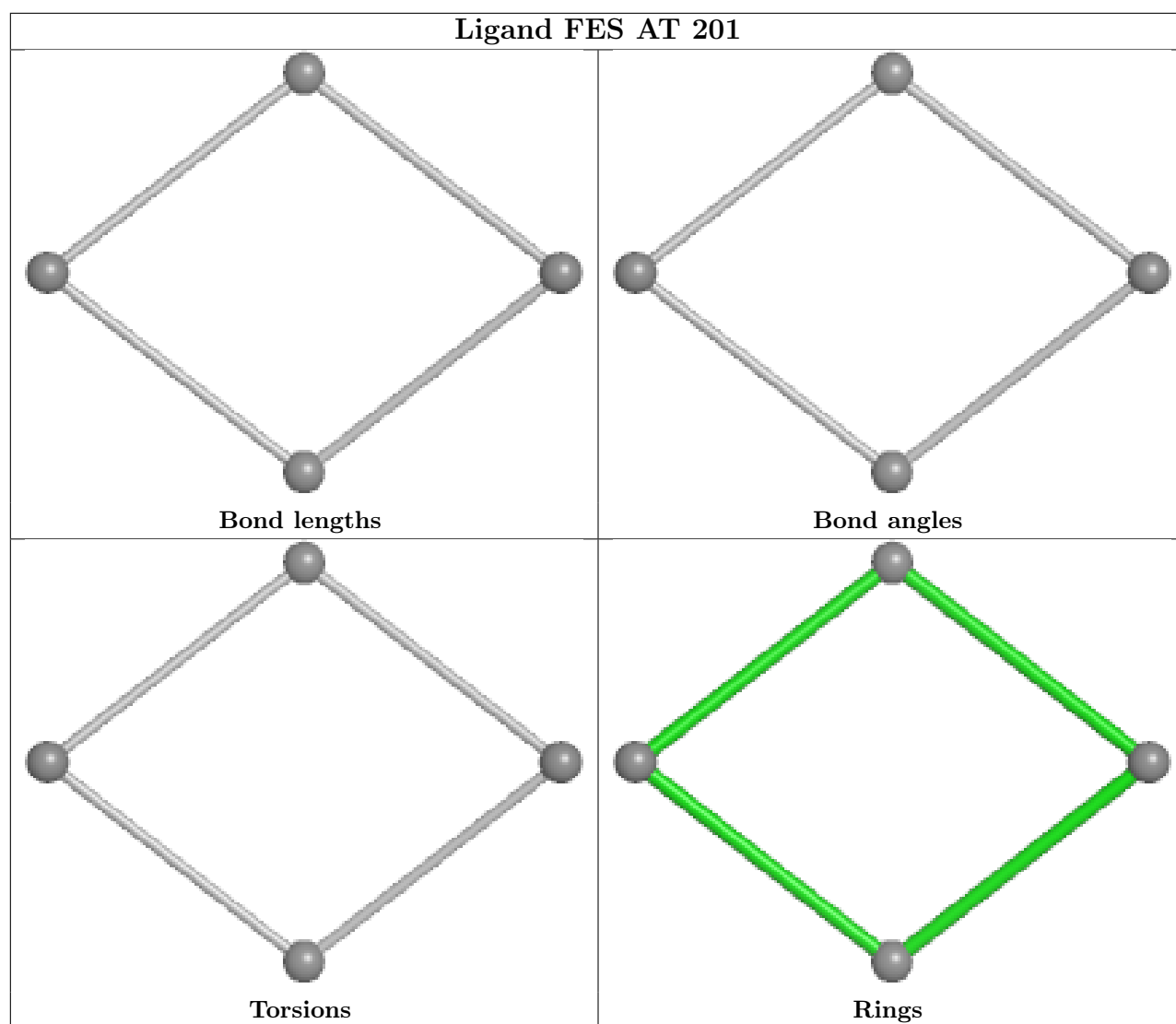
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

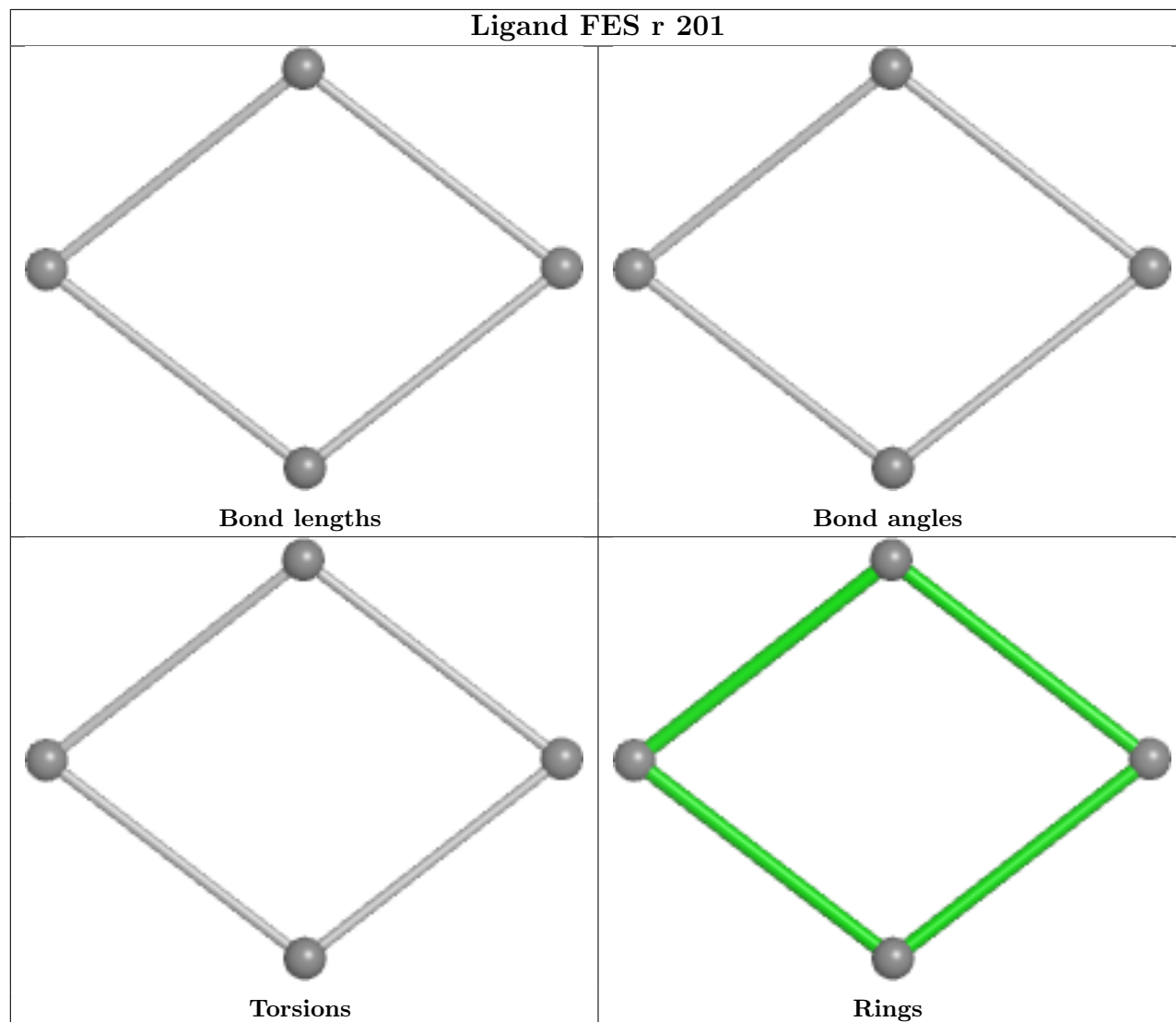
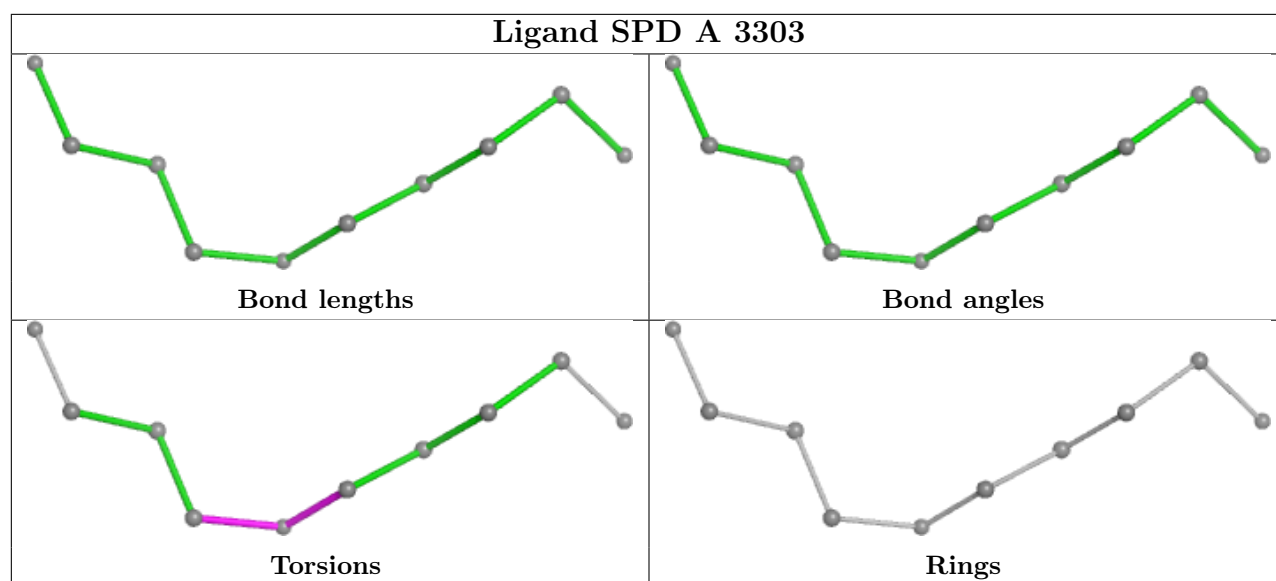


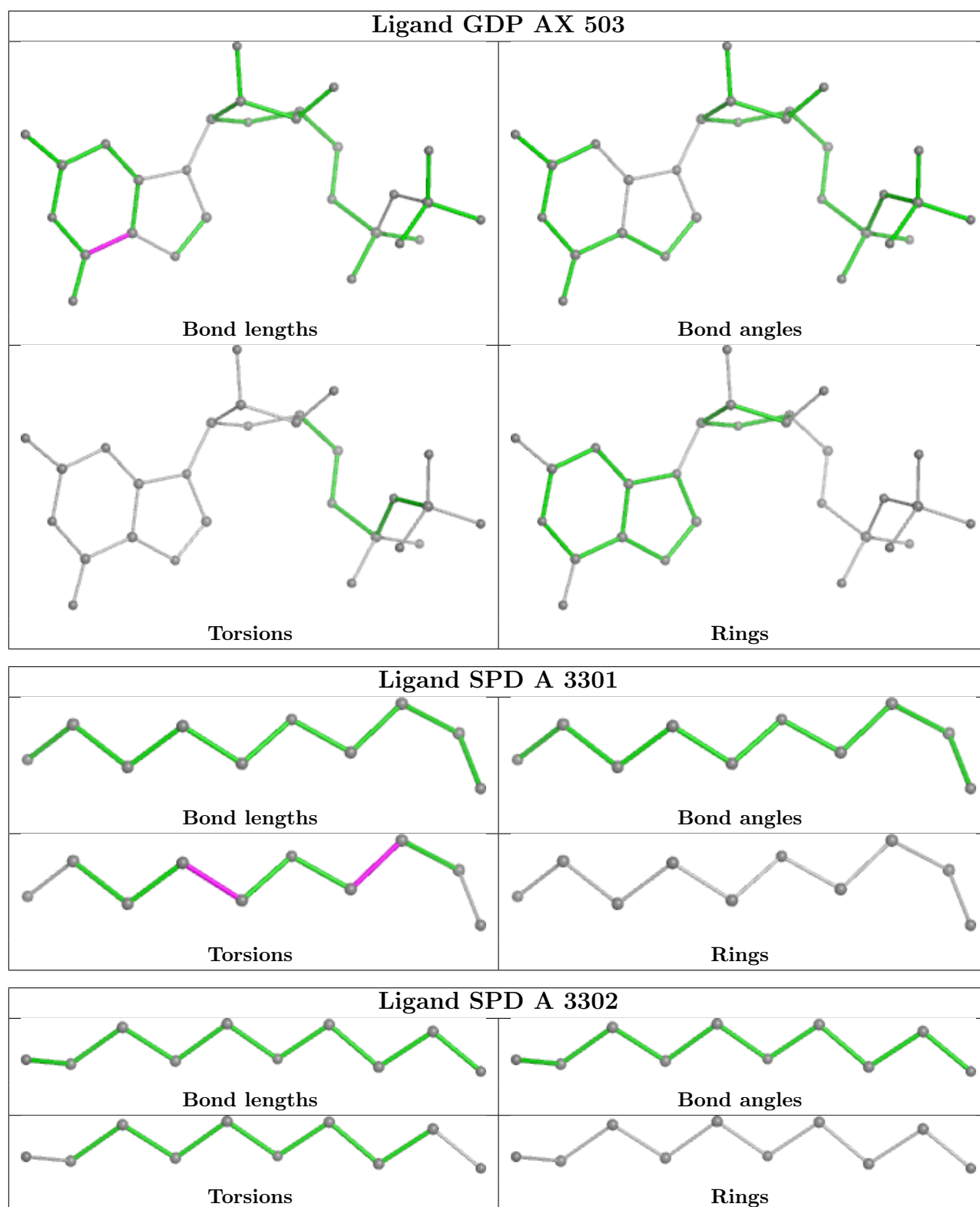
Ligand NAD AA 1701

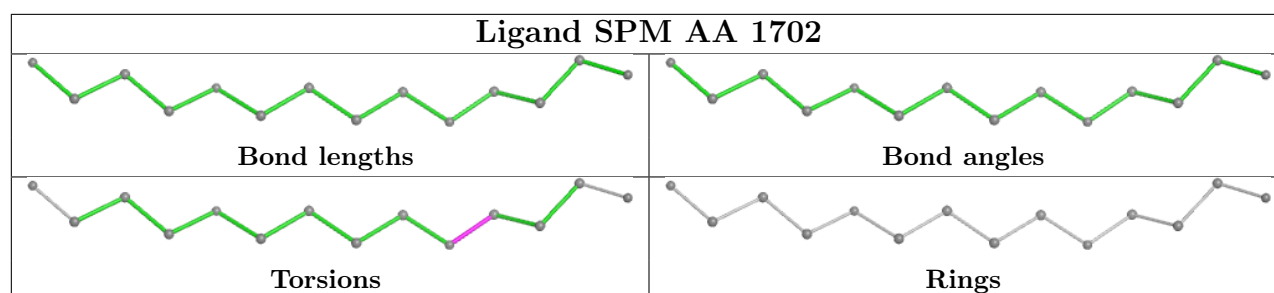












5.7 Other polymers [i](#)

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 |
|-----|-------|------------------|
| 89 | Ay | 3 |
| 32 | Aw | 1 |
| 35 | A | 1 |
| 33 | Ax | 1 |
| 34 | Az | 1 |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1 | Aw | 44:A | O3' | 74:C | P | 56.79 |
| 1 | Ay | 27:G | O3' | 43:C | P | 17.81 |
| 1 | Ay | 54:U | O3' | 58:A | P | 12.21 |
| 1 | A | 2357:C | O3' | 2361:G | P | 10.83 |
| 1 | Ax | 15:A | O3' | 21:A | P | 9.85 |
| 1 | Ay | 15:A | O3' | 21:A | P | 9.25 |
| 1 | Az | 3:A | O3' | 4:A | P | 3.05 |

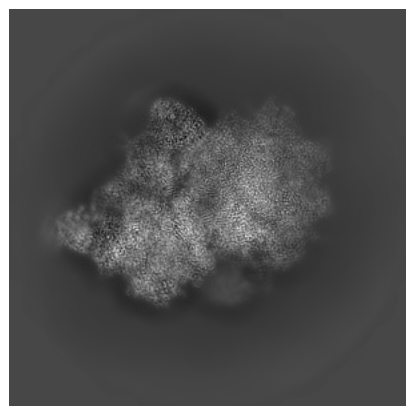
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13980. These allow visual inspection of the internal detail of the map and identification of artifacts.

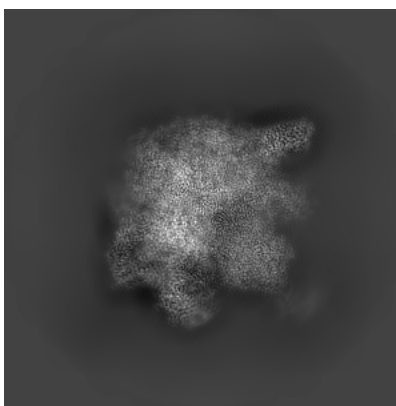
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

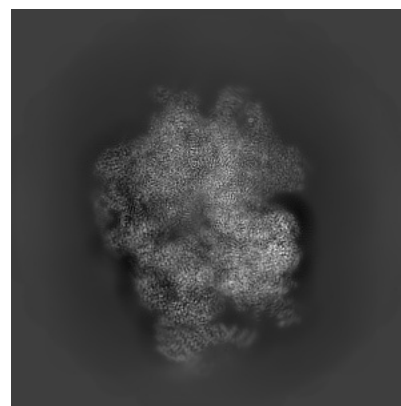
6.1.1 Primary map



X

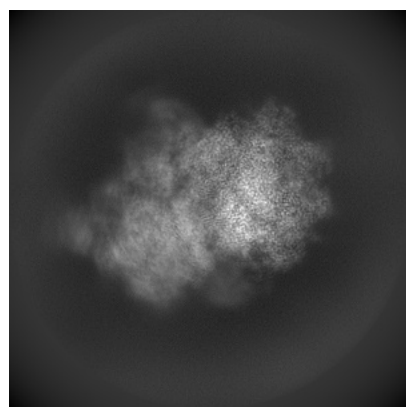


Y

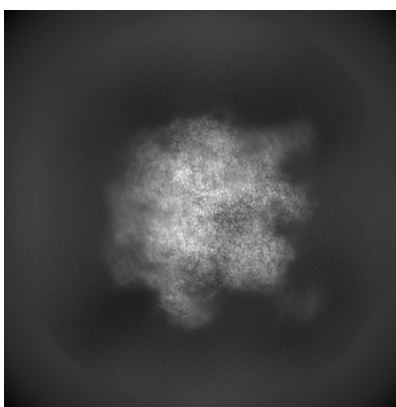


Z

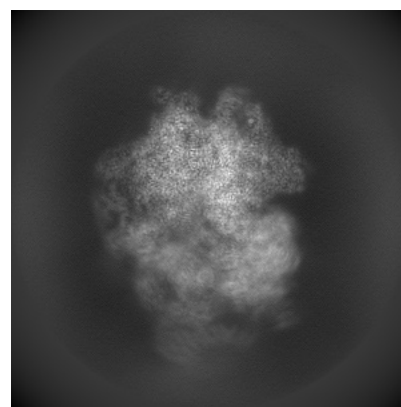
6.1.2 Raw map



X



Y

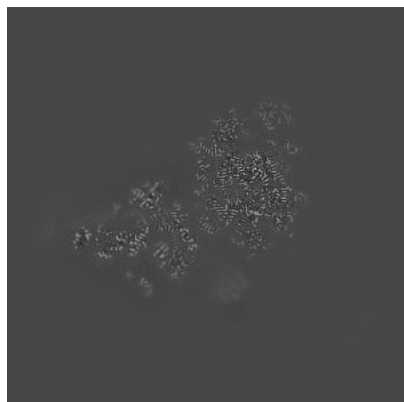


Z

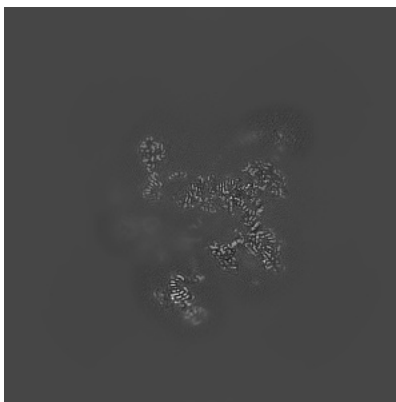
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

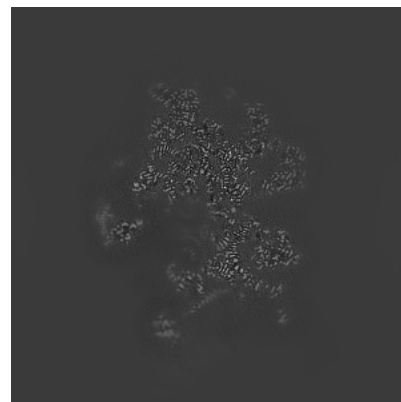
6.2.1 Primary map



X Index: 270

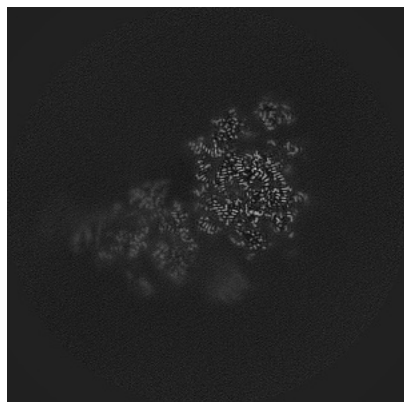


Y Index: 270

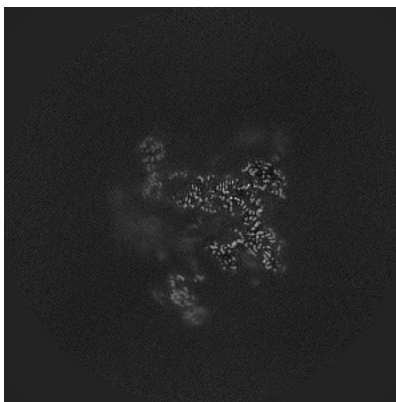


Z Index: 270

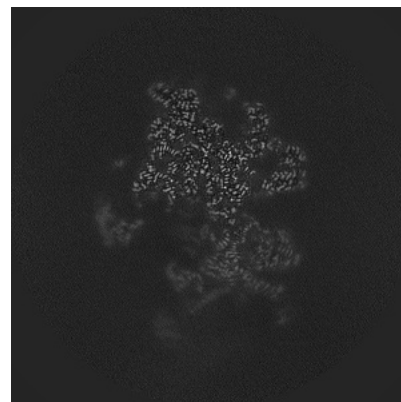
6.2.2 Raw map



X Index: 270



Y Index: 270

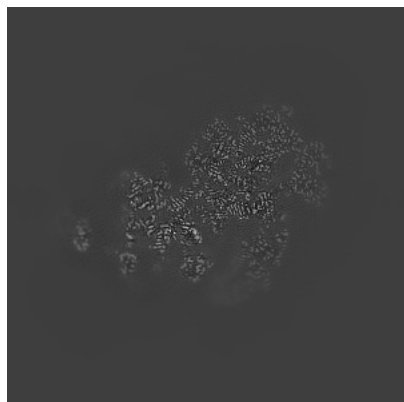


Z Index: 270

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

6.3 Largest variance slices [i](#)

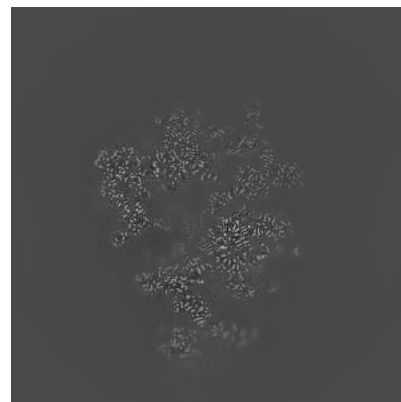
6.3.1 Primary map



X Index: 291

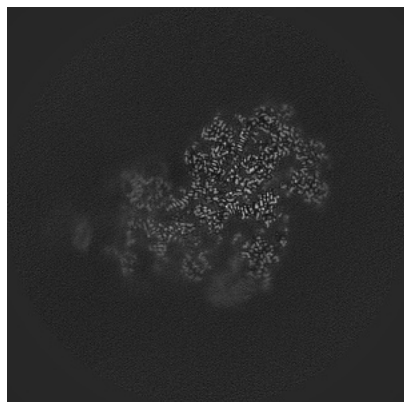


Y Index: 318

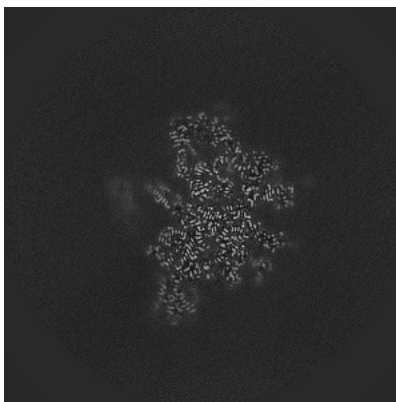


Z Index: 240

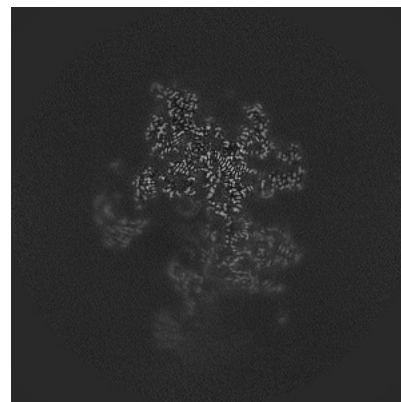
6.3.2 Raw map



X Index: 289



Y Index: 318

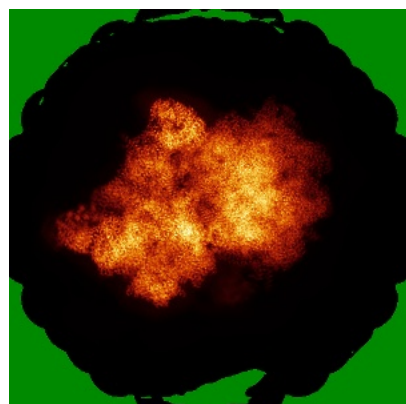


Z Index: 265

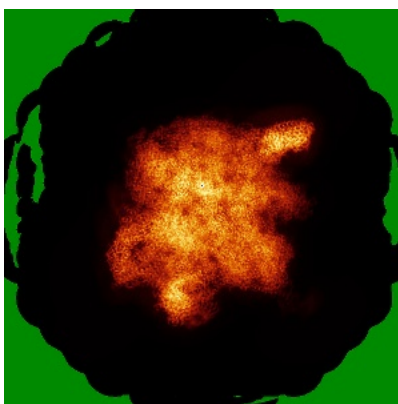
The images above show the largest variance slices of the map in three orthogonal directions.

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

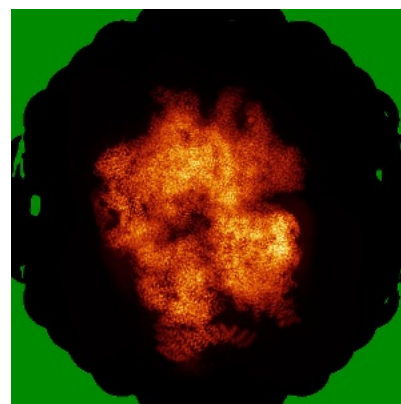
6.4.1 Primary map



X

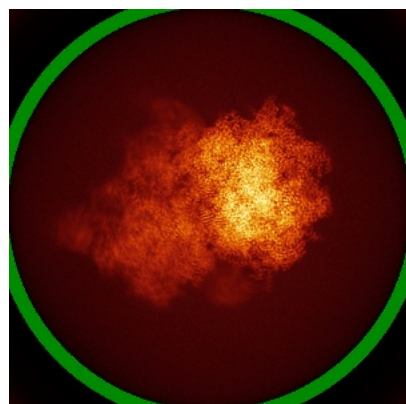


Y

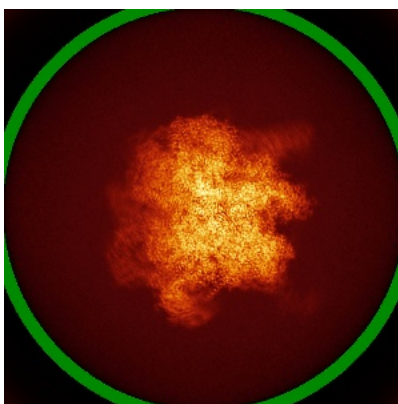


Z

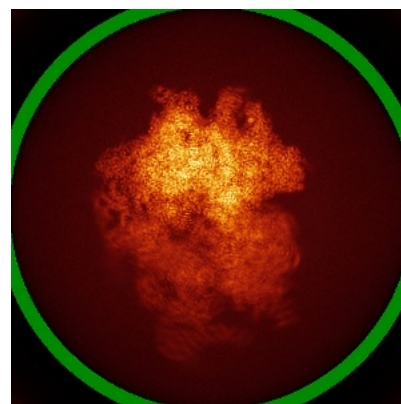
6.4.2 Raw map



X



Y

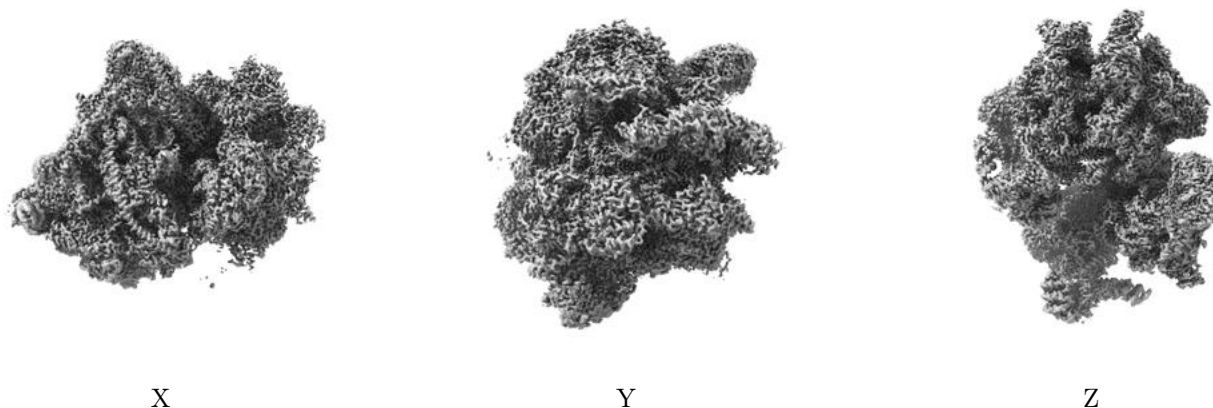


Z

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

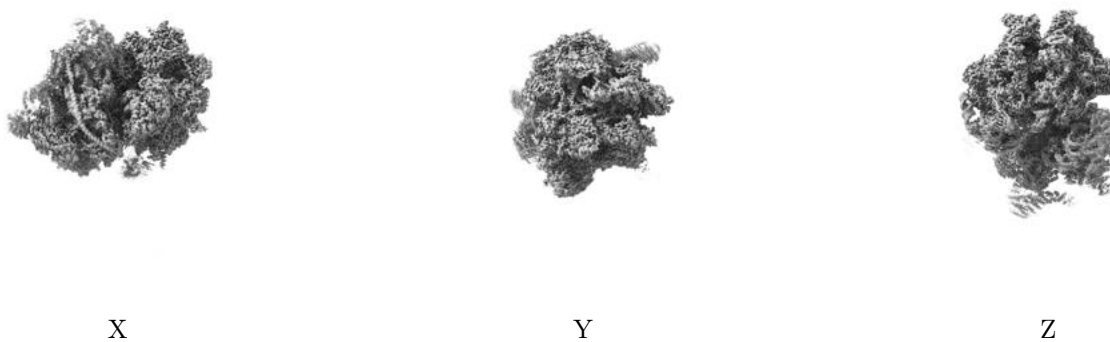
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 4.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

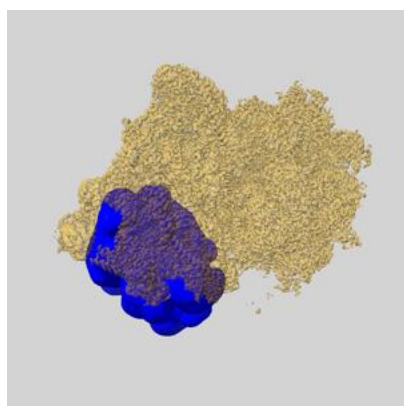
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

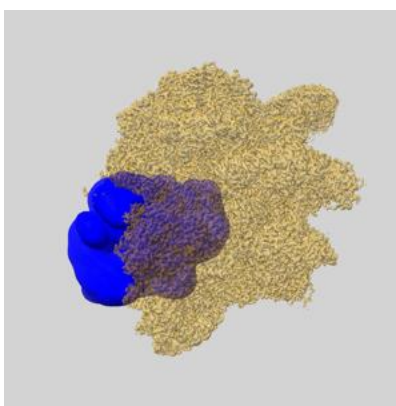
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

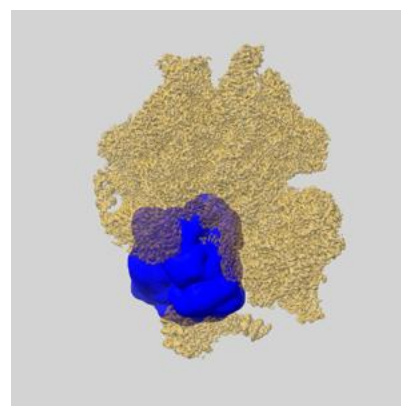
6.6.1 emd_13980_msk_1.map [i](#)



X

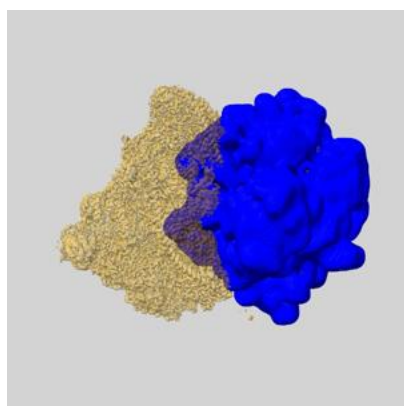


Y

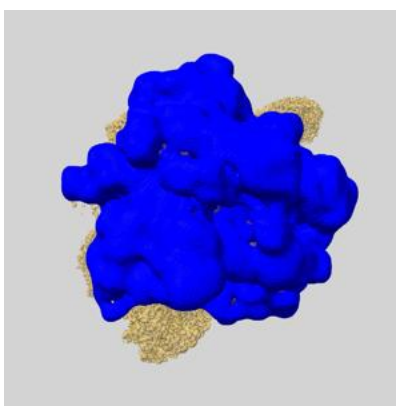


Z

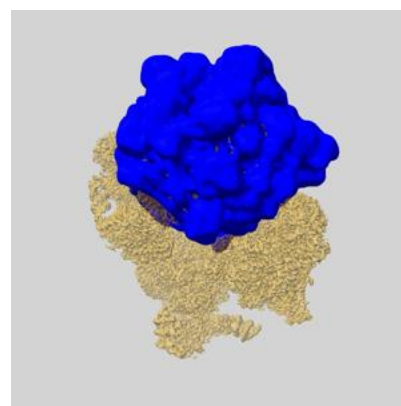
6.6.2 emd_13980_msk_2.map [i](#)



X

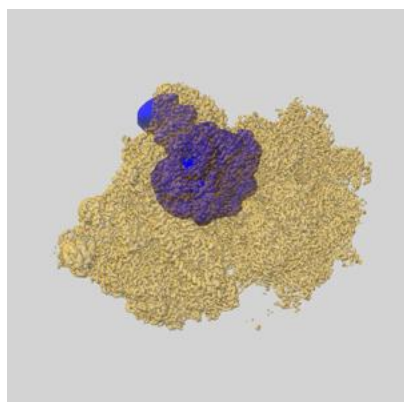


Y

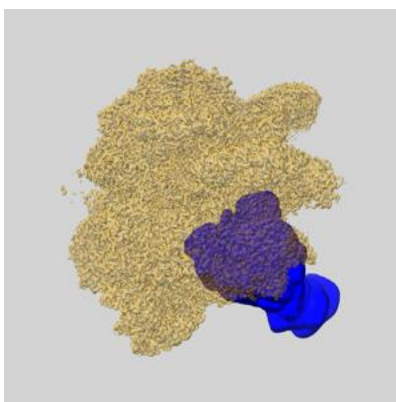


Z

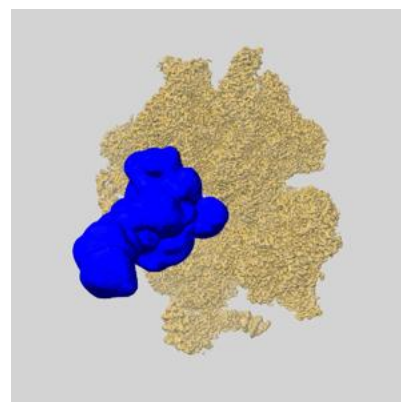
6.6.3 emd_13980_msk_3.map [i](#)



X

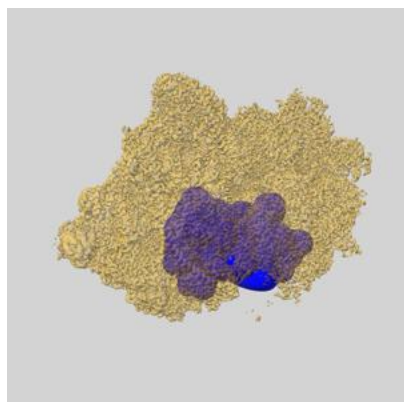


Y

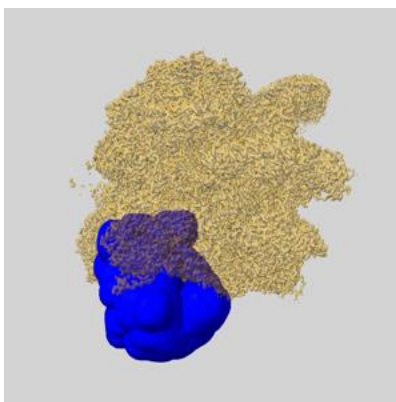


Z

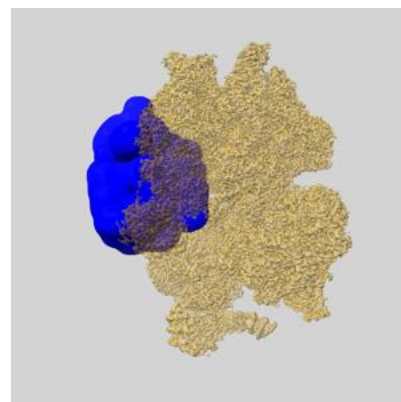
6.6.4 emd_13980_msk_4.map [i](#)



X

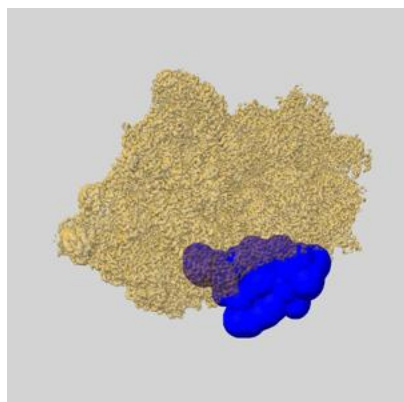


Y

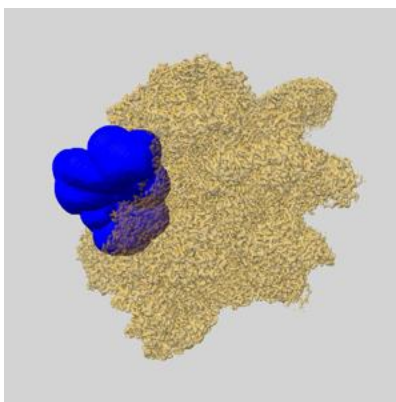


Z

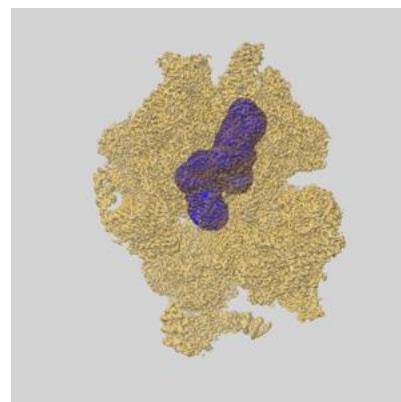
6.6.5 emd_13980_msk_5.map [i](#)



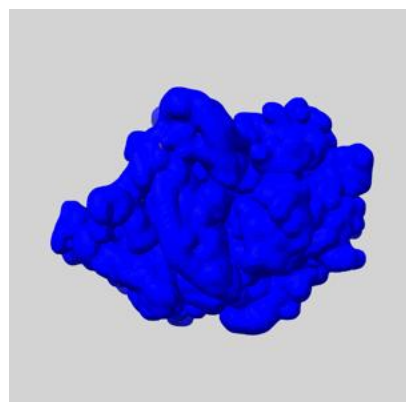
X



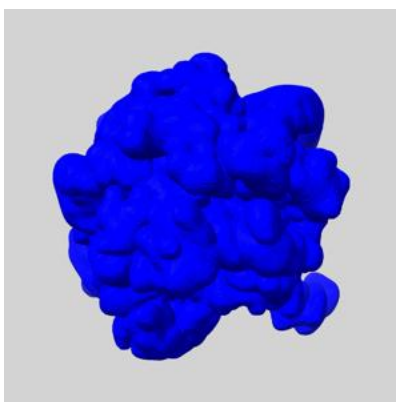
Y



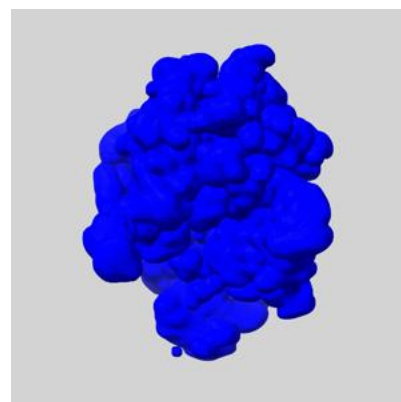
Z

6.6.6 emd_13980_msk_6.map [i](#)

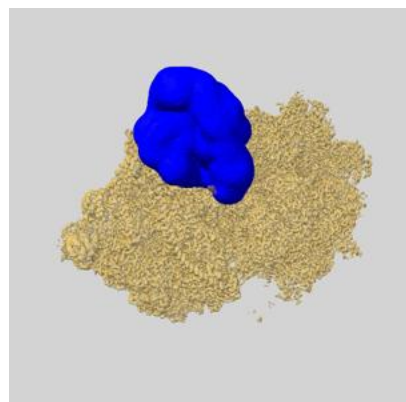
X



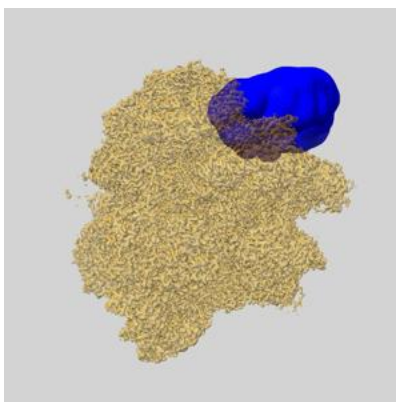
Y



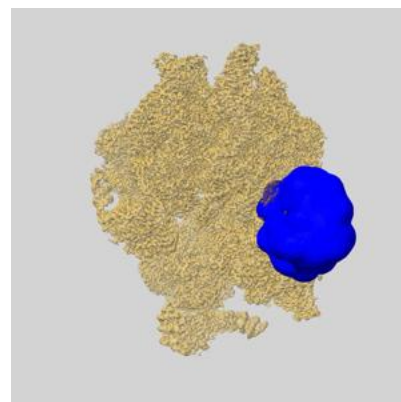
Z

6.6.7 emd_13980_msk_7.map [i](#)

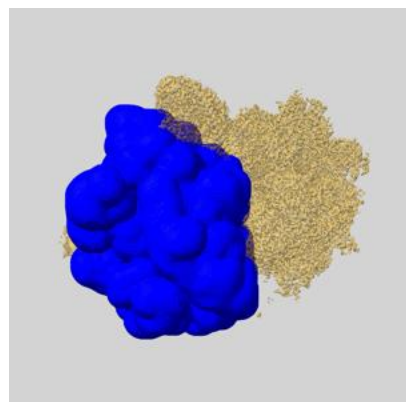
X



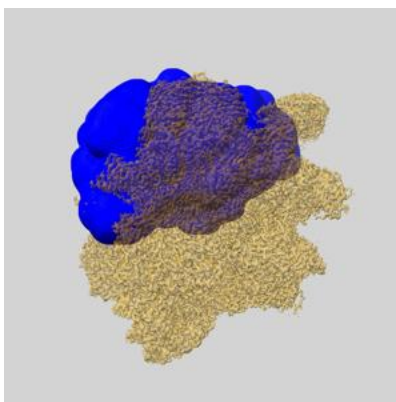
Y



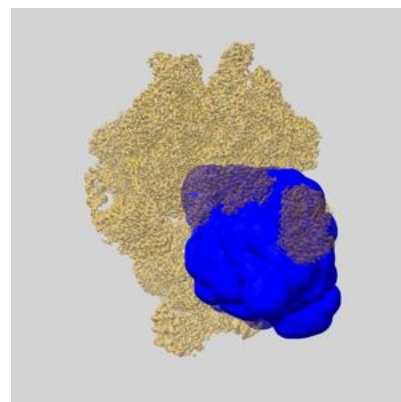
Z

6.6.8 emd_13980_msk_8.map [i](#)

X

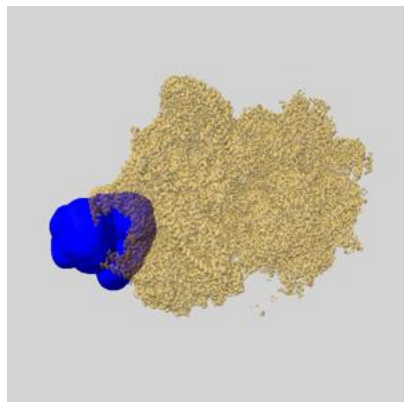


Y

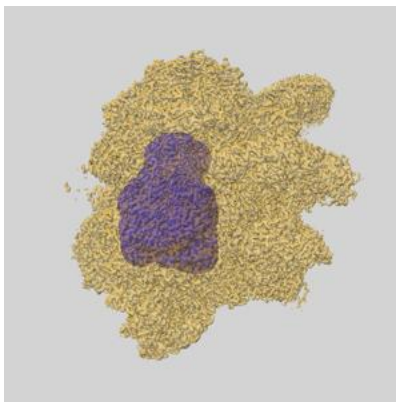


Z

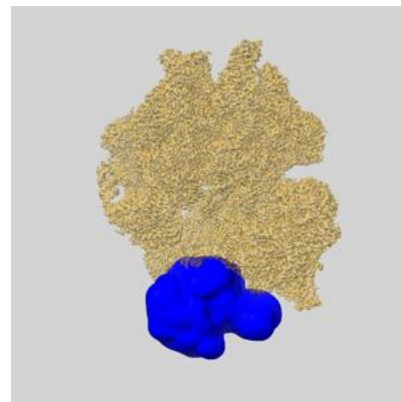
6.6.9 emd_13980_msk_9.map [i](#)



X



Y

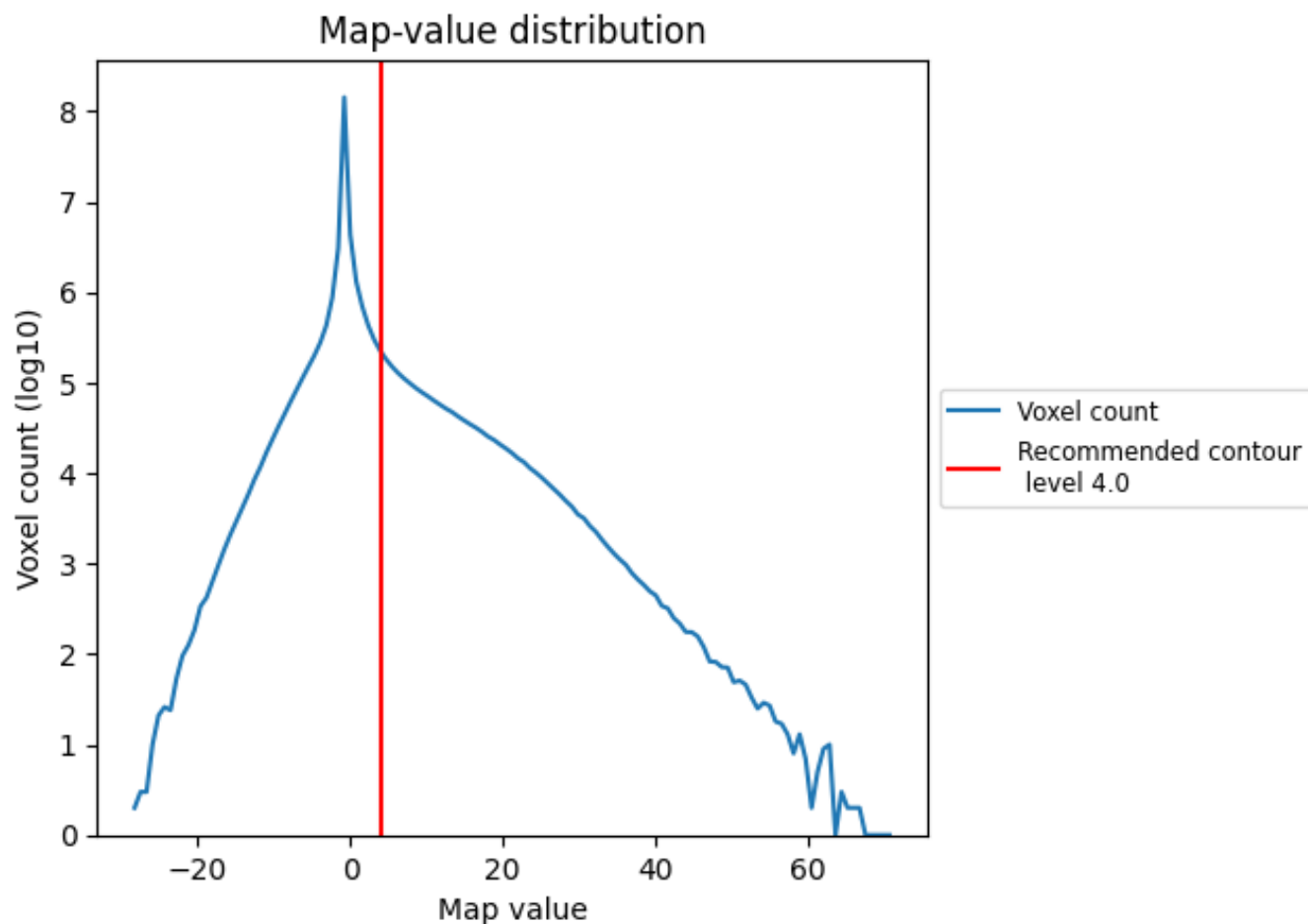


Z

7 Map analysis [i](#)

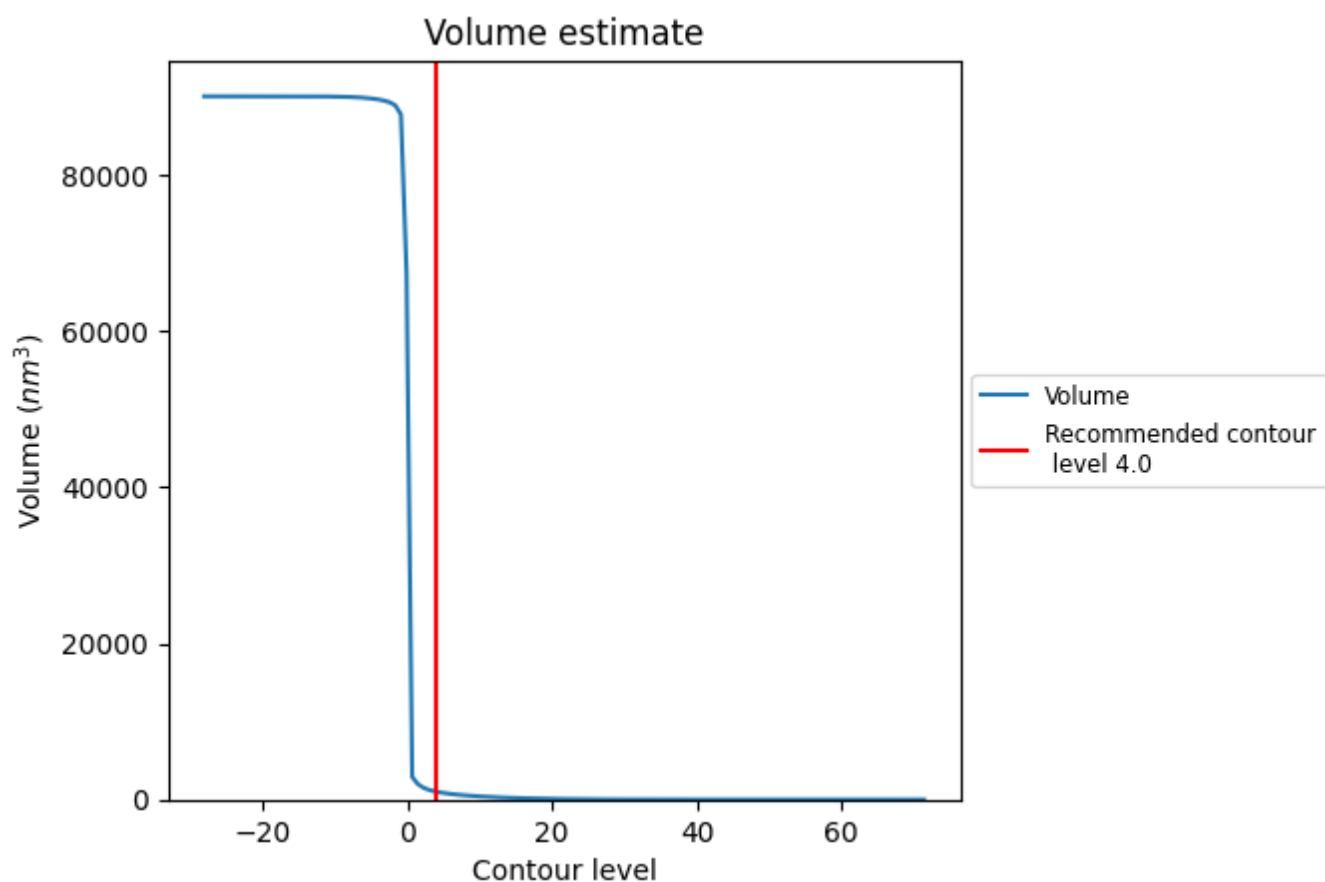
This section contains the results of statistical analysis of the map.

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.

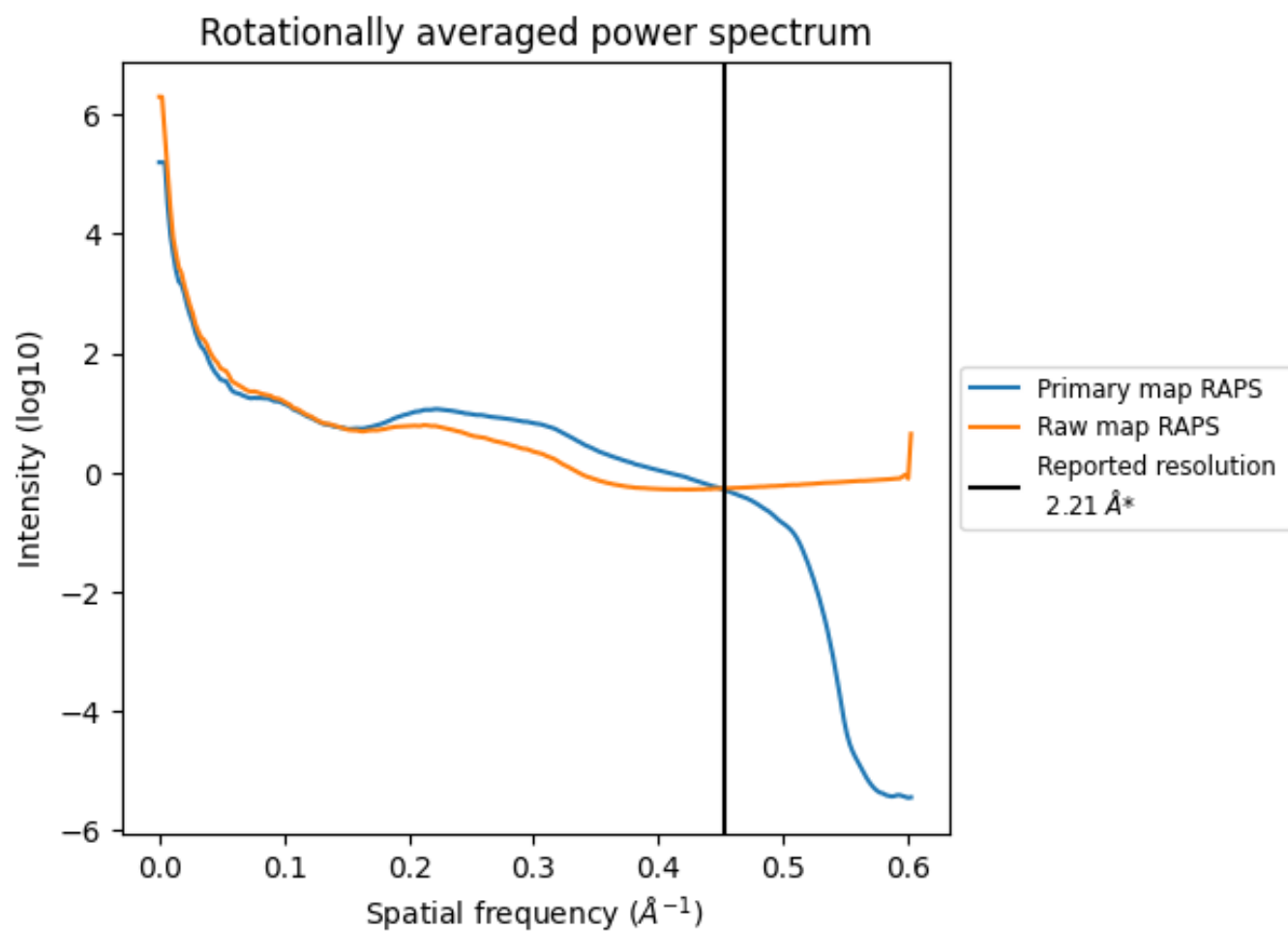
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 998 nm³; this corresponds to an approximate mass of 902 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

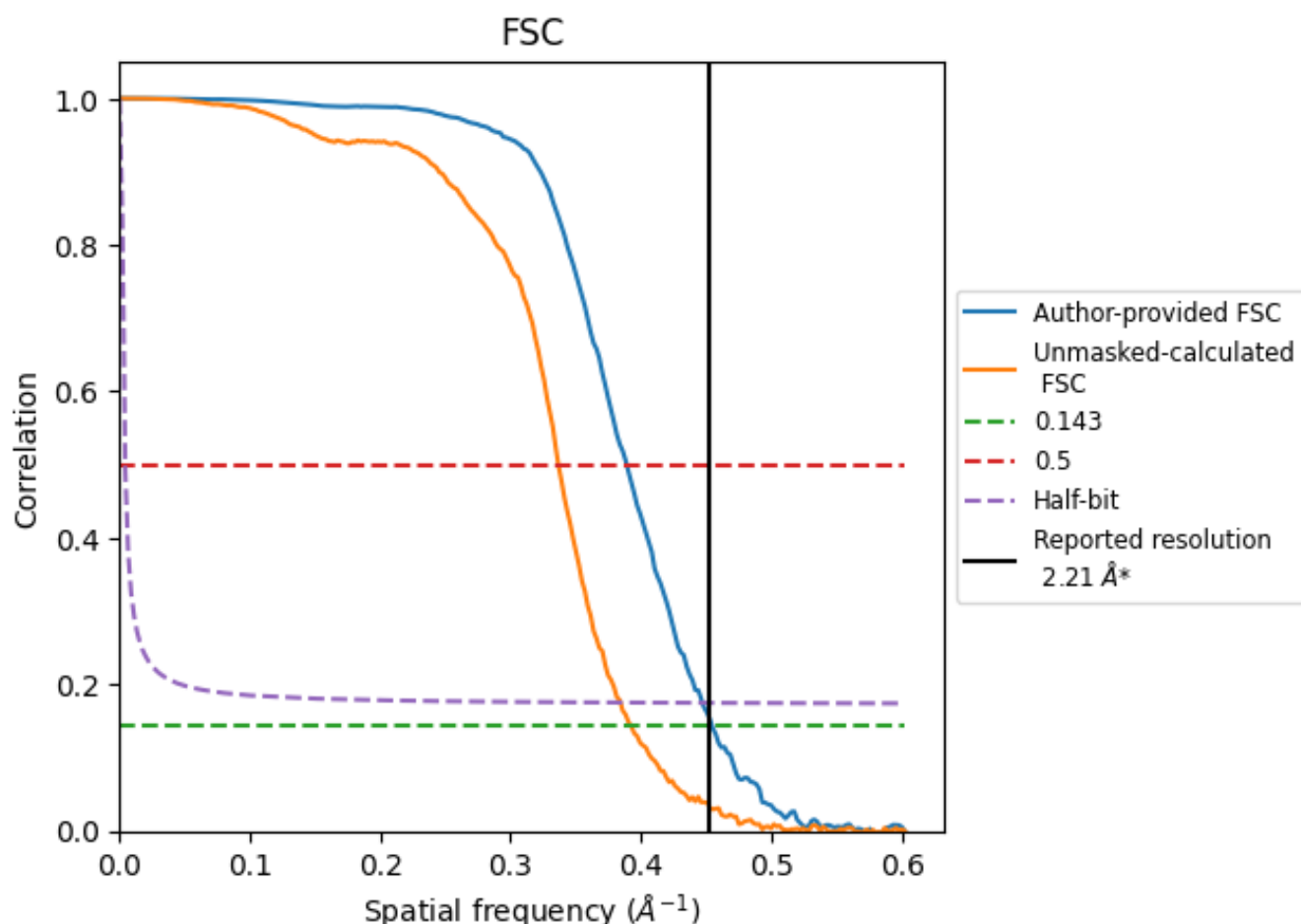


*Reported resolution corresponds to spatial frequency of 0.452 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.452 \AA^{-1}

8.2 Resolution estimates [i](#)

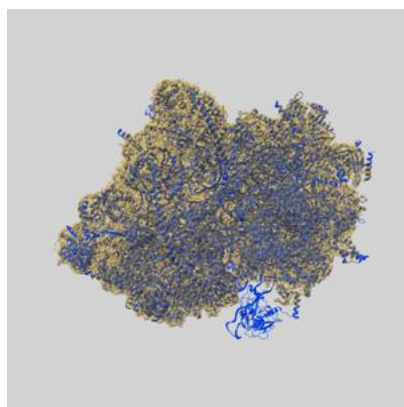
| Resolution estimate (Å) | Estimation criterion (FSC cut-off) | | |
|---------------------------|------------------------------------|------|----------|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | 2.21 | - | - |
| Author-provided FSC curve | 2.20 | 2.57 | 2.24 |
| Unmasked-calculated* | 2.55 | 2.97 | 2.60 |

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.55 differs from the reported value 2.21 by more than 10 %

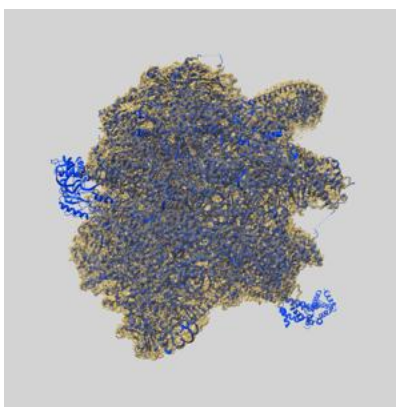
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-13980 and PDB model 7QI4. Per-residue inclusion information can be found in section 3 on page 31.

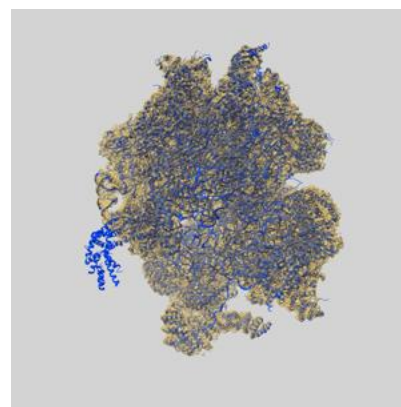
9.1 Map-model overlay [i](#)



X



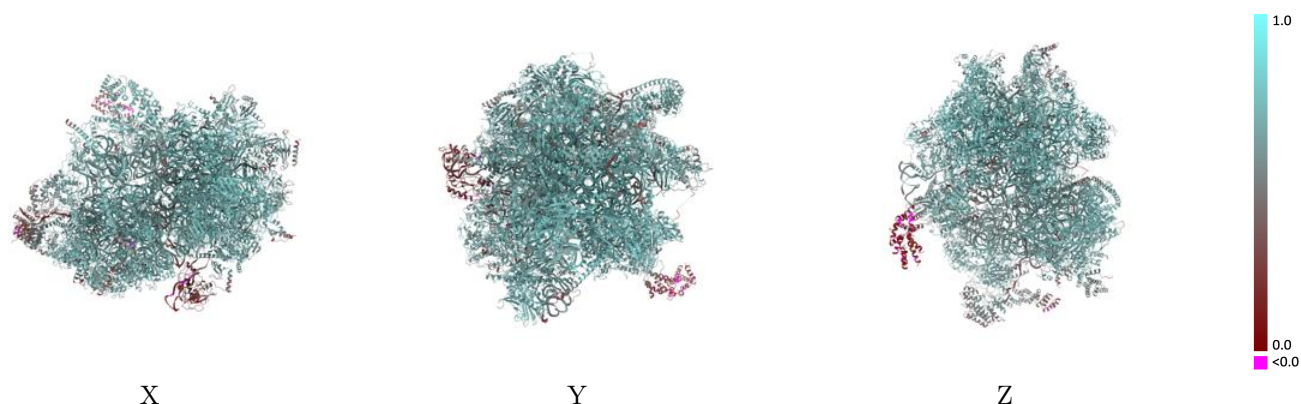
Y



Z

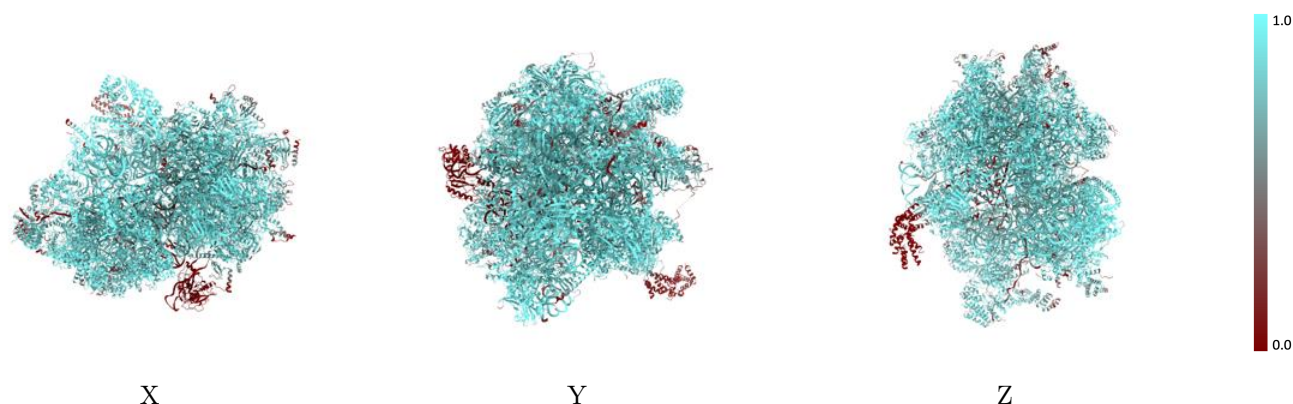
The images above show the 3D surface view of the map at the recommended contour level 4.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



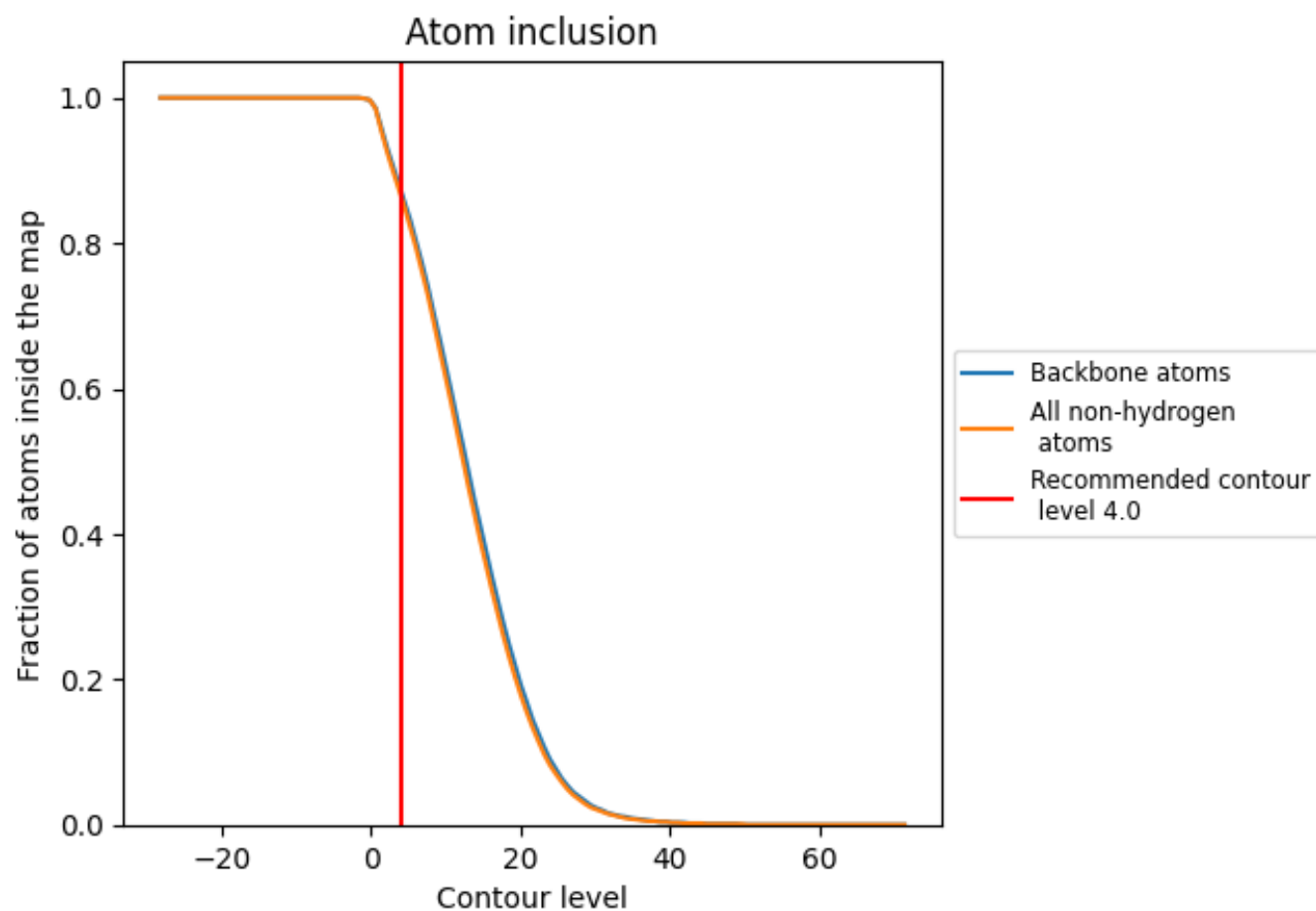
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (4.0).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 87% 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 (4.0) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|-------|--|--|
| All |  0.8660 |  0.6580 |
| 0 |  0.8910 |  0.7120 |
| 1 |  0.8340 |  0.6530 |
| 2 |  0.9970 |  0.7990 |
| 3 |  0.9800 |  0.7760 |
| 4 |  0.9570 |  0.7280 |
| 5 |  0.8920 |  0.6790 |
| 6 |  0.9470 |  0.6840 |
| 7 |  0.7770 |  0.6380 |
| 8 |  0.7300 |  0.5620 |
| 9 |  0.8140 |  0.6560 |
| A |  0.9310 |  0.7150 |
| A0 |  0.9350 |  0.6560 |
| A1 |  0.9030 |  0.6410 |
| A2 |  0.8240 |  0.6160 |
| A3 |  0.9400 |  0.6960 |
| A4 |  0.8330 |  0.5170 |
| AA |  0.9690 |  0.6790 |
| AB |  0.9370 |  0.6800 |
| AC |  0.9790 |  0.7080 |
| AD |  0.8780 |  0.6410 |
| AE |  0.9280 |  0.6750 |
| AF |  0.9240 |  0.6620 |
| AG |  0.8650 |  0.6250 |
| AH |  0.9420 |  0.6690 |
| AI |  0.9470 |  0.6810 |
| AJ |  0.9250 |  0.6580 |
| AK |  0.9770 |  0.7220 |
| AL |  0.8710 |  0.6390 |
| AM |  0.9230 |  0.6580 |
| AN |  0.9400 |  0.6820 |
| AO |  0.9200 |  0.6490 |
| AP |  0.9330 |  0.6880 |
| AQ |  0.9700 |  0.7130 |
| AR |  0.8420 |  0.5910 |







































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| Chain | Atom inclusion | Q-score |
|-------|--|--|
| AS |  0.8420 |  0.5980 |
| AT |  0.9180 |  0.6630 |
| AU |  0.8410 |  0.6050 |
| AV |  0.9450 |  0.6500 |
| AW |  0.9120 |  0.6420 |
| AX |  0.9440 |  0.6610 |
| AY |  0.8320 |  0.5840 |
| AZ |  0.9020 |  0.6580 |
| Aw |  0.4040 |  0.5580 |
| Ax |  0.3350 |  0.4630 |
| Ay |  0.0320 |  0.3360 |
| Az |  0.3840 |  0.3970 |
| B |  0.9290 |  0.6060 |
| D |  0.9450 |  0.7310 |
| E |  0.9310 |  0.7300 |
| F |  0.9500 |  0.7440 |
| H |  0.3380 |  0.4460 |
| I |  0.7310 |  0.5550 |
| J |  0.8260 |  0.5930 |
| K |  0.9680 |  0.7450 |
| L |  0.9410 |  0.7310 |
| M |  0.9400 |  0.7310 |
| N |  0.9210 |  0.6940 |
| O |  0.9380 |  0.7350 |
| P |  0.9700 |  0.7200 |
| Q |  0.8570 |  0.6850 |
| R |  0.9550 |  0.7670 |
| S |  0.9370 |  0.7330 |
| T |  0.9450 |  0.7360 |
| U |  0.8140 |  0.6740 |
| V |  0.7520 |  0.6230 |
| W |  0.9560 |  0.7350 |
| X |  0.8590 |  0.6760 |
| Y |  0.9190 |  0.7130 |
| Z |  0.9310 |  0.7310 |
| a |  0.8030 |  0.6550 |
| b |  0.9450 |  0.7370 |
| c |  0.8580 |  0.6730 |
| d |  0.6790 |  0.5740 |
| e |  0.8310 |  0.5750 |
| f |  0.8300 |  0.6020 |
| g |  0.8990 |  0.7070 |

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| Chain | Atom inclusion | Q-score |
|-------|--|--|
| h |  0.7470 |  0.6260 |
| i |  0.9710 |  0.7750 |
| j |  0.8340 |  0.6530 |
| k |  0.9150 |  0.6390 |
| l |  0.8770 |  0.6230 |
| m |  0.6820 |  0.5220 |
| o |  0.9670 |  0.7590 |
| p |  0.7550 |  0.5880 |
| q |  0.6110 |  0.5270 |
| r |  0.9320 |  0.6980 |
| s |  0.9060 |  0.7060 |
| t |  0.1870 |  0.3060 |
| u |  0.1050 |  0.2870 |
| v |  0.0000 |  0.1330 |
| w |  0.0000 |  0.0340 |
| x |  0.0000 |  0.0990 |
| y |  0.0000 |  0.0580 |
| z |  0.0080 |  0.2250 |