



wwPDB EM Validation Summary Report ⓘ

Dec 17, 2022 – 03:23 pm GMT

PDB ID : 6ZSB
EMDB ID : EMD-11392
Title : Human mitochondrial ribosome in complex with mRNA and P-site tRNA
Authors : Aibara, S.; Singh, V.; Modelska, A.; Amunts, A.
Deposited on : 2020-07-15
Resolution : 4.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

| | | |
|--------------------------------|---|--|
| EMDB validation analysis | : | 0.0.1.dev43 |
| 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 | : | FAILED |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.31.3 |

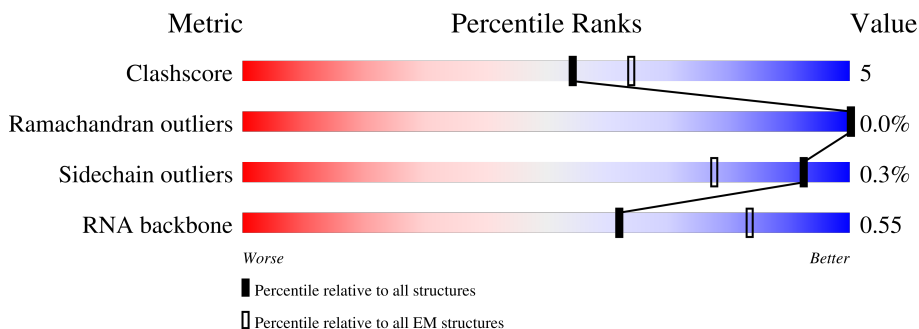
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.50 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 $\leq 5\%$.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | 0 | 188 | 49% 8% 43% |
| 2 | 1 | 65 | 68% 14% 18% |
| 3 | 2 | 92 | 43% 7% 50% |
| 4 | 3 | 188 | 39% 12% 49% |
| 5 | 4 | 103 | 33% . 63% |
| 6 | 5 | 423 | 80% 13% 7% |
| 7 | 6 | 380 | 79% 14% 7% |







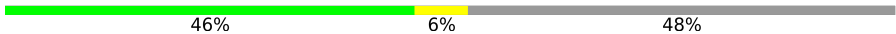


















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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 8 | 7 | 338 | |
| 9 | 8 | 206 | |
| 10 | 9 | 137 | |
| 11 | XA | 1561 | |
| 12 | A0 | 218 | |
| 13 | A1 | 323 | |
| 14 | A2 | 118 | |
| 15 | A3 | 199 | |
| 16 | A4 | 689 | |
| 17 | AA | 954 | |
| 18 | AB | 296 | |
| 19 | AC | 167 | |
| 20 | AD | 430 | |
| 21 | AE | 125 | |
| 22 | AF | 242 | |
| 23 | AG | 396 | |
| 24 | AH | 201 | |
| 25 | AI | 194 | |
| 26 | AJ | 138 | |
| 27 | AK | 128 | |
| 28 | AL | 257 | |
| 29 | AM | 137 | |
| 30 | AN | 130 | |
| 31 | AO | 258 | |
| 32 | AP | 142 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 33 | AQ | 87 |  |
| 34 | AR | 360 |  |
| 35 | AS | 190 |  |
| 36 | AT | 173 |  |
| 37 | AU | 205 |  |
| 38 | AV | 414 |  |
| 39 | AW | 187 |  |
| 40 | AX | 398 |  |
| 41 | AY | 395 |  |
| 42 | AZ | 106 |  |
| 43 | XB | 72 |  |
| 44 | XD | 305 |  |
| 45 | XE | 348 |  |
| 46 | XF | 311 |  |
| 47 | XH | 267 |  |
| 48 | XI | 261 |  |
| 49 | XJ | 192 |  |
| 50 | XK | 178 |  |
| 51 | XL | 145 |  |
| 52 | XM | 296 |  |
| 53 | XN | 251 |  |
| 54 | XO | 175 |  |
| 55 | XP | 180 |  |
| 56 | XQ | 292 |  |
| 57 | XR | 149 |  |

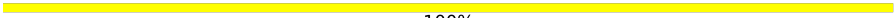
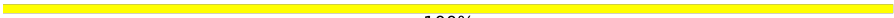







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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 58 | XS | 205 | |
| 59 | XT | 206 | |
| 60 | XU | 153 | |
| 61 | XV | 216 | |
| 62 | XW | 148 | |
| 63 | XX | 256 | |
| 64 | XY | 250 | |
| 65 | XZ | 161 | |
| 66 | a | 142 | |
| 67 | b | 215 | |
| 68 | c | 332 | |
| 69 | d | 306 | |
| 70 | e | 279 | |
| 71 | f | 212 | |
| 72 | g | 166 | |
| 73 | h | 158 | |
| 74 | i | 128 | |
| 75 | j | 123 | |
| 76 | k | 112 | |
| 77 | l | 138 | |
| 78 | m | 128 | |
| 79 | o | 102 | |
| 80 | p | 206 | |
| 81 | q | 222 | |
| 82 | r | 196 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 83 | r1 | 4 |  100% |
| 84 | r3 | 75 |  100% |
| 85 | s | 439 |  84% 16% |
| 86 | t1 | 198 |  23% 77% |
| 86 | t2 | 198 |  15% 85% |
| 86 | t3 | 198 |  15% 85% |
| 86 | t4 | 198 |  15% 85% |
| 86 | t5 | 198 |  15% 85% |
| 86 | t6 | 198 |  14% 86% |

2 Entry composition

There are 91 unique types of molecules in this entry. The entry contains 312096 atoms, of which 143062 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 39S ribosomal protein L32, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 1 | 0 | 108 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1783 | 545 | 903 | 172 | 157 | 6 | | |
| | | | | | | | | | | |

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

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|----|---|---------|-------|
| 2 | 1 | 53 | Total | C | H | N | O | S | 0 | 0 |
| | | | 919 | 281 | 480 | 84 | 72 | 2 | | |
| | | | | | | | | | | |

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

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|----|---|---------|-------|
| 3 | 2 | 46 | Total | C | H | N | O | S | 0 | 0 |
| | | | 782 | 233 | 406 | 83 | 59 | 1 | | |
| | | | | | | | | | | |

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

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 4 | 3 | 95 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1714 | 539 | 883 | 162 | 127 | 3 | | |
| | | | | | | | | | | |

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

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|----|---|---------|-------|
| 5 | 4 | 38 | Total | C | H | N | O | S | 0 | 0 |
| | | | 703 | 217 | 362 | 72 | 48 | 4 | | |
| | | | | | | | | | | |

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

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|-------|
| 6 | 5 | 393 | Total | C | H | N | O | S | 0 | 0 |
| | | | 6404 | 2070 | 3200 | 559 | 564 | 11 | | |
| | | | | | | | | | | |

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

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|---------|-------|
| 7 | 6 | 354 | Total | C | H | N | O | S | 0 | 0 |
| | | | 5786 | 1881 | 2839 | 525 | 532 | 9 | | |

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

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|-------|
| 8 | 7 | 291 | Total | C | H | N | O | S | 0 | 0 |
| | | | 4738 | 1514 | 2373 | 401 | 432 | 18 | | |

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

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 9 | 8 | 139 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2377 | 747 | 1202 | 208 | 218 | 2 | | |

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

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 10 | 9 | 124 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1983 | 644 | 987 | 170 | 180 | 2 | | |

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

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|------|-------|------|---------|-------|
| 11 | XA | 1499 | Total | C | H | N | O | P | 0 | 0 |
| | | | 48002 | 14284 | 16169 | 5756 | 10294 | 1499 | | |

- Molecule 12 is a protein called 28S ribosomal protein S34, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|---------|-------|
| 12 | A0 | 201 | Total | C | H | N | O | S | 0 | 0 |
| | | | 3369 | 1065 | 1685 | 322 | 292 | 5 | | |

- Molecule 13 is a protein called 28S ribosomal protein S35, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|-------|
| 13 | A1 | 275 | Total | C | H | N | O | S | 0 | 0 |
| | | | 4491 | 1414 | 2261 | 380 | 425 | 11 | | |

- Molecule 14 is a protein called Coiled-coil-helix-coiled-coil-helix domain-containing protein 1.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 14 | A2 | 116 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1889 | 574 | 964 | 181 | 162 | 8 | | |

- Molecule 15 is a protein called Aurora kinase A-interacting protein.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---|---------|-------|
| 15 | A3 | 69 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1292 | 393 | 682 | 130 | 86 | 1 | | |

- Molecule 16 is a protein called Pentatricopeptide repeat domain-containing protein 3, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|-------|
| 16 | A4 | 552 | Total | C | H | N | O | S | 0 | 0 |
| | | | 8955 | 2866 | 4485 | 756 | 820 | 28 | | |

- Molecule 17 is a RNA chain called 12S mitochondrial rRNA.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|------|-----|---------|-------|
| 17 | AA | 924 | Total | C | H | N | O | P | 0 | 0 |
| | | | 29598 | 8800 | 9970 | 3540 | 6364 | 924 | | |

- Molecule 18 is a protein called 28S ribosomal protein S2, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|-------|
| 18 | AB | 218 | Total | C | H | N | O | S | 0 | 0 |
| | | | 3545 | 1135 | 1769 | 322 | 309 | 10 | | |

- Molecule 19 is a protein called 28S ribosomal protein S24, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 19 | AC | 132 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2170 | 699 | 1088 | 195 | 184 | 4 | | |

- Molecule 20 is a protein called 28S ribosomal protein S5, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|-------|
| 20 | AD | 343 | Total | C | H | N | O | S | 0 | 0 |
| | | | 5501 | 1706 | 2785 | 515 | 482 | 13 | | |

- Molecule 21 is a protein called 28S ribosomal protein S6, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 21 | AE | 122 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1973 | 614 | 1001 | 177 | 177 | 4 | | |

- Molecule 22 is a protein called 28S ribosomal protein S7, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|-------|
| 22 | AF | 201 | Total | C | H | N | O | S | 0 | 0 |
| | | | 3383 | 1069 | 1715 | 305 | 283 | 11 | | |

- Molecule 23 is a protein called 28S ribosomal protein S9, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|-------|
| 23 | AG | 304 | Total | C | H | N | O | S | 0 | 0 |
| | | | 4996 | 1593 | 2491 | 444 | 454 | 14 | | |

- Molecule 24 is a protein called 28S ribosomal protein S10, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 24 | AH | 135 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2241 | 712 | 1136 | 187 | 203 | 3 | | |

- Molecule 25 is a protein called 28S ribosomal protein S11, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 25 | AI | 136 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2063 | 637 | 1052 | 192 | 178 | 4 | | |

- Molecule 26 is a protein called 28S ribosomal protein S12, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 26 | AJ | 108 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1725 | 521 | 887 | 169 | 142 | 6 | | |

- Molecule 27 is a protein called 28S ribosomal protein S14, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 27 | AK | 101 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1746 | 537 | 885 | 179 | 140 | 5 | | |

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

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 28 | AL | 164 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2854 | 883 | 1472 | 257 | 235 | 7 | | |

- Molecule 29 is a protein called 28S ribosomal protein S16, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 29 | AM | 116 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1871 | 582 | 951 | 182 | 150 | 6 | | |

- Molecule 30 is a protein called 28S ribosomal protein S17, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 30 | AN | 107 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1754 | 549 | 908 | 153 | 141 | 3 | | |

- Molecule 31 is a protein called 28S ribosomal protein S18b, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 31 | AO | 185 | Total | C | H | N | O | S | 0 | 0 |
| | | | 3018 | 970 | 1490 | 285 | 267 | 6 | | |

- Molecule 32 is a protein called 28S ribosomal protein S18c, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 32 | AP | 95 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1561 | 493 | 796 | 132 | 132 | 8 | | |

- Molecule 33 is a protein called 28S ribosomal protein S21, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 33 | AQ | 85 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1483 | 455 | 749 | 149 | 123 | 7 | | |

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 34 is a protein called 28S ribosomal protein S22, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|---------|-------|
| 34 | AR | 250 | Total | C | H | N | O | S | 0 | 0 |
| | | | 4134 | 1314 | 2074 | 353 | 385 | 8 | | |

- Molecule 35 is a protein called 28S ribosomal protein S23, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 35 | AS | 133 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2203 | 709 | 1103 | 196 | 194 | 1 | | |

- Molecule 36 is a protein called 28S ribosomal protein S25, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|----|---------|-------|
| 36 | AT | 162 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2673 | 850 | 1343 | 231 | 238 | 11 | | |

- Molecule 37 is a protein called 28S ribosomal protein S26, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 37 | AU | 173 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2932 | 900 | 1471 | 294 | 263 | 4 | | |

- Molecule 38 is a protein called 28S ribosomal protein S27, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|-------|
| 38 | AV | 349 | Total | C | H | N | O | S | 0 | 0 |
| | | | 5729 | 1841 | 2862 | 478 | 536 | 12 | | |

- Molecule 39 is a protein called 28S ribosomal protein S28, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 39 | AW | 97 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1551 | 486 | 785 | 137 | 139 | 4 | | |

- Molecule 40 is a protein called 28S ribosomal protein S29, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|-------|
| 40 | AX | 348 | Total | C | H | N | O | S | 0 | 0 |
| | | | 5619 | 1802 | 2805 | 491 | 510 | 11 | | |

- Molecule 41 is a protein called 28S ribosomal protein S31, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 41 | AY | 113 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1868 | 621 | 912 | 157 | 176 | 2 | | |

- Molecule 42 is a protein called 28S ribosomal protein S33, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 42 | AZ | 86 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1465 | 467 | 734 | 131 | 129 | 4 | | |

- Molecule 43 is a RNA chain called mitochondrial tRNA^{Val}.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|----|---------|-------|
| 43 | XB | 59 | Total | C | H | N | O | P | 0 | 0 |
| | | | 1895 | 563 | 640 | 227 | 406 | 59 | | |

- Molecule 44 is a protein called 39S ribosomal protein L2, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|---------|-------|
| 44 | XD | 236 | Total | C | H | N | O | S | 0 | 0 |
| | | | 3738 | 1145 | 1896 | 373 | 315 | 9 | | |

- Molecule 45 is a protein called 39S ribosomal protein L3, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|-------|
| 45 | XE | 304 | Total | C | H | N | O | S | 0 | 0 |
| | | | 4798 | 1539 | 2402 | 416 | 430 | 11 | | |

- Molecule 46 is a protein called 39S ribosomal protein L4, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|---------|-------|
| 46 | XF | 250 | Total | C | H | N | O | S | 0 | 0 |
| | | | 4058 | 1294 | 2045 | 365 | 348 | 6 | | |

- Molecule 47 is a protein called 39S ribosomal protein L9, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|--|---------|-------|
| 47 | XH | 95 | Total | C | H | N | O | | 0 | 0 |
| | | | 1616 | 498 | 832 | 152 | 134 | | | |

- Molecule 48 is a protein called 39S ribosomal protein L10, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|-------|
| 48 | XI | 211 | Total | C | H | N | O | S | 0 | 0 |
| | | | 3474 | 1086 | 1783 | 303 | 291 | 11 | | |

- Molecule 49 is a protein called 39S ribosomal protein L11, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 49 | XJ | 170 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2658 | 825 | 1367 | 230 | 234 | 2 | | |

- Molecule 50 is a protein called 39S ribosomal protein L13, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 50 | XK | 177 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2899 | 934 | 1448 | 259 | 251 | 7 | | |

- Molecule 51 is a protein called 39S ribosomal protein L14, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 51 | XL | 115 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1830 | 559 | 941 | 171 | 154 | 5 | | |

- Molecule 52 is a protein called 39S ribosomal protein L15, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|---------|-------|
| 52 | XM | 287 | Total | C | H | N | O | S | 0 | 0 |
| | | | 4683 | 1472 | 2378 | 425 | 402 | 6 | | |

- Molecule 53 is a protein called 39S ribosomal protein L16, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|-------|
| 53 | XN | 221 | Total | C | H | N | O | S | 0 | 0 |
| | | | 3586 | 1138 | 1808 | 325 | 305 | 10 | | |

- Molecule 54 is a protein called 39S ribosomal protein L17, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 54 | XO | 152 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2528 | 784 | 1283 | 239 | 215 | 7 | | |

- Molecule 55 is a protein called 39S ribosomal protein L18, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 55 | XP | 143 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2326 | 729 | 1162 | 223 | 207 | 5 | | |

- Molecule 56 is a protein called 39S ribosomal protein L19, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|---------|-------|
| 56 | XQ | 238 | Total | C | H | N | O | S | 0 | 0 |
| | | | 4000 | 1268 | 2022 | 352 | 349 | 9 | | |

- Molecule 57 is a protein called 39S ribosomal protein L20, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 57 | XR | 140 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2367 | 732 | 1214 | 231 | 186 | 4 | | |

- Molecule 58 is a protein called 39S ribosomal protein L21, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 58 | XS | 160 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2638 | 829 | 1354 | 226 | 225 | 4 | | |

- Molecule 59 is a protein called 39S ribosomal protein L22, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 59 | XT | 166 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2778 | 875 | 1410 | 254 | 232 | 7 | | |

- Molecule 60 is a protein called 39S ribosomal protein L23, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 60 | XU | 141 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2335 | 743 | 1164 | 222 | 203 | 3 | | |

- Molecule 61 is a protein called 39S ribosomal protein L24, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|---------|-------|
| 61 | XV | 202 | Total | C | H | N | O | S | 0 | 0 |
| | | | 3304 | 1051 | 1656 | 294 | 295 | 8 | | |

- Molecule 62 is a protein called 39S ribosomal protein L27, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 62 | XW | 111 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1769 | 558 | 898 | 164 | 146 | 3 | | |

- Molecule 63 is a protein called 39S ribosomal protein L28, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|---------|-------|
| 63 | XX | 243 | Total | C | H | N | O | S | 0 | 0 |
| | | | 4089 | 1317 | 2054 | 351 | 362 | 5 | | |

- Molecule 64 is a protein called 39S ribosomal protein L47, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 64 | XY | 178 | Total | C | H | N | O | S | 0 | 0 |
| | | | 3109 | 981 | 1575 | 295 | 254 | 4 | | |

- Molecule 65 is a protein called 39S ribosomal protein L30, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 65 | XZ | 120 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2008 | 626 | 1030 | 183 | 166 | 3 | | |

- Molecule 66 is a protein called 39S ribosomal protein L42, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 66 | a | 97 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1590 | 512 | 777 | 145 | 151 | 5 | | |

- Molecule 67 is a protein called 39S ribosomal protein L43, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 67 | b | 148 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2358 | 733 | 1180 | 229 | 213 | 3 | | |

- Molecule 68 is a protein called 39S ribosomal protein L44, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|---------|-------|
| 68 | c | 275 | Total | C | H | N | O | S | 0 | 0 |
| | | | 4437 | 1415 | 2220 | 383 | 410 | 9 | | |

- Molecule 69 is a protein called 39S ribosomal protein L45, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|-------|
| 69 | d | 216 | Total | C | H | N | O | S | 0 | 0 |
| | | | 3501 | 1125 | 1743 | 305 | 315 | 13 | | |

- Molecule 70 is a protein called 39S ribosomal protein L46, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|---------|-------|
| 70 | e | 217 | Total | C | H | N | O | S | 0 | 0 |
| | | | 3529 | 1124 | 1767 | 310 | 323 | 5 | | |

- Molecule 71 is a protein called 39S ribosomal protein L48, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 71 | f | 143 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2314 | 737 | 1165 | 187 | 221 | 4 | | |

- Molecule 72 is a protein called 39S ribosomal protein L49, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 72 | g | 132 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2183 | 710 | 1086 | 191 | 194 | 2 | | |

- Molecule 73 is a protein called 39S ribosomal protein L50, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 73 | h | 108 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1748 | 560 | 866 | 154 | 165 | 3 | | |

- Molecule 74 is a protein called 39S ribosomal protein L51, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 74 | i | 97 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1684 | 532 | 857 | 165 | 126 | 4 | | |

- Molecule 75 is a protein called 39S ribosomal protein L52, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 75 | j | 86 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1367 | 426 | 678 | 134 | 127 | 2 | | |

- Molecule 76 is a protein called 39S ribosomal protein L53, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 76 | k | 95 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1477 | 456 | 745 | 139 | 132 | 5 | | |

- Molecule 77 is a protein called 39S ribosomal protein L54, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 77 | l | 80 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1327 | 427 | 654 | 118 | 125 | 3 | | |

- Molecule 78 is a protein called 39S ribosomal protein L55, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---|---------|-------|
| 78 | m | 60 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1025 | 309 | 525 | 104 | 85 | 2 | | |

- Molecule 79 is a protein called Ribosomal protein 63, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 79 | o | 94 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1601 | 501 | 804 | 165 | 128 | 3 | | |

- Molecule 80 is a protein called Peptidyl-tRNA hydrolase ICT1, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 80 | p | 127 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2141 | 661 | 1083 | 201 | 192 | 4 | | |

- Molecule 81 is a protein called Growth arrest and DNA damage-inducible proteins-interacting protein 1.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 81 | q | 164 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2737 | 858 | 1358 | 267 | 249 | 5 | | |

- Molecule 82 is a protein called 39S ribosomal protein S18a, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 82 | r | 152 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2514 | 792 | 1267 | 239 | 208 | 8 | | |

- Molecule 83 is a RNA chain called mRNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|----|---|----|---|---------|-------|
| 83 | r1 | 4 | Total | C | N | O | P | 0 | 0 |
| | | | 72 | 36 | 8 | 24 | 4 | | |

- Molecule 84 is a RNA chain called P-site tRNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 84 | r3 | 75 | Total | C | N | O | P | 0 | 0 |
| | | | 1459 | 711 | 222 | 451 | 75 | | |

- Molecule 85 is a protein called 39S ribosomal protein S30, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|-------|
| 85 | s | 370 | Total | C | H | N | O | S | 0 | 0 |
| | | | 6058 | 1946 | 3022 | 542 | 534 | 14 | | |

- Molecule 86 is a protein called 39S ribosomal protein L12, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|----|---------|-------|
| 86 | t1 | 46 | Total | C | H | N | O | 2 | 0 |
| | | | 733 | 228 | 379 | 56 | 70 | | |
| 86 | t2 | 30 | Total | C | H | N | O | 0 | 0 |
| | | | 506 | 154 | 268 | 38 | 46 | | |
| 86 | t3 | 30 | Total | C | H | N | O | 0 | 0 |
| | | | 506 | 154 | 268 | 38 | 46 | | |
| 86 | t4 | 29 | Total | C | H | N | O | 0 | 0 |
| | | | 484 | 148 | 255 | 36 | 45 | | |
| 86 | t5 | 29 | Total | C | H | N | O | 0 | 0 |
| | | | 484 | 148 | 255 | 36 | 45 | | |
| 86 | t6 | 27 | Total | C | H | N | O | 0 | 0 |
| | | | 450 | 137 | 236 | 34 | 43 | | |

- Molecule 87 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|----|---------|
| 87 | 0 | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |
| 87 | 4 | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |
| 87 | AB | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |
| 87 | AO | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |

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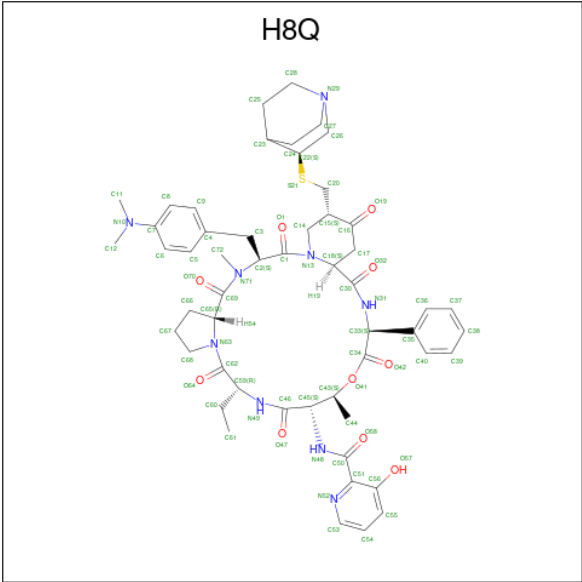
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| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|------------|---------|---------|
| 87 | AP | 1 | Total 1 | Zn 1 | 0 |
| 87 | AT | 1 | Total 1 | Zn 1 | 0 |
| 87 | r | 1 | Total 1 | Zn 1 | 0 |

- Molecule 88 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

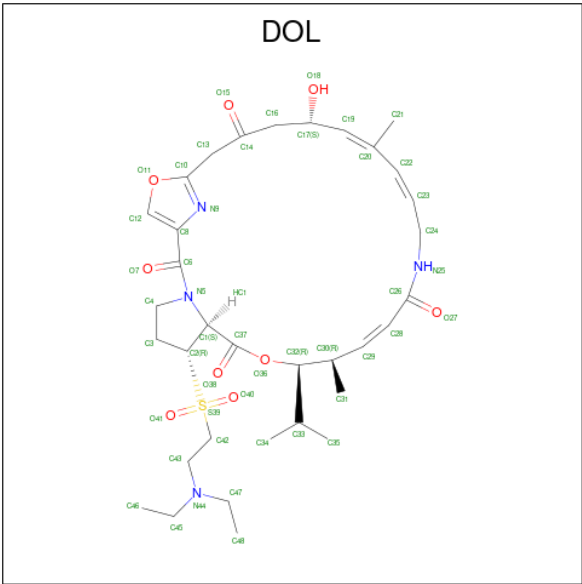
| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|--------------|-----------|---------|
| 88 | 9 | 1 | Total 1 | Mg 1 | 0 |
| 88 | XA | 142 | Total 142 | Mg 142 | 0 |
| 88 | A2 | 1 | Total 1 | Mg 1 | 0 |
| 88 | AA | 45 | Total 45 | Mg 45 | 0 |
| 88 | XD | 1 | Total 1 | Mg 1 | 0 |
| 88 | XE | 1 | Total 1 | Mg 1 | 0 |
| 88 | XM | 2 | Total 2 | Mg 2 | 0 |
| 88 | XW | 1 | Total 1 | Mg 1 | 0 |
| 88 | g | 1 | Total 1 | Mg 1 | 0 |

- Molecule 89 is {N}-[(3 {S},6 {R},12 {R},15 {S},16 {S},19 {S},22 {S},25 {S})-25-[(3 {S})-1-azabicyclo[2.2.2]octan-3-yl]sulfanylmethyl]-3-[[4-(dimethylamino)phenyl]methyl]-12-ethyl-4,16-dimethyl-2,5,11,14,18,21,24-heptakis(oxidanylidene)-19-phenyl-17-oxa-1,4,10,13,20-pentazatricyclo[20.4.0.0[^]{6,10}]hexacosan-15-yl]-3-oxidanyl-pyridine-2-carboxamide (three-letter code: H8Q) (formula: C₅₃H₆₇N₉O₁₀S).



| Mol | Chain | Residues | Atoms | | | | | | AltConf |
|-----|-------|----------|-------|----|----|---|----|---|---------|
| 89 | XA | 1 | Total | C | H | N | O | S | 0 |
| | | | 140 | 53 | 67 | 9 | 10 | 1 | |

- Molecule 90 is 5-(2-DIETHYLAMINO-ETHANESULFONYL)-21-HYDROXY-10-ISOPROPYL-11,19-DIMETHYL-9,26-DIOXA-3,15,28-TRIAZA-TRICYCLO[23.2.1.00,255]OCTACOSA-1(27),12,17,19,25(28)-PENTAENE-2,8,14,23-TETRAONE (three-letter code: DOL) (formula: C₃₄H₅₀N₄O₉S).



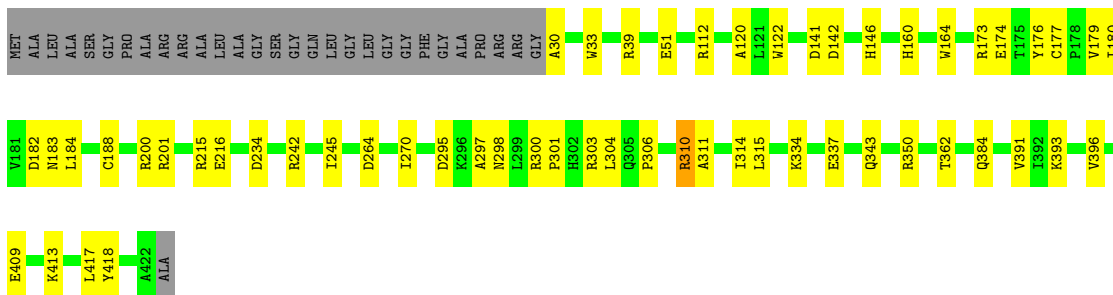
| Mol | Chain | Residues | Atoms | | | | | AltConf | |
|-----|-------|----------|-------|----|----|---|---|---------|---|
| 90 | XA | 1 | Total | C | H | N | O | S | 0 |
| | | | 98 | 34 | 50 | 4 | 9 | 1 | |


-
- The image displays the chemical structure of Guanosine Triphosphate (GTP). It consists of a guanine base (a purine ring system with an amino group at C2) linked to a ribose sugar via a glycosidic bond. The ribose sugar is further linked to a chain of three phosphate groups (gamma, beta, and alpha phosphates) via a triphosphate chain. The structure is color-coded: the guanine base is blue, the ribose sugar is green, and the phosphate groups are red. Stereochemistry is indicated with wedges and dashes. The label 'GTP' is centered above the structure.

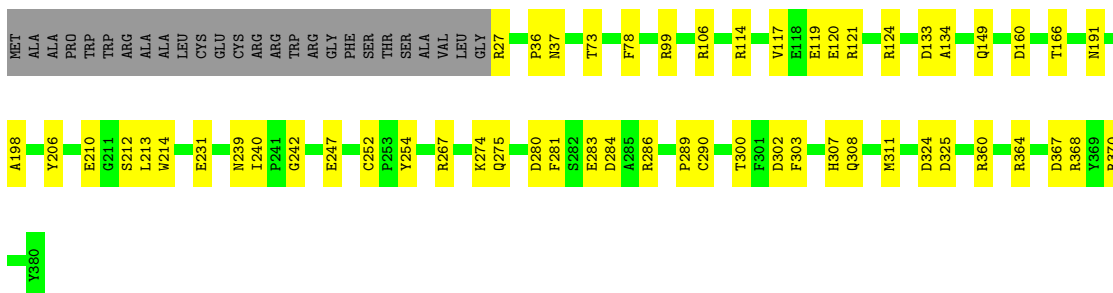




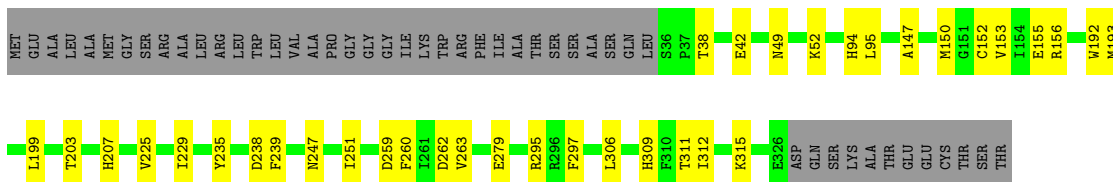
- Chain 5: 80% 13% 7%



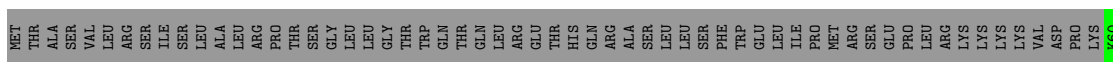
- Chain 6:  79% 14% 7%



- Chain 7:  75% 11% 14%



- Chain 8:  61% 6% 33%





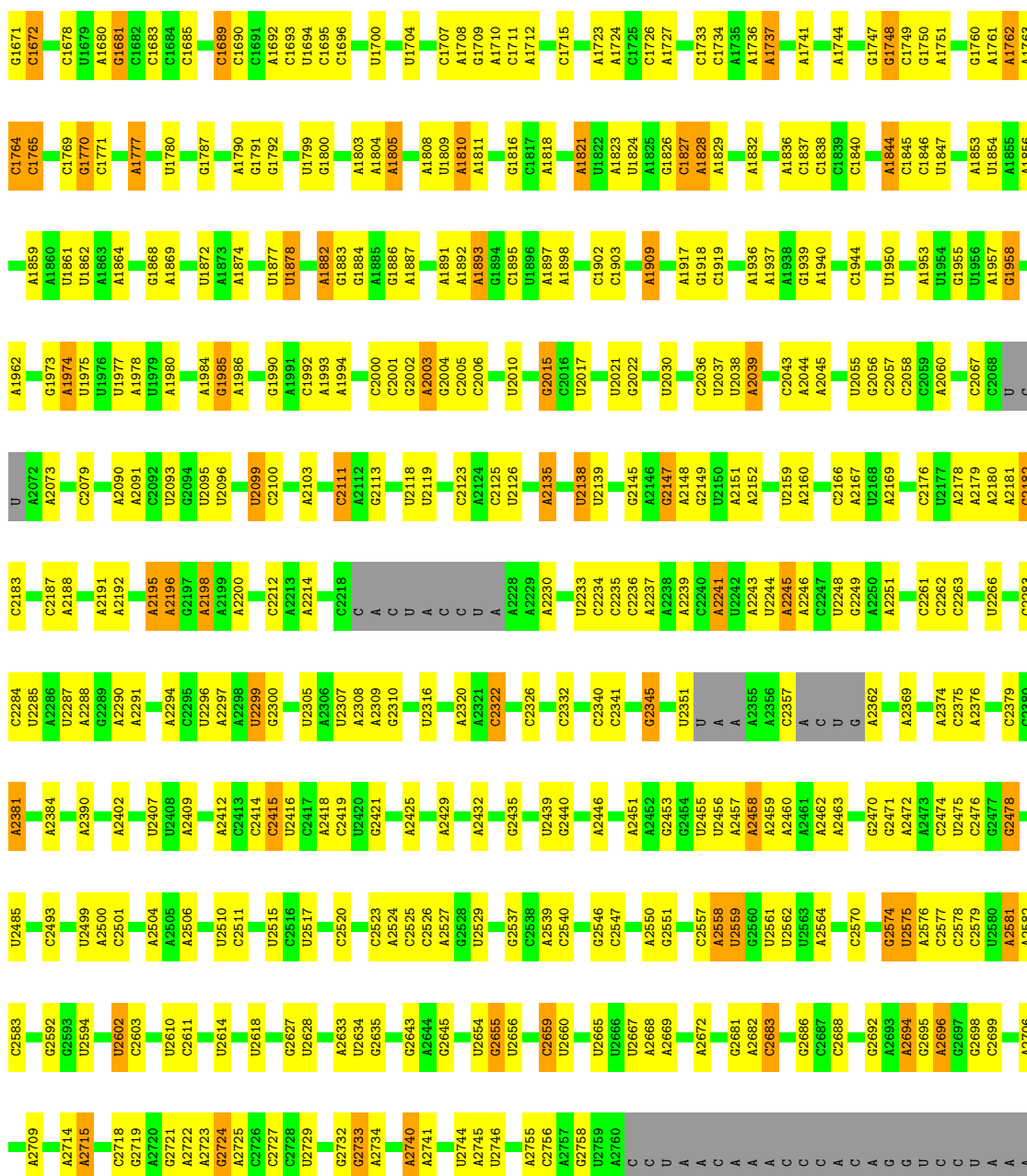
- Molecule 10: 39S ribosomal protein L41, mitochondrial

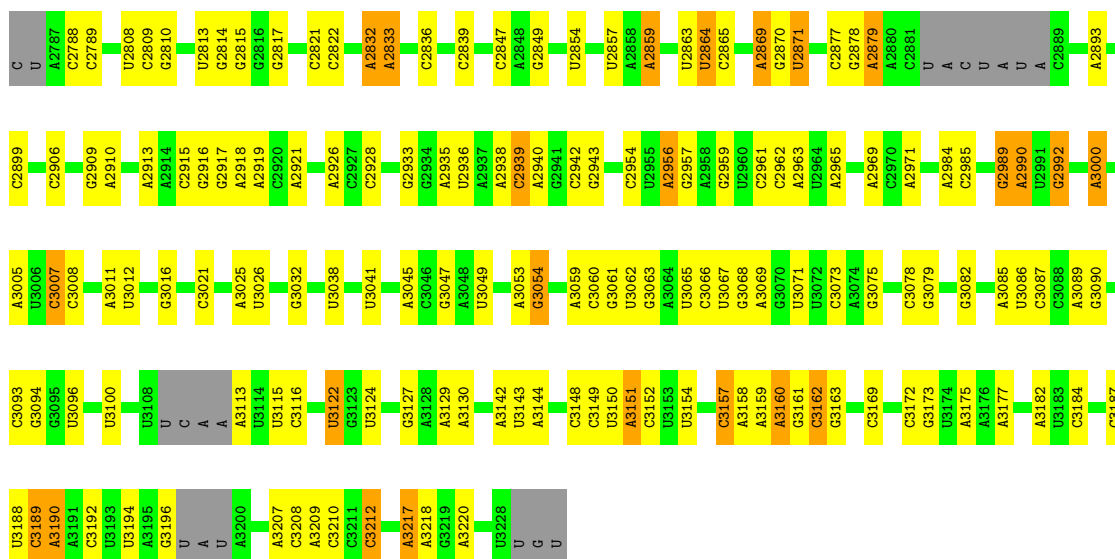
Chain 9: 81% 9% 9%



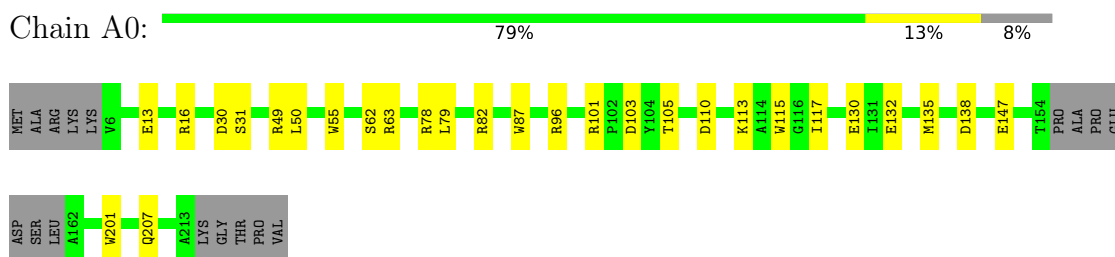
- Molecule 11: 16S mitochondrial rRNA

Chain XA: 61% 30% 5%

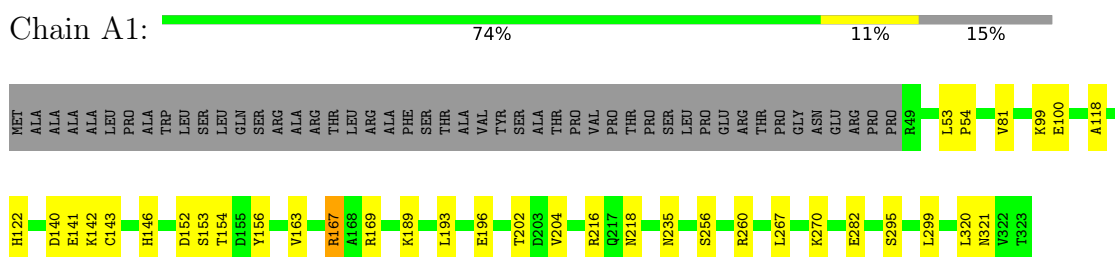




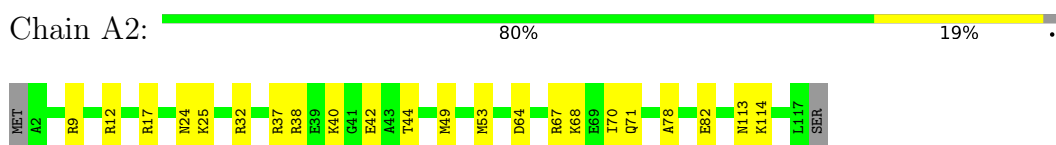
- Molecule 12: 28S ribosomal protein S34, mitochondrial



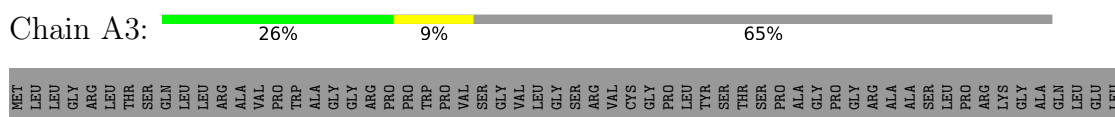
- Molecule 13: 28S ribosomal protein S35, mitochondrial



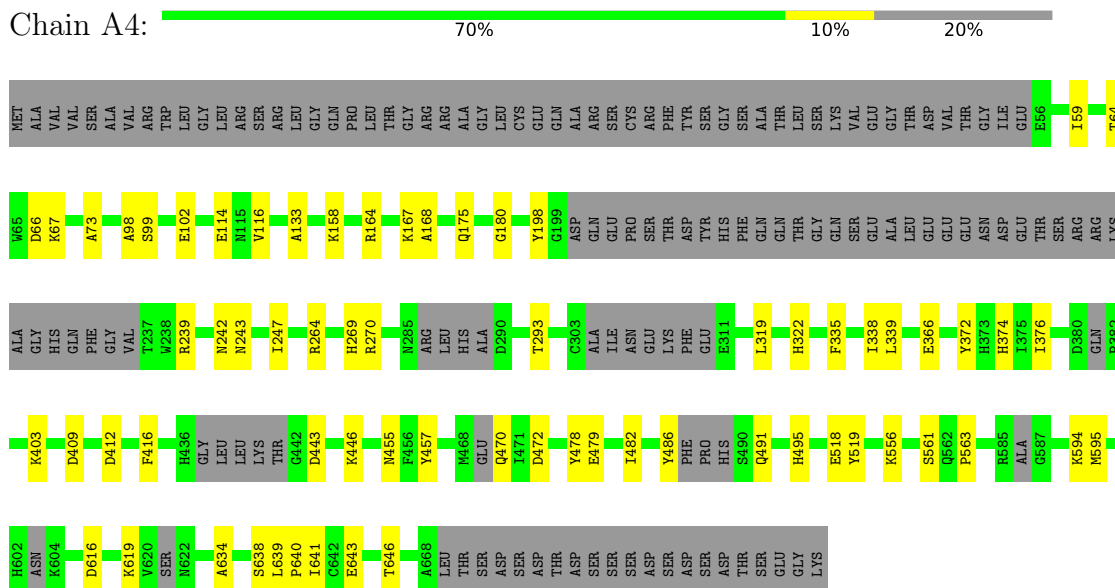
- Molecule 14: Coiled-coil-helix-coiled-coil-helix domain-containing protein 1



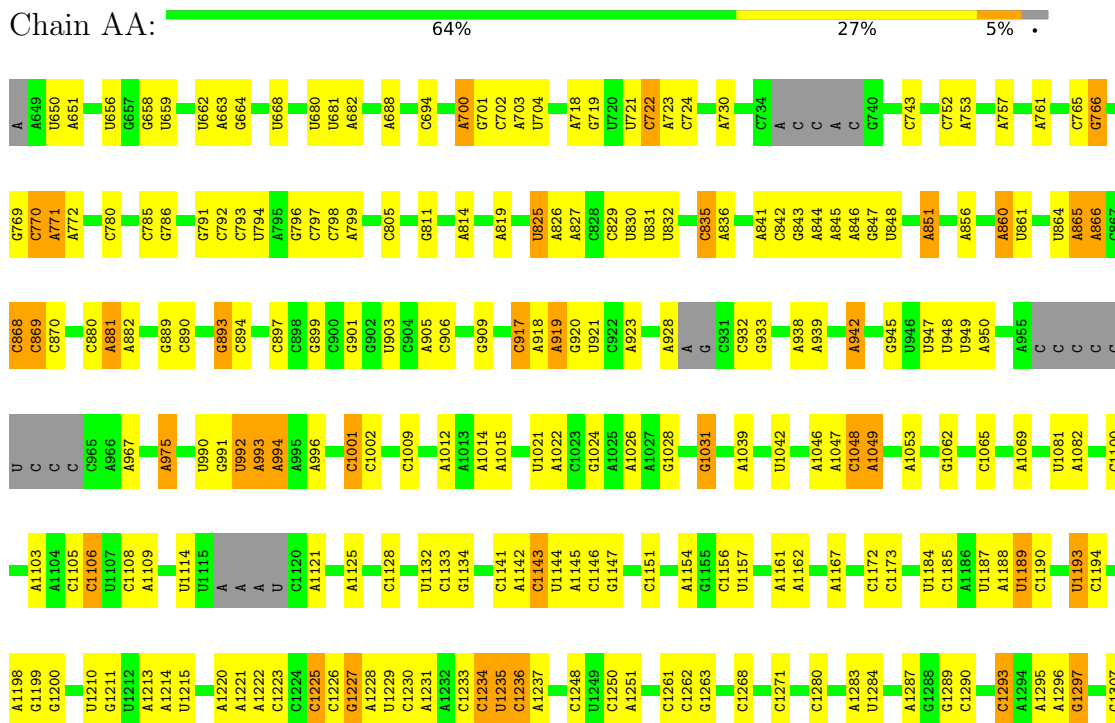
- Molecule 15: Aurora kinase A-interacting protein

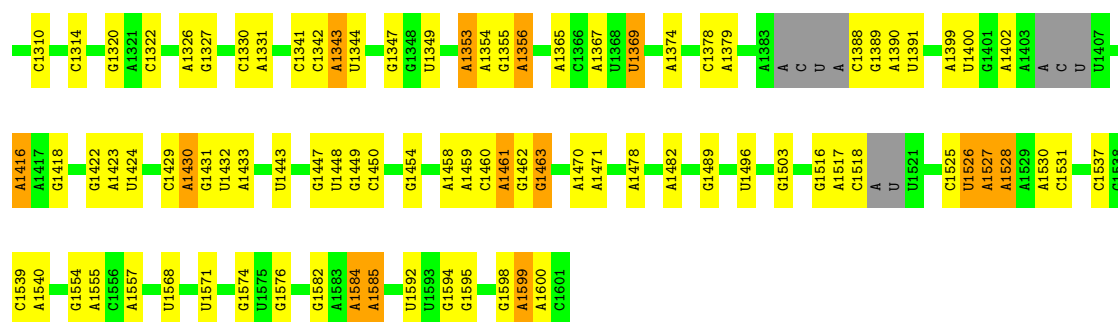


- Molecule 16: Pentatricopeptide repeat domain-containing protein 3, mitochondrial



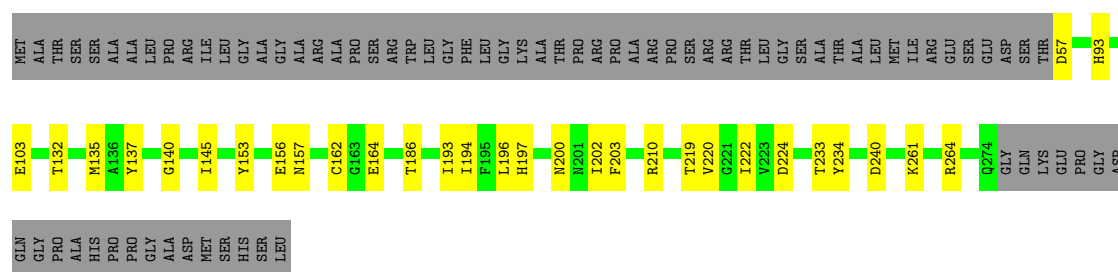
- Molecule 17: 12S mitochondrial rRNA





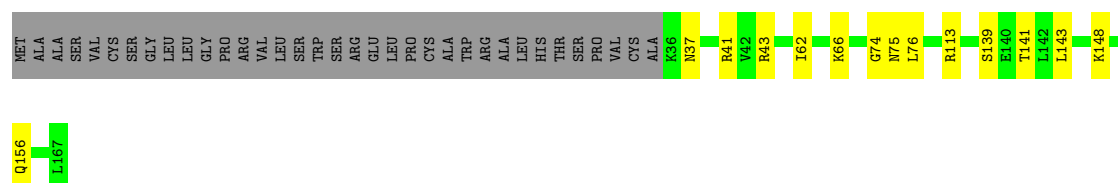
- Molecule 18: 28S ribosomal protein S2, mitochondrial

Chain AB: 63% 10% 26%



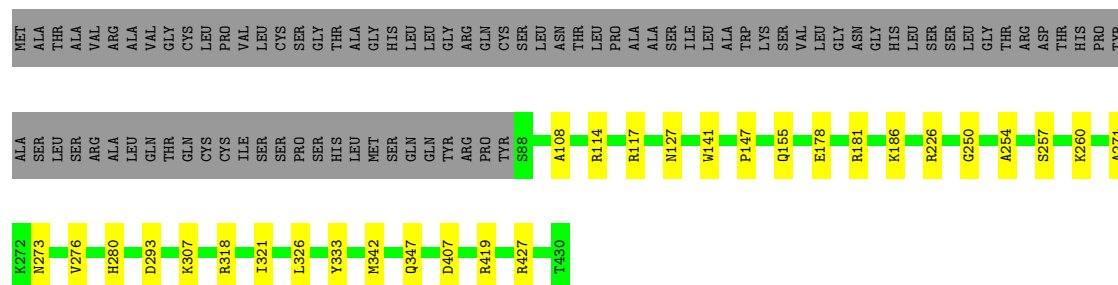
- Molecule 19: 28S ribosomal protein S24, mitochondrial

Chain AC: 71% 8% 21%



- Molecule 20: 28S ribosomal protein S5, mitochondrial

Chain AD: 73% 7% 20%



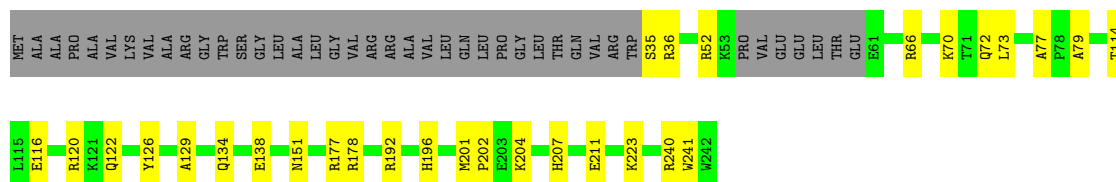
- Molecule 21: 28S ribosomal protein S6, mitochondrial

Chain AE: 81% 17% 2%



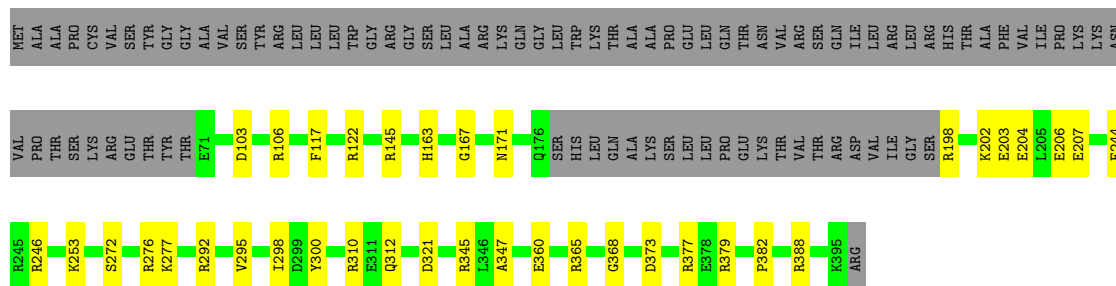
- Molecule 22: 28S ribosomal protein S7, mitochondrial

Chain AF: 71% 12% 17%



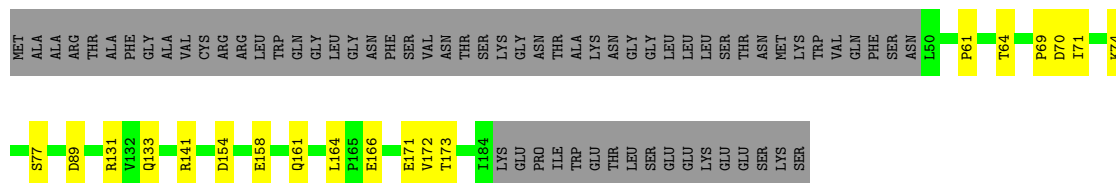
- Molecule 23: 28S ribosomal protein S9, mitochondrial

Chain AG: 67% 9% 23%



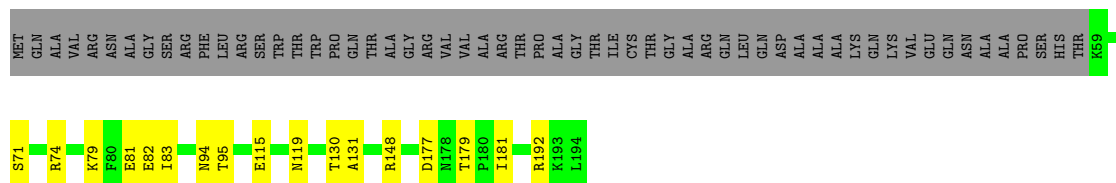
- Molecule 24: 28S ribosomal protein S10, mitochondrial

Chain AH: 58% 9% 33%



- Molecule 25: 28S ribosomal protein S11, mitochondrial

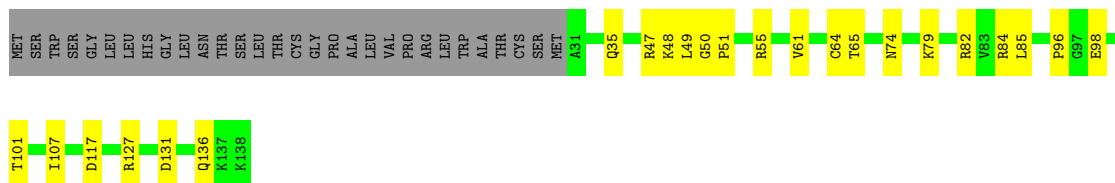
Chain AI: 61% 9% 30%



- Molecule 26: 28S ribosomal protein S12, mitochondrial

Chain AJ: 62% 17% 22%





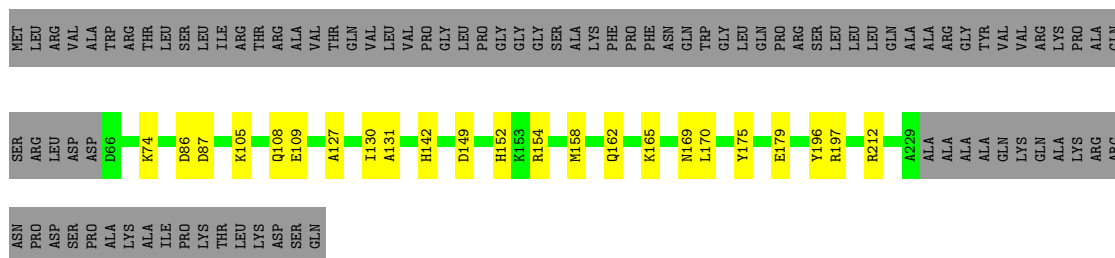
- Molecule 27: 28S ribosomal protein S14, mitochondrial

Chain AK: 62% 17% 21%



- Molecule 28: 28S ribosomal protein S15, mitochondrial

Chain AL: 55% 9% 36%



- Molecule 29: 28S ribosomal protein S16, mitochondrial

Chain AM: 74% 11% 15%



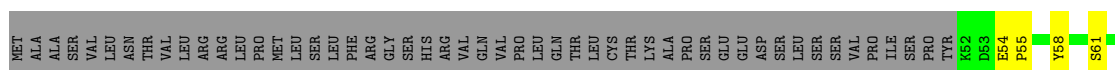
- Molecule 30: 28S ribosomal protein S17, mitochondrial

Chain AN: 72% 10% 18%



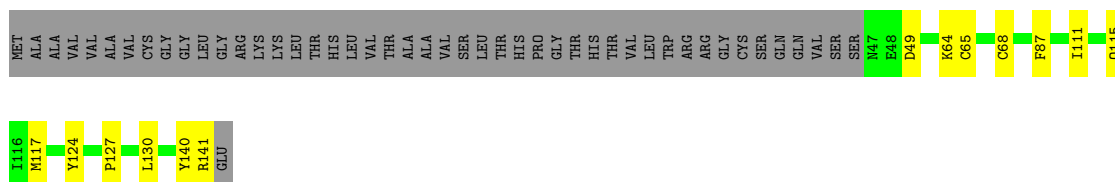
- Molecule 31: 28S ribosomal protein S18b, mitochondrial

Chain AO: 62% 9% 28%





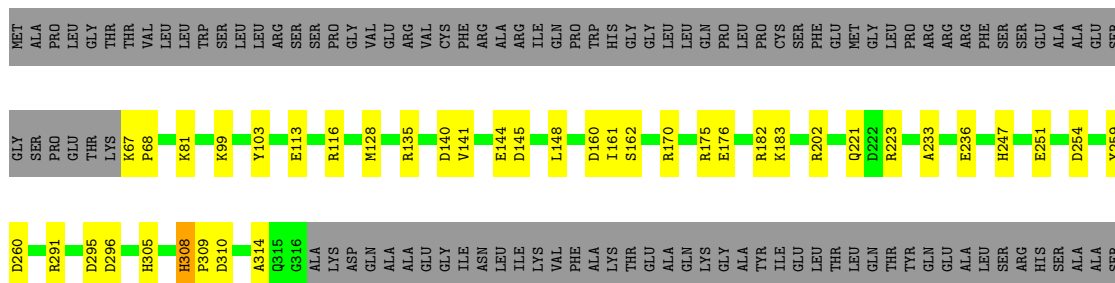
- Molecule 32: 28S ribosomal protein S18c, mitochondrial



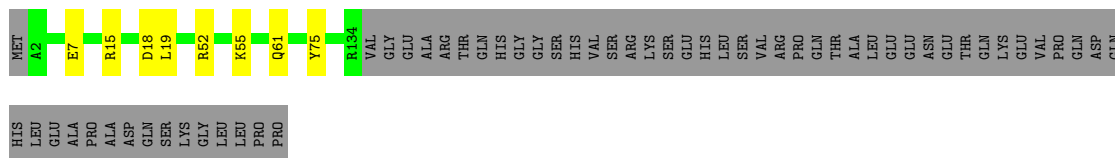
- Molecule 33: 28S ribosomal protein S21, mitochondrial



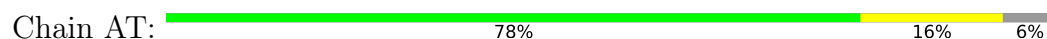
- Molecule 34: 28S ribosomal protein S22, mitochondrial



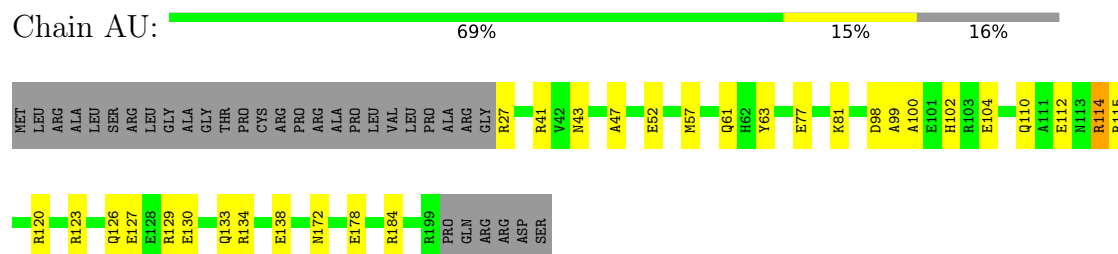
- Molecule 35: 28S ribosomal protein S23, mitochondrial



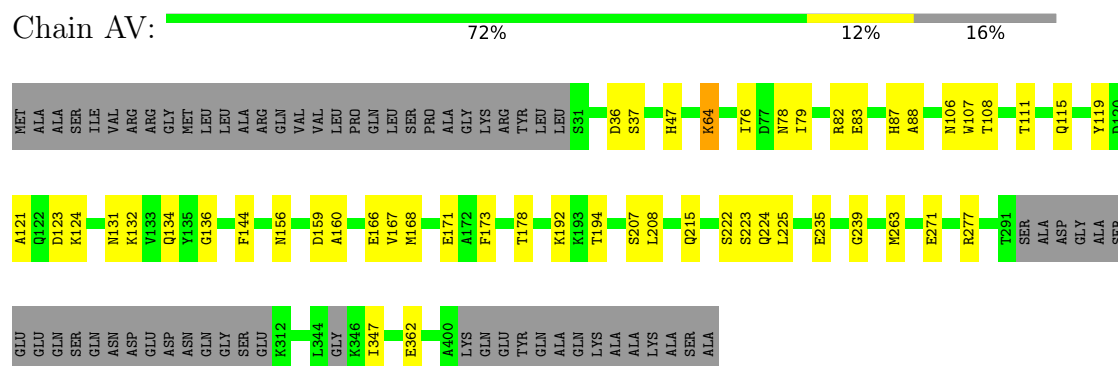
- Molecule 36: 28S ribosomal protein S25, mitochondrial



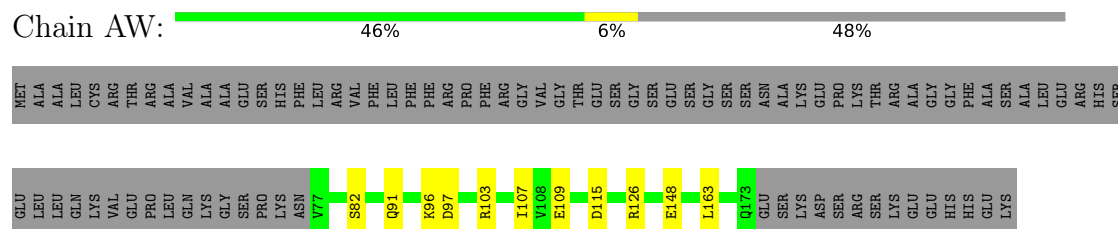
- Molecule 37: 28S ribosomal protein S26, mitochondrial



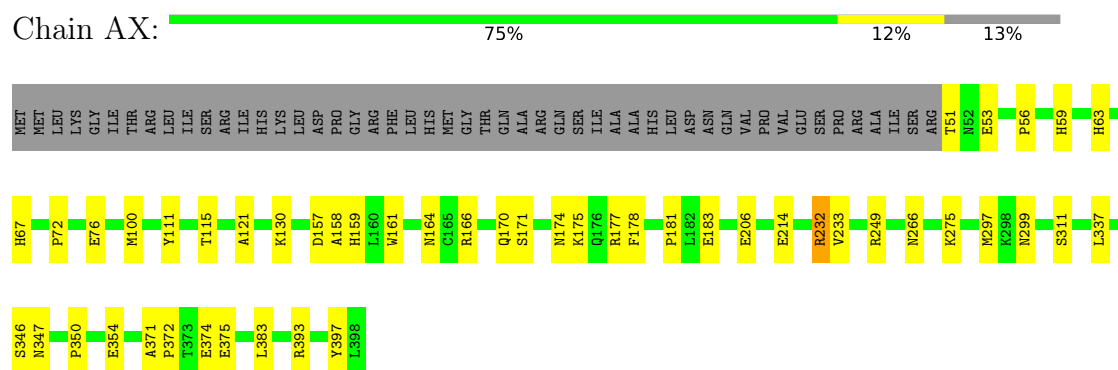
- Molecule 38: 28S ribosomal protein S27, mitochondrial



- Molecule 39: 28S ribosomal protein S28, mitochondrial

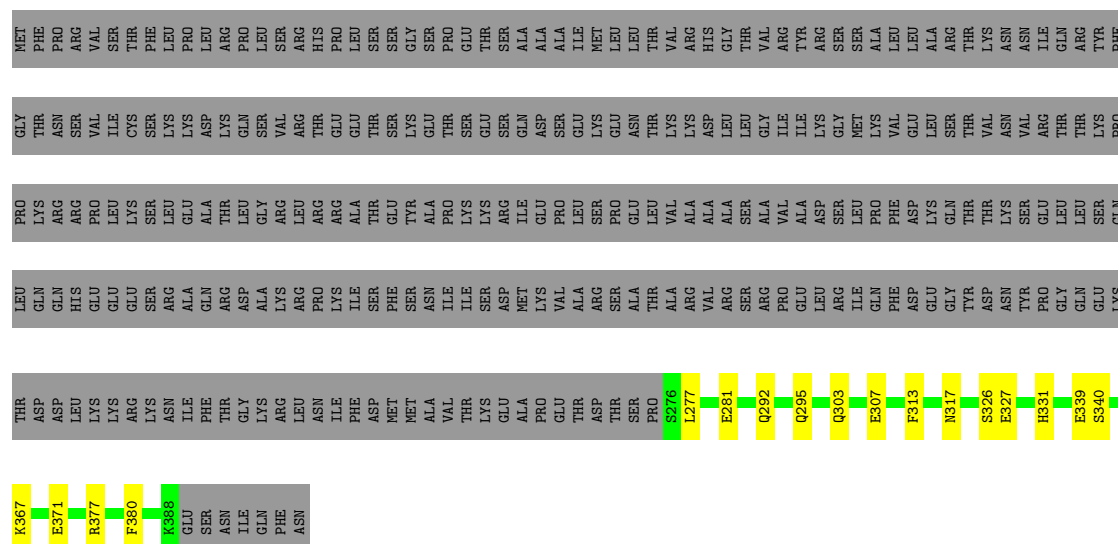


- Molecule 40: 28S ribosomal protein S29, mitochondrial



- Molecule 41: 28S ribosomal protein S31, mitochondrial





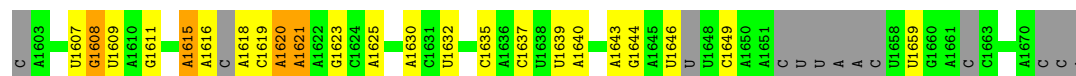
- Molecule 42: 28S ribosomal protein S33, mitochondrial

Chain AZ: 71% 10% 19%



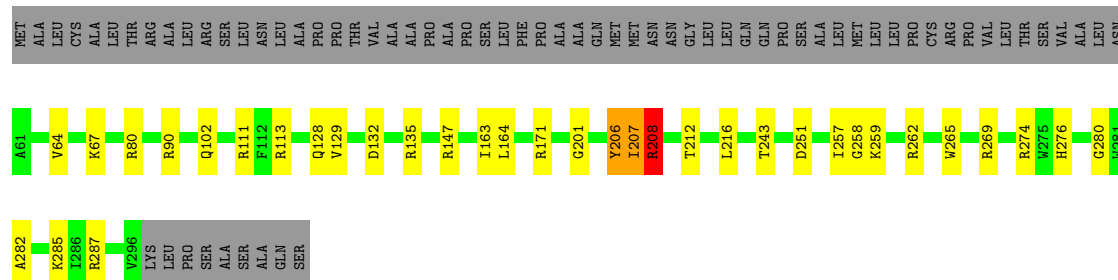
- Molecule 43: mitochondrial tRNA^{Val}

Chain XB: 50% 26% 6% 18%



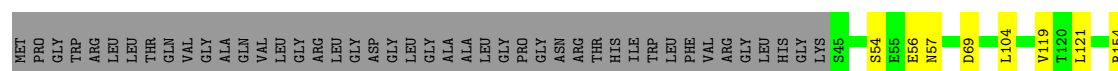
- Molecule 44: 39S ribosomal protein L2, mitochondrial

Chain XD: 66% 10% 23%



- Molecule 45: 39S ribosomal protein L3, mitochondrial

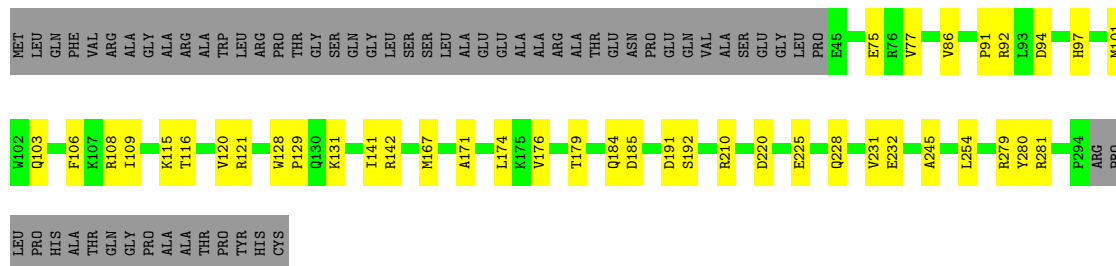
Chain XE: 79% 8% 13%





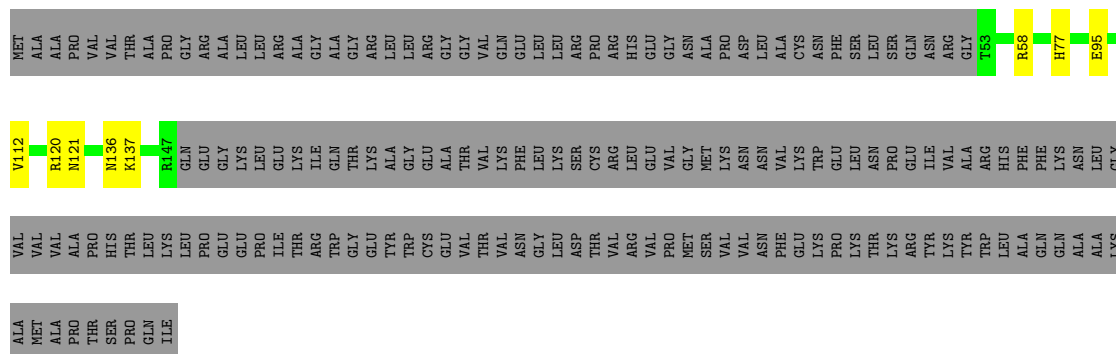
- Molecule 46: 39S ribosomal protein L4, mitochondrial

Chain XF: 67% 13% 20%



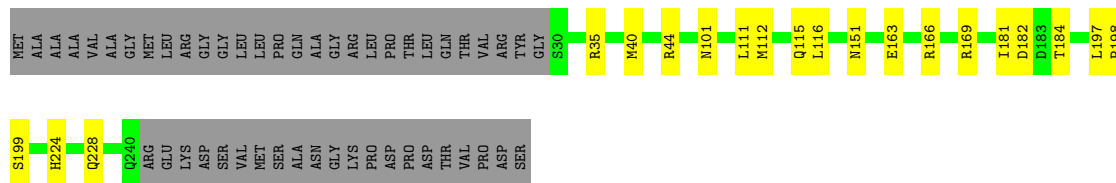
- Molecule 47: 39S ribosomal protein L9, mitochondrial

Chain XH: 33% 64%



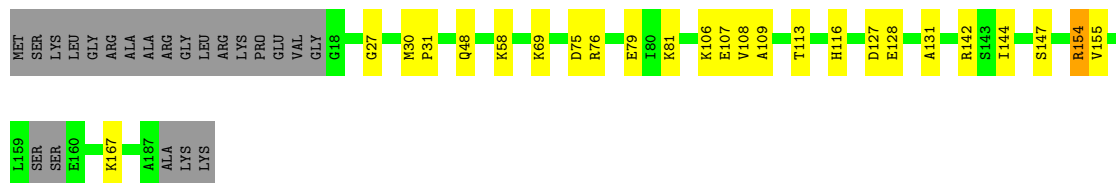
- Molecule 48: 39S ribosomal protein L10, mitochondrial

Chain XI: 73% 8% 19%



- Molecule 49: 39S ribosomal protein L11, mitochondrial

Chain XJ: 76% 12% 11%



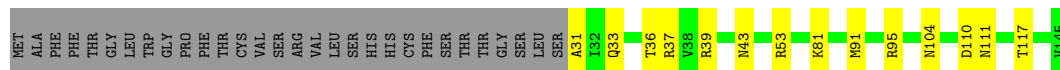
- Molecule 50: 39S ribosomal protein L13, mitochondrial

Chain XK:  87% 12% ..




- Molecule 51: 39S ribosomal protein L14, mitochondrial

Chain XL:  70% 10% 21%




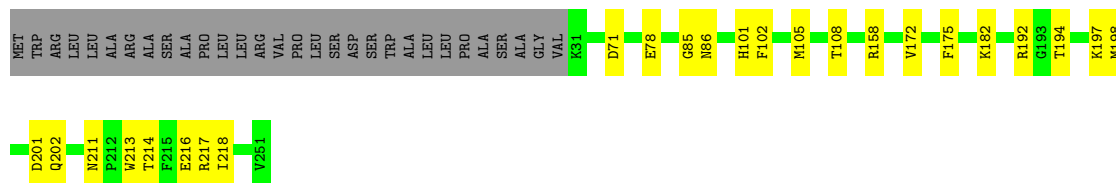
- Molecule 52: 39S ribosomal protein L15, mitochondrial

Chain XM:  81% 16% .



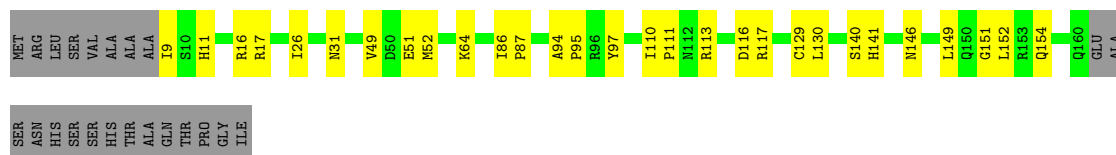
- Molecule 53: 39S ribosomal protein L16, mitochondrial

Chain XN:  78% 10% 12%



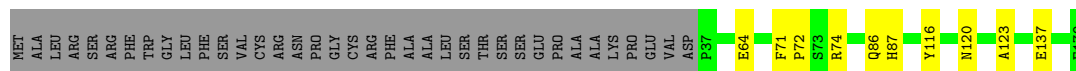
- Molecule 54: 39S ribosomal protein L17, mitochondrial

Chain XO:  70% 17% 13%



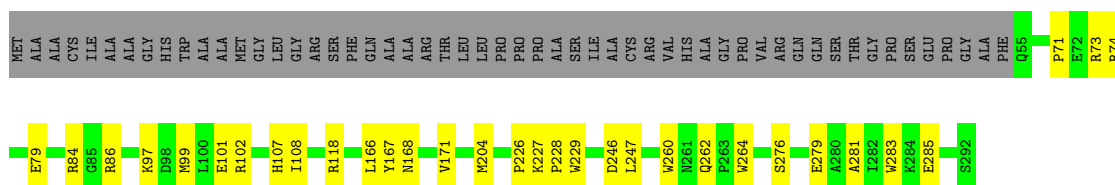
- Molecule 55: 39S ribosomal protein L18, mitochondrial

Chain XP:  74% 6% 21%




- Molecule 56: 39S ribosomal protein L19, mitochondrial

Chain XQ:  71% 11% 18%




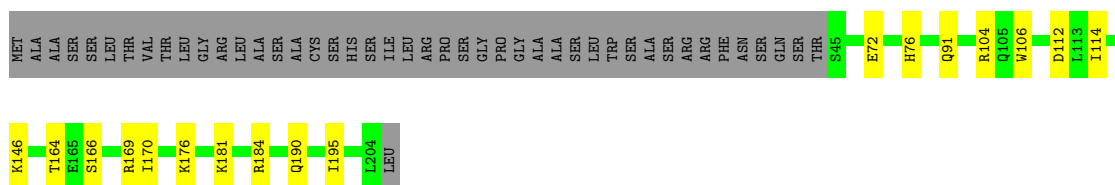
- Molecule 57: 39S ribosomal protein L20, mitochondrial

Chain XR:  76% 18% 6%



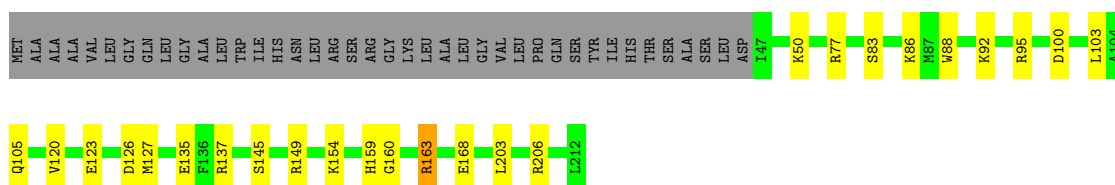
- Molecule 58: 39S ribosomal protein L21, mitochondrial

Chain XS:  70% 8% 22%




- Molecule 59: 39S ribosomal protein L22, mitochondrial

Chain XT:  68% 12% 19%




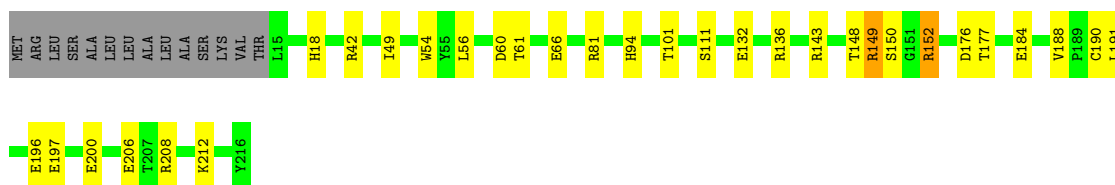
- Molecule 60: 39S ribosomal protein L23, mitochondrial

Chain XU:  78% 14% 8%



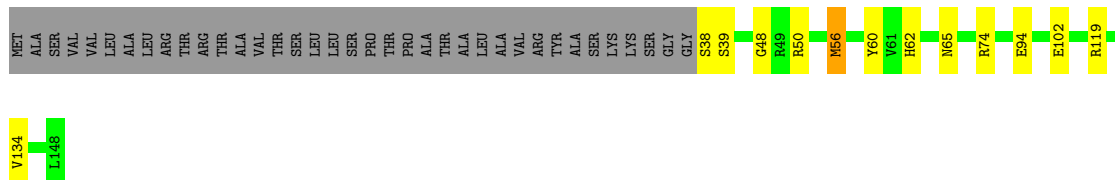
- Molecule 61: 39S ribosomal protein L24, mitochondrial

Chain XV:  79% 13% 6%



- Molecule 62: 39S ribosomal protein L27, mitochondrial

Chain XW: 66% 8% 25%



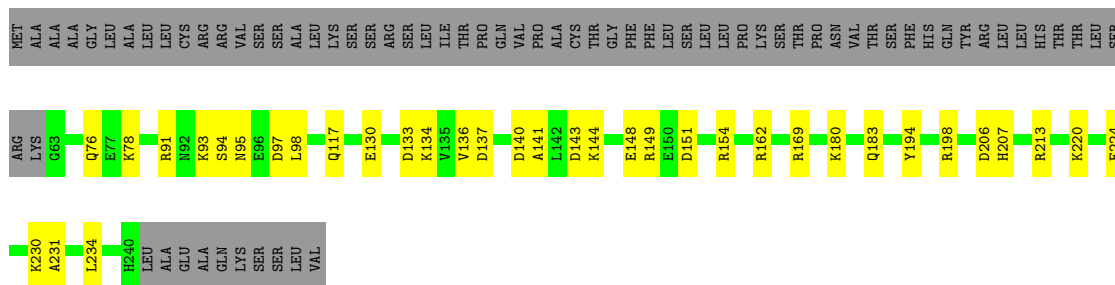
- Molecule 63: 39S ribosomal protein L28, mitochondrial

Chain XX: 84% 11% 5%



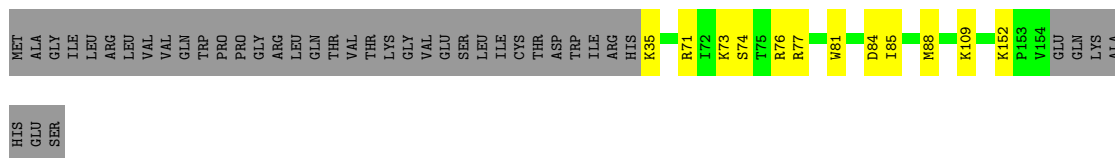
- Molecule 64: 39S ribosomal protein L47, mitochondrial

Chain XY: 57% 14% 29%




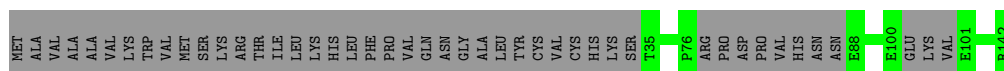
- Molecule 65: 39S ribosomal protein L30, mitochondrial

Chain XZ: 67% 7% 25%



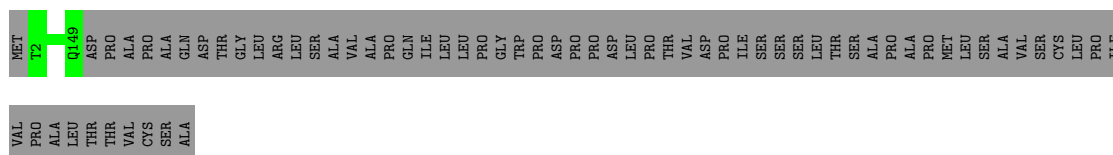
- Molecule 66: 39S ribosomal protein L42, mitochondrial

Chain a:  68% 32%




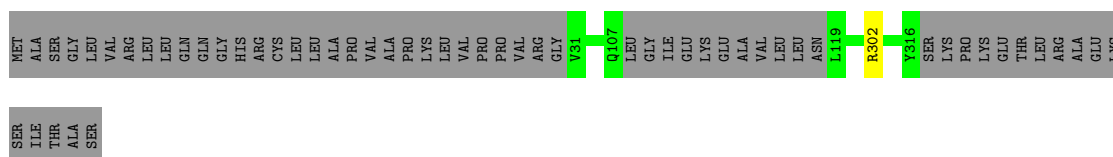
- Molecule 67: 39S ribosomal protein L43, mitochondrial

Chain b:  69% 31%



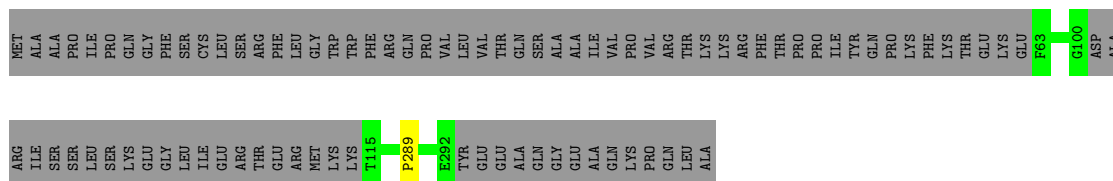
- Molecule 68: 39S ribosomal protein L44, mitochondrial

Chain c:  83% 17%




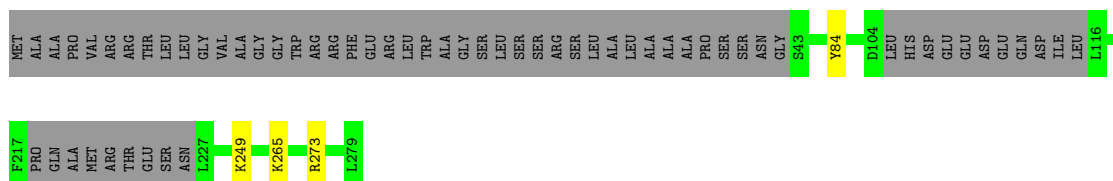
- Molecule 69: 39S ribosomal protein L45, mitochondrial

Chain d:  70% 29%



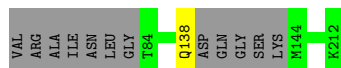
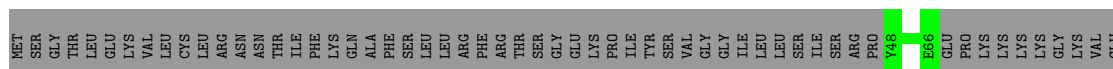
- Molecule 70: 39S ribosomal protein L46, mitochondrial

Chain e:  76% 22%




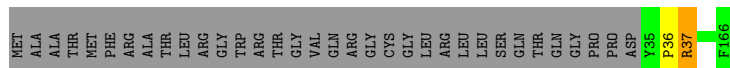
- Molecule 71: 39S ribosomal protein L48, mitochondrial

Chain f:  67% 33%



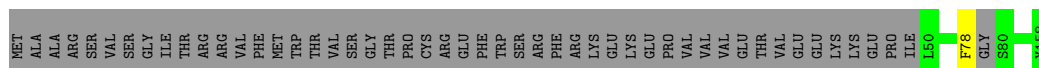
- Molecule 72: 39S ribosomal protein L49, mitochondrial

Chain g:  78% 20%




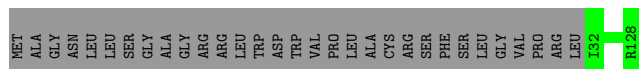
- Molecule 73: 39S ribosomal protein L50, mitochondrial

Chain h:  68% 32%



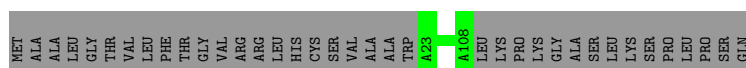
- Molecule 74: 39S ribosomal protein L51, mitochondrial

Chain i:  76% 24%




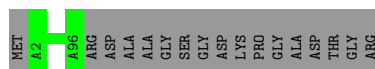
- Molecule 75: 39S ribosomal protein L52, mitochondrial

Chain j:  70% 30%



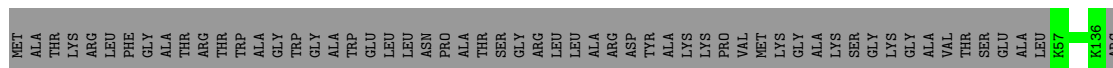
- Molecule 76: 39S ribosomal protein L53, mitochondrial

Chain k:  85% 15%



- Molecule 77: 39S ribosomal protein L54, mitochondrial

Chain l:  58% 42%



LEU

- Molecule 78: 39S ribosomal protein L55, mitochondrial

Chain m:  47% 53%

MET ALA ALA VAL GLY SER LEU LEU GLY ARG LEU ARG GLN SER THR VAL VAL LYS ALA THR GLY PRO ALA LEU ARG ARG LEU HIS THR SER SER TRP ARG ALA ASP S35 T83 LEU S84 K94 ARG GLU ALA GLN LEU GLN SER ARG LYS GLU TYR GLU GLN SER ASP LEU

HIS VAL GLU ARG TYR ARG GLN PHE TRP THR ARG THR LYS

- Molecule 79: Ribosomal protein 63, mitochondrial

Chain o:  92% 8%

MET PHE LEU THR ALA LEU LEU TRP R9 S102

- Molecule 80: Peptidyl-tRNA hydrolase ICT1, mitochondrial

Chain p:  62% 38%

MET ALA ALA THR ARG CYS LEU ARG TRP GLY LEU SER ARG ALA GLY VAL TRP LEU LEU PRO PRO PRO ALA ARG CYS PRO ARG ALA LEU HIS GLN LYS ASP GLY THR E38 V61 PRO ASN GLY ALA LYS GLN ALA ASP SER D70 S83 SER GLY PRO GLY GLN ASN VAL

ASN LYS Y95 Q163 THR PRO LYS GLU PRO THR LYS GLU ASP VAL K174 T193 HIS SER ALA VAL LYS THR ARG ARG VAL ASP MET ASP


- Molecule 81: Growth arrest and DNA damage-inducible proteins-interacting protein 1

Chain q:  73% 26%

MET ALA ALA SER VAL ARG GLN ALA ARG SER SER LEU GLY VAL ALA ALA THR LEU LEU ALA PRO GLY SER ARG Y25 R155 K188 ARG LEU LYS GLU LYS GLN LYS ARG LYS LYS GLU ALA ARG ALA ALA LEU ALA ALA VAL VAL ASP GLN PRO PRO ALA

PRO SER SER

- Molecule 82: 39S ribosomal protein S18a, mitochondrial

Chain r:  78% 22%

MET ALA ALA LEU LYS VAL LEU VAL SER GLY CYS GLY ARG LEU LEU GLY THR LEU LEU ALA GLY PRO PRO ALA ARG ARG THR SER TRP ARG LEU ALA GLY F35 T41 GLN E83 P136 GLY VAL VAL PRO LYS SER LYS PRO Q146 H196

- Molecule 83: mRNA

Chain r1:  100%

YSP46
YSP47
YSP48
YSP49

- Molecule 84: P-site tRNA

Chain r3:

100%

YSP1 YSP2 A3 A4 A5 A6 YSP7 A8 A9 A10 A11 YSP12 YSP13 A14 A15 YSP16 YSP17 A17A A18 A19 YSP20 A21 A22 A23 YSP24 YSP25 A26 YSP27 YSP28 A29 A30 A31 YSP32 YSP33 YSP34 A35 YSP36 A37 YSP38 YSP39 YSP40 YSP41 A42 A43 A44 A45 A46 YSP47 A48 YSP49 YSP50 A51 A52 YSP53 YSP54 A55 YSP56 A57 YSP59

YSP60 YSP61 YSP62 YSP63 YSP64 YSP65 A66 YSP67 A68 YSP69 YSP70 A71 YSP72 YSP73 A74

- Molecule 85: 39S ribosomal protein S30, mitochondrial

Chain s:

84%

16%

MET ALA ALA ALA ARG CYS TRP ARG ARG PRO LEU LEU GLY ARG CYS PRO ARG A15 YSP16 YSP17 A17A A18 A19 YSP20 A21 A22 A23 YSP24 YSP25 A26 YSP27 YSP28 A29 A30 A31 YSP32 YSP33 YSP34 A35 YSP36 A37 YSP38 YSP39 YSP40 YSP41 A42 A43 A44 A45 A46 YSP47 A48 YSP49 YSP50 A51 A52 YSP53 YSP54 A55 YSP56 A57 YSP59

LEU ASP LEU A140 K430 GLU GLU LYS SER LEU LEU GLU ASN

- Molecule 86: 39S ribosomal protein L12, mitochondrial

Chain t1:

23%

77%

MET LEU PRO ALA ALA ARG PRO PRO LEU LEU GLY ARG CYS PRO ARG A15 YSP16 YSP17 A17A A18 A19 YSP20 A21 A22 A23 YSP24 YSP25 A26 YSP27 YSP28 A29 A30 A31 YSP32 YSP33 YSP34 A35 YSP36 A37 YSP38 YSP39 YSP40 YSP41 A42 A43 A44 A45 A46 YSP47 A48 YSP49 YSP50 A51 A52 YSP53 YSP54 A55 YSP56 A57 YSP59

GLY VAL MET SER GLY VAL PRO PRO LEU LEU GLY ARG CYS PRO ARG A15 YSP16 YSP17 A17A A18 A19 YSP20 A21 A22 A23 YSP24 YSP25 A26 YSP27 YSP28 A29 A30 A31 YSP32 YSP33 YSP34 A35 YSP36 A37 YSP38 YSP39 YSP40 YSP41 A42 A43 A44 A45 A46 YSP47 A48 YSP49 YSP50 A51 A52 YSP53 YSP54 A55 YSP56 A57 YSP59

LYS LYS LEU VAL SER LEU PRO PRO LEU LEU GLY ARG CYS PRO ARG A15 YSP16 YSP17 A17A A18 A19 YSP20 A21 A22 A23 YSP24 YSP25 A26 YSP27 YSP28 A29 A30 A31 YSP32 YSP33 YSP34 A35 YSP36 A37 YSP38 YSP39 YSP40 YSP41 A42 A43 A44 A45 A46 YSP47 A48 YSP49 YSP50 A51 A52 YSP53 YSP54 A55 YSP56 A57 YSP59

- Molecule 86: 39S ribosomal protein L12, mitochondrial

Chain t2:

15%

85%

MET LEU PRO ALA ALA ARG PRO PRO LEU LEU GLY ARG CYS PRO ARG A15 YSP16 YSP17 A17A A18 A19 YSP20 A21 A22 A23 YSP24 YSP25 A26 YSP27 YSP28 A29 A30 A31 YSP32 YSP33 YSP34 A35 YSP36 A37 YSP38 YSP39 YSP40 YSP41 A42 A43 A44 A45 A46 YSP47 A48 YSP49 YSP50 A51 A52 YSP53 YSP54 A55 YSP56 A57 YSP59

PRO P1 K30 GLN ASP VAL VAL LEU LEU VAL PRO PRO LEU LEU GLY ARG CYS PRO ARG A15 YSP16 YSP17 A17A A18 A19 YSP20 A21 A22 A23 YSP24 YSP25 A26 YSP27 YSP28 A29 A30 A31 YSP32 YSP33 YSP34 A35 YSP36 A37 YSP38 YSP39 YSP40 YSP41 A42 A43 A44 A45 A46 YSP47 A48 YSP49 YSP50 A51 A52 YSP53 YSP54 A55 YSP56 A57 YSP59

GLU ILE LYS ASN TYR THR GLN GLY VAL VAL LEU LEU VAL PRO PRO LEU LEU GLY ARG CYS PRO ARG A15 YSP16 YSP17 A17A A18 A19 YSP20 A21 A22 A23 YSP24 YSP25 A26 YSP27 YSP28 A29 A30 A31 YSP32 YSP33 YSP34 A35 YSP36 A37 YSP38 YSP39 YSP40 YSP41 A42 A43 A44 A45 A46 YSP47 A48 YSP49 YSP50 A51 A52 YSP53 YSP54 A55 YSP56 A57 YSP59

- Molecule 86: 39S ribosomal protein L12, mitochondrial

Chain t3:

15%

85%

4 Experimental information

| Property | Value | Source |
|--------------------------------------|---|-----------|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 6692 | 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) | Not provided | |
| Maximum defocus (nm) | Not provided | |
| Magnification | Not provided | |
| Image detector | GATAN K2 SUMMIT (4k x 4k) | Depositor |

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: P5P, Y5P, GTP, H8Q, MG, ZN, DOL

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

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|---------------|-------------|----------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 1 | 0 | 0.27 | 0/895 | 0.44 | 0/1201 |
| 2 | 1 | 0.26 | 0/444 | 0.45 | 0/591 |
| 3 | 2 | 0.32 | 0/382 | 0.42 | 0/507 |
| 4 | 3 | 0.32 | 0/852 | 0.46 | 0/1136 |
| 5 | 4 | 0.27 | 0/349 | 0.44 | 0/461 |
| 6 | 5 | 0.26 | 0/3298 | 0.43 | 0/4492 |
| 7 | 6 | 0.27 | 0/3042 | 0.42 | 0/4140 |
| 8 | 7 | 0.25 | 0/2420 | 0.41 | 0/3270 |
| 9 | 8 | 1.81 | 1/1199 (0.1%) | 0.46 | 2/1612 (0.1%) |
| 10 | 9 | 0.28 | 0/1024 | 0.43 | 0/1379 |
| 11 | XA | 0.35 | 0/35615 | 0.79 | 0/55429 |
| 12 | A0 | 0.23 | 0/1727 | 0.42 | 0/2338 |
| 13 | A1 | 0.24 | 0/2276 | 0.40 | 0/3079 |
| 14 | A2 | 0.25 | 0/939 | 0.43 | 0/1256 |
| 15 | A3 | 0.28 | 0/621 | 0.44 | 0/820 |
| 16 | A4 | 0.25 | 0/4559 | 0.41 | 0/6149 |
| 17 | AA | 0.23 | 0/21952 | 0.76 | 1/34164 (0.0%) |
| 18 | AB | 0.25 | 0/1819 | 0.41 | 0/2462 |
| 19 | AC | 0.25 | 0/1112 | 0.41 | 0/1505 |
| 20 | AD | 0.25 | 0/2768 | 0.43 | 0/3707 |
| 21 | AE | 0.25 | 0/989 | 0.44 | 0/1335 |
| 22 | AF | 0.24 | 0/1708 | 0.39 | 0/2291 |
| 23 | AG | 0.25 | 0/2559 | 0.41 | 0/3429 |
| 24 | AH | 0.25 | 0/1128 | 0.43 | 0/1529 |
| 25 | AI | 0.25 | 0/1031 | 0.42 | 0/1390 |
| 26 | AJ | 0.25 | 0/854 | 0.46 | 0/1148 |
| 27 | AK | 0.23 | 0/879 | 0.41 | 0/1182 |
| 28 | AL | 0.25 | 0/1406 | 0.40 | 0/1878 |
| 29 | AM | 0.25 | 0/941 | 0.41 | 0/1265 |
| 30 | AN | 0.25 | 0/864 | 0.44 | 0/1169 |
| 31 | AO | 0.24 | 0/1580 | 0.40 | 0/2150 |
| 32 | AP | 0.25 | 0/782 | 0.38 | 0/1050 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|---------------|-------------|---------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 33 | AQ | 0.24 | 0/746 | 0.43 | 0/993 |
| 34 | AR | 0.30 | 1/2103 (0.0%) | 0.52 | 3/2842 (0.1%) |
| 35 | AS | 0.25 | 0/1127 | 0.39 | 0/1518 |
| 36 | AT | 0.25 | 0/1361 | 0.42 | 0/1829 |
| 37 | AU | 0.24 | 0/1482 | 0.41 | 0/1987 |
| 38 | AV | 0.24 | 0/2925 | 0.40 | 0/3948 |
| 39 | AW | 0.25 | 0/778 | 0.45 | 0/1048 |
| 40 | AX | 0.25 | 0/2886 | 0.43 | 0/3909 |
| 41 | AY | 0.25 | 0/985 | 0.37 | 0/1329 |
| 42 | AZ | 0.25 | 0/748 | 0.39 | 0/1000 |
| 43 | XB | 0.20 | 0/1400 | 0.73 | 0/2168 |
| 44 | XD | 0.28 | 0/1879 | 0.46 | 0/2527 |
| 45 | XE | 0.29 | 0/2465 | 0.44 | 0/3344 |
| 46 | XF | 0.32 | 0/2071 | 0.49 | 0/2817 |
| 47 | XH | 0.26 | 0/798 | 0.44 | 0/1073 |
| 48 | XI | 0.26 | 0/1727 | 0.44 | 0/2340 |
| 49 | XJ | 0.24 | 0/1309 | 0.40 | 0/1764 |
| 50 | XK | 0.29 | 0/1495 | 0.42 | 0/2029 |
| 51 | XL | 0.27 | 0/904 | 0.44 | 0/1218 |
| 52 | XM | 0.31 | 0/2359 | 0.45 | 0/3185 |
| 53 | XN | 0.28 | 0/1825 | 0.45 | 0/2458 |
| 54 | XO | 0.26 | 0/1269 | 0.44 | 0/1708 |
| 55 | XP | 0.26 | 0/1190 | 0.42 | 0/1611 |
| 56 | XQ | 0.26 | 0/2026 | 0.44 | 0/2734 |
| 57 | XR | 0.33 | 0/1174 | 0.45 | 0/1572 |
| 58 | XS | 0.29 | 0/1311 | 0.47 | 0/1778 |
| 59 | XT | 0.31 | 0/1402 | 0.44 | 0/1886 |
| 60 | XU | 0.28 | 0/1200 | 0.43 | 0/1623 |
| 61 | XV | 0.26 | 0/1693 | 0.45 | 0/2297 |
| 62 | XW | 0.29 | 0/893 | 0.45 | 0/1204 |
| 63 | XX | 0.29 | 1/2090 (0.0%) | 0.43 | 0/2825 |
| 64 | XY | 0.27 | 0/1571 | 0.43 | 0/2106 |
| 65 | XZ | 0.29 | 0/1003 | 0.44 | 0/1354 |
| 66 | a | 0.27 | 0/838 | 0.45 | 0/1138 |
| 67 | b | 0.29 | 0/1202 | 0.47 | 0/1626 |
| 68 | c | 0.26 | 0/2264 | 0.41 | 0/3059 |
| 69 | d | 0.25 | 0/1807 | 0.42 | 0/2450 |
| 70 | e | 1.42 | 6/1797 (0.3%) | 0.43 | 0/2422 |
| 71 | f | 0.26 | 0/1169 | 0.42 | 0/1576 |
| 72 | g | 0.44 | 2/1134 (0.2%) | 0.45 | 0/1547 |
| 73 | h | 0.25 | 0/905 | 0.43 | 0/1233 |
| 74 | i | 0.32 | 0/849 | 0.48 | 0/1135 |
| 75 | j | 0.27 | 0/703 | 0.41 | 0/947 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|------------------|-------------|-----------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 76 | k | 0.24 | 0/743 | 0.45 | 0/1003 |
| 77 | l | 0.24 | 0/692 | 0.38 | 0/939 |
| 78 | m | 0.23 | 0/508 | 0.44 | 0/682 |
| 79 | o | 0.28 | 0/818 | 0.46 | 0/1097 |
| 80 | p | 0.23 | 0/1071 | 0.42 | 0/1433 |
| 81 | q | 0.26 | 0/1413 | 0.42 | 0/1906 |
| 82 | r | 0.26 | 0/1282 | 0.41 | 0/1734 |
| 85 | s | 0.26 | 0/3114 | 0.44 | 0/4225 |
| 86 | t1 | 0.26 | 0/366 | 0.39 | 0/497 |
| 86 | t2 | 0.22 | 0/238 | 0.38 | 0/319 |
| 86 | t3 | 0.22 | 0/238 | 0.37 | 0/319 |
| 86 | t4 | 0.22 | 0/229 | 0.37 | 0/308 |
| 86 | t5 | 0.23 | 0/229 | 0.37 | 0/308 |
| 86 | t6 | 0.24 | 0/213 | 0.40 | 0/286 |
| All | All | 0.35 | 11/176031 (0.0%) | 0.58 | 6/249727 (0.0%) |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 44 | XD | 0 | 1 |
| 48 | XI | 0 | 1 |
| 50 | XK | 0 | 1 |
| 70 | e | 0 | 1 |
| 71 | f | 0 | 1 |
| 72 | g | 0 | 1 |
| 73 | h | 0 | 1 |
| All | All | 0 | 7 |

The worst 5 of 11 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 9 | 8 | 99 | ARG | CG-CD | 61.84 | 3.06 | 1.51 |
| 70 | e | 84 | TYR | CD2-CE2 | 31.66 | 1.86 | 1.39 |
| 70 | e | 84 | TYR | CD1-CE1 | 31.19 | 1.86 | 1.39 |
| 70 | e | 84 | TYR | CE2-CZ | 21.63 | 1.66 | 1.38 |
| 70 | e | 84 | TYR | CE1-CZ | 21.08 | 1.66 | 1.38 |

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

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 34 | AR | 309 | PRO | O-C-N | 11.63 | 141.32 | 122.70 |
| 34 | AR | 309 | PRO | CA-C-N | -8.78 | 97.89 | 117.20 |
| 9 | 8 | 99 | ARG | CG-CD-NE | 5.94 | 124.27 | 111.80 |
| 34 | AR | 309 | PRO | C-N-CA | -5.91 | 106.92 | 121.70 |
| 9 | 8 | 99 | ARG | CB-CG-CD | 5.59 | 126.12 | 111.60 |

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 44 | XD | 206 | TYR | Peptide |
| 48 | XI | 197 | LEU | Peptide |
| 50 | XK | 137 | ILE | Peptide |
| 70 | e | 265 | LYS | Peptide |
| 71 | f | 138 | GLN | Peptide |

5.2 Too-close contacts [i](#)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | 0 | 880 | 903 | 903 | 13 | 0 |
| 2 | 1 | 439 | 480 | 480 | 7 | 0 |
| 3 | 2 | 376 | 406 | 406 | 7 | 0 |
| 4 | 3 | 831 | 883 | 883 | 16 | 0 |
| 5 | 4 | 341 | 362 | 361 | 3 | 0 |
| 6 | 5 | 3204 | 3200 | 3200 | 35 | 0 |
| 7 | 6 | 2947 | 2839 | 2841 | 37 | 0 |
| 8 | 7 | 2365 | 2373 | 2372 | 23 | 0 |
| 9 | 8 | 1175 | 1202 | 1202 | 8 | 0 |
| 10 | 9 | 996 | 987 | 987 | 12 | 0 |
| 11 | XA | 31833 | 16169 | 16167 | 296 | 0 |
| 12 | A0 | 1684 | 1685 | 1685 | 17 | 0 |
| 13 | A1 | 2230 | 2261 | 2261 | 26 | 0 |
| 14 | A2 | 925 | 964 | 964 | 14 | 0 |
| 15 | A3 | 610 | 682 | 682 | 16 | 0 |
| 16 | A4 | 4470 | 4485 | 4486 | 43 | 0 |
| 17 | AA | 19628 | 9970 | 9971 | 163 | 0 |
| 18 | AB | 1776 | 1769 | 1769 | 21 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 19 | AC | 1082 | 1088 | 1088 | 12 | 0 |
| 20 | AD | 2716 | 2785 | 2785 | 21 | 0 |
| 21 | AE | 972 | 1001 | 1001 | 14 | 0 |
| 22 | AF | 1668 | 1715 | 1716 | 24 | 0 |
| 23 | AG | 2505 | 2491 | 2490 | 29 | 0 |
| 24 | AH | 1105 | 1136 | 1136 | 15 | 0 |
| 25 | AI | 1011 | 1052 | 1052 | 11 | 0 |
| 26 | AJ | 838 | 887 | 887 | 20 | 0 |
| 27 | AK | 861 | 885 | 885 | 17 | 0 |
| 28 | AL | 1382 | 1472 | 1472 | 16 | 0 |
| 29 | AM | 920 | 951 | 951 | 13 | 0 |
| 30 | AN | 846 | 908 | 908 | 10 | 0 |
| 31 | AO | 1528 | 1490 | 1490 | 18 | 0 |
| 32 | AP | 765 | 796 | 796 | 9 | 0 |
| 33 | AQ | 734 | 749 | 749 | 6 | 0 |
| 34 | AR | 2060 | 2074 | 2074 | 30 | 0 |
| 35 | AS | 1100 | 1103 | 1103 | 7 | 0 |
| 36 | AT | 1330 | 1343 | 1343 | 16 | 0 |
| 37 | AU | 1461 | 1471 | 1471 | 23 | 0 |
| 38 | AV | 2867 | 2862 | 2862 | 29 | 0 |
| 39 | AW | 766 | 785 | 785 | 7 | 0 |
| 40 | AX | 2814 | 2805 | 2804 | 28 | 0 |
| 41 | AY | 956 | 912 | 911 | 13 | 0 |
| 42 | AZ | 731 | 734 | 734 | 8 | 0 |
| 43 | XB | 1255 | 640 | 640 | 12 | 0 |
| 44 | XD | 1842 | 1896 | 1896 | 25 | 0 |
| 45 | XE | 2396 | 2402 | 2402 | 21 | 0 |
| 46 | XF | 2013 | 2045 | 2044 | 32 | 0 |
| 47 | XH | 784 | 832 | 832 | 5 | 0 |
| 48 | XI | 1691 | 1783 | 1783 | 12 | 0 |
| 49 | XJ | 1291 | 1367 | 1364 | 16 | 0 |
| 50 | XK | 1451 | 1448 | 1448 | 16 | 0 |
| 51 | XL | 889 | 941 | 941 | 10 | 0 |
| 52 | XM | 2305 | 2378 | 2378 | 32 | 0 |
| 53 | XN | 1778 | 1808 | 1808 | 15 | 0 |
| 54 | XO | 1245 | 1283 | 1283 | 20 | 0 |
| 55 | XP | 1164 | 1162 | 1162 | 9 | 0 |
| 56 | XQ | 1978 | 2022 | 2022 | 21 | 0 |
| 57 | XR | 1153 | 1214 | 1214 | 23 | 0 |
| 58 | XS | 1284 | 1354 | 1354 | 14 | 0 |
| 59 | XT | 1368 | 1410 | 1410 | 18 | 0 |
| 60 | XU | 1171 | 1164 | 1164 | 15 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 61 | XV | 1648 | 1656 | 1654 | 26 | 0 |
| 62 | XW | 871 | 898 | 898 | 9 | 0 |
| 63 | XX | 2035 | 2054 | 2054 | 19 | 0 |
| 64 | XY | 1534 | 1575 | 1575 | 29 | 0 |
| 65 | XZ | 978 | 1030 | 1030 | 9 | 0 |
| 66 | a | 813 | 777 | 777 | 0 | 0 |
| 67 | b | 1178 | 1180 | 1180 | 0 | 0 |
| 68 | c | 2217 | 2220 | 2220 | 0 | 0 |
| 69 | d | 1758 | 1743 | 1742 | 0 | 0 |
| 70 | e | 1762 | 1767 | 1767 | 0 | 0 |
| 71 | f | 1149 | 1165 | 1165 | 0 | 0 |
| 72 | g | 1097 | 1086 | 1084 | 0 | 0 |
| 73 | h | 882 | 866 | 867 | 0 | 0 |
| 74 | i | 827 | 857 | 857 | 0 | 0 |
| 75 | j | 689 | 678 | 678 | 0 | 0 |
| 76 | k | 732 | 745 | 745 | 0 | 0 |
| 77 | l | 673 | 654 | 653 | 0 | 0 |
| 78 | m | 500 | 525 | 525 | 0 | 0 |
| 79 | o | 797 | 804 | 804 | 0 | 0 |
| 80 | p | 1058 | 1083 | 1083 | 0 | 0 |
| 81 | q | 1379 | 1358 | 1359 | 0 | 0 |
| 82 | r | 1247 | 1267 | 1267 | 0 | 0 |
| 83 | r1 | 72 | 0 | 49 | 0 | 0 |
| 84 | r3 | 1459 | 0 | 829 | 0 | 0 |
| 85 | s | 3036 | 3022 | 3022 | 0 | 0 |
| 86 | t1 | 354 | 379 | 374 | 0 | 0 |
| 86 | t2 | 238 | 268 | 270 | 0 | 0 |
| 86 | t3 | 238 | 268 | 270 | 0 | 0 |
| 86 | t4 | 229 | 255 | 257 | 0 | 0 |
| 86 | t5 | 229 | 255 | 257 | 0 | 0 |
| 86 | t6 | 214 | 236 | 236 | 0 | 0 |
| 87 | 0 | 1 | 0 | 0 | 0 | 0 |
| 87 | 4 | 1 | 0 | 0 | 0 | 0 |
| 87 | AB | 1 | 0 | 0 | 0 | 0 |
| 87 | AO | 1 | 0 | 0 | 0 | 0 |
| 87 | AP | 1 | 0 | 0 | 0 | 0 |
| 87 | AT | 1 | 0 | 0 | 0 | 0 |
| 87 | r | 1 | 0 | 0 | 0 | 0 |
| 88 | 9 | 1 | 0 | 0 | 0 | 0 |
| 88 | A2 | 1 | 0 | 0 | 0 | 0 |
| 88 | AA | 45 | 0 | 0 | 0 | 0 |
| 88 | XA | 142 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 88 | XD | 1 | 0 | 0 | 0 | 0 |
| 88 | XE | 1 | 0 | 0 | 0 | 0 |
| 88 | XM | 2 | 0 | 0 | 0 | 0 |
| 88 | XW | 1 | 0 | 0 | 0 | 0 |
| 88 | g | 1 | 0 | 0 | 0 | 0 |
| 89 | XA | 73 | 67 | 0 | 3 | 0 |
| 90 | XA | 48 | 50 | 50 | 4 | 0 |
| 91 | AX | 32 | 10 | 12 | 1 | 0 |
| All | All | 169034 | 143062 | 143868 | 1265 | 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 5.

The worst 5 of 1265 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) |
|-------------------|--------------------|--------------------------|-------------------|
| 63:XX:144:TYR:O | 63:XX:148:THR:HG23 | 1.56 | 1.05 |
| 4:3:104:ARG:NH1 | 4:3:160:LYS:O | 2.03 | 0.90 |
| 11:XA:2517:U:OP1 | 44:XD:287:ARG:NH2 | 2.04 | 0.90 |
| 23:AG:276:ARG:NH1 | 23:AG:373:ASP:OD2 | 2.04 | 0.90 |
| 45:XE:216:GLN:NE2 | 45:XE:261:MET:SD | 2.45 | 0.90 |

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 | |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 1 | 0 | 106/188 (56%) | 103 (97%) | 3 (3%) | 0 | 100 | 100 |
| 2 | 1 | 51/65 (78%) | 50 (98%) | 1 (2%) | 0 | 100 | 100 |
| 3 | 2 | 44/92 (48%) | 43 (98%) | 1 (2%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 4 | 3 | 93/188 (50%) | 93 (100%) | 0 | 0 | 100 | 100 |
| 5 | 4 | 36/103 (35%) | 35 (97%) | 1 (3%) | 0 | 100 | 100 |
| 6 | 5 | 389/423 (92%) | 365 (94%) | 24 (6%) | 0 | 100 | 100 |
| 7 | 6 | 352/380 (93%) | 325 (92%) | 27 (8%) | 0 | 100 | 100 |
| 8 | 7 | 285/338 (84%) | 265 (93%) | 20 (7%) | 0 | 100 | 100 |
| 9 | 8 | 137/206 (66%) | 131 (96%) | 6 (4%) | 0 | 100 | 100 |
| 10 | 9 | 122/137 (89%) | 115 (94%) | 7 (6%) | 0 | 100 | 100 |
| 12 | A0 | 197/218 (90%) | 189 (96%) | 8 (4%) | 0 | 100 | 100 |
| 13 | A1 | 273/323 (84%) | 258 (94%) | 15 (6%) | 0 | 100 | 100 |
| 14 | A2 | 114/118 (97%) | 110 (96%) | 4 (4%) | 0 | 100 | 100 |
| 15 | A3 | 67/199 (34%) | 66 (98%) | 1 (2%) | 0 | 100 | 100 |
| 16 | A4 | 526/689 (76%) | 493 (94%) | 33 (6%) | 0 | 100 | 100 |
| 18 | AB | 216/296 (73%) | 211 (98%) | 5 (2%) | 0 | 100 | 100 |
| 19 | AC | 130/167 (78%) | 128 (98%) | 2 (2%) | 0 | 100 | 100 |
| 20 | AD | 341/430 (79%) | 325 (95%) | 16 (5%) | 0 | 100 | 100 |
| 21 | AE | 120/125 (96%) | 116 (97%) | 4 (3%) | 0 | 100 | 100 |
| 22 | AF | 197/242 (81%) | 195 (99%) | 2 (1%) | 0 | 100 | 100 |
| 23 | AG | 300/396 (76%) | 288 (96%) | 12 (4%) | 0 | 100 | 100 |
| 24 | AH | 133/201 (66%) | 124 (93%) | 9 (7%) | 0 | 100 | 100 |
| 25 | AI | 134/194 (69%) | 126 (94%) | 8 (6%) | 0 | 100 | 100 |
| 26 | AJ | 106/138 (77%) | 98 (92%) | 8 (8%) | 0 | 100 | 100 |
| 27 | AK | 99/128 (77%) | 97 (98%) | 2 (2%) | 0 | 100 | 100 |
| 28 | AL | 162/257 (63%) | 156 (96%) | 6 (4%) | 0 | 100 | 100 |
| 29 | AM | 114/137 (83%) | 113 (99%) | 1 (1%) | 0 | 100 | 100 |
| 30 | AN | 105/130 (81%) | 103 (98%) | 2 (2%) | 0 | 100 | 100 |
| 31 | AO | 183/258 (71%) | 179 (98%) | 4 (2%) | 0 | 100 | 100 |
| 32 | AP | 93/142 (66%) | 86 (92%) | 7 (8%) | 0 | 100 | 100 |
| 33 | AQ | 83/87 (95%) | 78 (94%) | 5 (6%) | 0 | 100 | 100 |
| 34 | AR | 248/360 (69%) | 239 (96%) | 9 (4%) | 0 | 100 | 100 |
| 35 | AS | 131/190 (69%) | 123 (94%) | 8 (6%) | 0 | 100 | 100 |
| 36 | AT | 160/173 (92%) | 150 (94%) | 10 (6%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 37 | AU | 171/205 (83%) | 168 (98%) | 3 (2%) | 0 | 100 | 100 |
| 38 | AV | 341/414 (82%) | 318 (93%) | 23 (7%) | 0 | 100 | 100 |
| 39 | AW | 95/187 (51%) | 90 (95%) | 5 (5%) | 0 | 100 | 100 |
| 40 | AX | 346/398 (87%) | 328 (95%) | 18 (5%) | 0 | 100 | 100 |
| 41 | AY | 111/395 (28%) | 106 (96%) | 5 (4%) | 0 | 100 | 100 |
| 42 | AZ | 84/106 (79%) | 81 (96%) | 3 (4%) | 0 | 100 | 100 |
| 44 | XD | 234/305 (77%) | 217 (93%) | 15 (6%) | 2 (1%) | 17 | 56 |
| 45 | XE | 302/348 (87%) | 291 (96%) | 11 (4%) | 0 | 100 | 100 |
| 46 | XF | 248/311 (80%) | 237 (96%) | 11 (4%) | 0 | 100 | 100 |
| 47 | XH | 93/267 (35%) | 89 (96%) | 4 (4%) | 0 | 100 | 100 |
| 48 | XI | 209/261 (80%) | 193 (92%) | 16 (8%) | 0 | 100 | 100 |
| 49 | XJ | 168/192 (88%) | 156 (93%) | 12 (7%) | 0 | 100 | 100 |
| 50 | XK | 175/178 (98%) | 167 (95%) | 8 (5%) | 0 | 100 | 100 |
| 51 | XL | 113/145 (78%) | 108 (96%) | 5 (4%) | 0 | 100 | 100 |
| 52 | XM | 285/296 (96%) | 273 (96%) | 12 (4%) | 0 | 100 | 100 |
| 53 | XN | 219/251 (87%) | 208 (95%) | 11 (5%) | 0 | 100 | 100 |
| 54 | XO | 150/175 (86%) | 142 (95%) | 8 (5%) | 0 | 100 | 100 |
| 55 | XP | 141/180 (78%) | 131 (93%) | 10 (7%) | 0 | 100 | 100 |
| 56 | XQ | 236/292 (81%) | 222 (94%) | 14 (6%) | 0 | 100 | 100 |
| 57 | XR | 138/149 (93%) | 131 (95%) | 7 (5%) | 0 | 100 | 100 |
| 58 | XS | 158/205 (77%) | 151 (96%) | 7 (4%) | 0 | 100 | 100 |
| 59 | XT | 164/206 (80%) | 159 (97%) | 5 (3%) | 0 | 100 | 100 |
| 60 | XU | 137/153 (90%) | 130 (95%) | 7 (5%) | 0 | 100 | 100 |
| 61 | XV | 200/216 (93%) | 191 (96%) | 9 (4%) | 0 | 100 | 100 |
| 62 | XW | 109/148 (74%) | 105 (96%) | 4 (4%) | 0 | 100 | 100 |
| 63 | XX | 241/256 (94%) | 230 (95%) | 10 (4%) | 1 (0%) | 34 | 72 |
| 64 | XY | 176/250 (70%) | 168 (96%) | 8 (4%) | 0 | 100 | 100 |
| 65 | XZ | 118/161 (73%) | 112 (95%) | 6 (5%) | 0 | 100 | 100 |
| 66 | a | 93/142 (66%) | 86 (92%) | 7 (8%) | 0 | 100 | 100 |
| 67 | b | 146/215 (68%) | 132 (90%) | 14 (10%) | 0 | 100 | 100 |
| 68 | c | 271/332 (82%) | 257 (95%) | 14 (5%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-------------------|-------------|----------|----------|-------------|-----|
| 69 | d | 212/306 (69%) | 200 (94%) | 11 (5%) | 1 (0%) | 29 | 68 |
| 70 | e | 211/279 (76%) | 203 (96%) | 8 (4%) | 0 | 100 | 100 |
| 71 | f | 139/212 (66%) | 133 (96%) | 6 (4%) | 0 | 100 | 100 |
| 72 | g | 130/166 (78%) | 124 (95%) | 6 (5%) | 0 | 100 | 100 |
| 73 | h | 106/158 (67%) | 99 (93%) | 7 (7%) | 0 | 100 | 100 |
| 74 | i | 95/128 (74%) | 93 (98%) | 2 (2%) | 0 | 100 | 100 |
| 75 | j | 84/123 (68%) | 83 (99%) | 1 (1%) | 0 | 100 | 100 |
| 76 | k | 93/112 (83%) | 88 (95%) | 5 (5%) | 0 | 100 | 100 |
| 77 | l | 78/138 (56%) | 73 (94%) | 5 (6%) | 0 | 100 | 100 |
| 78 | m | 58/128 (45%) | 52 (90%) | 6 (10%) | 0 | 100 | 100 |
| 79 | o | 92/102 (90%) | 89 (97%) | 3 (3%) | 0 | 100 | 100 |
| 80 | p | 119/206 (58%) | 113 (95%) | 6 (5%) | 0 | 100 | 100 |
| 81 | q | 162/222 (73%) | 155 (96%) | 7 (4%) | 0 | 100 | 100 |
| 82 | r | 144/196 (74%) | 139 (96%) | 5 (4%) | 0 | 100 | 100 |
| 85 | s | 366/439 (83%) | 346 (94%) | 20 (6%) | 0 | 100 | 100 |
| 86 | t1 | 45/198 (23%) | 39 (87%) | 6 (13%) | 0 | 100 | 100 |
| 86 | t2 | 28/198 (14%) | 28 (100%) | 0 | 0 | 100 | 100 |
| 86 | t3 | 28/198 (14%) | 27 (96%) | 1 (4%) | 0 | 100 | 100 |
| 86 | t4 | 27/198 (14%) | 26 (96%) | 1 (4%) | 0 | 100 | 100 |
| 86 | t5 | 27/198 (14%) | 26 (96%) | 1 (4%) | 0 | 100 | 100 |
| 86 | t6 | 25/198 (13%) | 25 (100%) | 0 | 0 | 100 | 100 |
| All | All | 13788/19160 (72%) | 13114 (95%) | 670 (5%) | 4 (0%) | 100 | 100 |

All (4) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 63 | XX | 150 | LYS |
| 44 | XD | 208 | ARG |
| 44 | XD | 207 | ILE |
| 69 | d | 289 | PRO |

5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|---------------|------------|----------|-------------|-----|
| 1 | 0 | 97/164 (59%) | 97 (100%) | 0 | 100 | 100 |
| 2 | 1 | 50/60 (83%) | 50 (100%) | 0 | 100 | 100 |
| 3 | 2 | 40/72 (56%) | 40 (100%) | 0 | 100 | 100 |
| 4 | 3 | 88/166 (53%) | 88 (100%) | 0 | 100 | 100 |
| 5 | 4 | 37/89 (42%) | 37 (100%) | 0 | 100 | 100 |
| 6 | 5 | 353/368 (96%) | 352 (100%) | 1 (0%) | 92 | 95 |
| 7 | 6 | 313/332 (94%) | 312 (100%) | 1 (0%) | 92 | 95 |
| 8 | 7 | 267/303 (88%) | 267 (100%) | 0 | 100 | 100 |
| 9 | 8 | 128/190 (67%) | 127 (99%) | 1 (1%) | 81 | 89 |
| 10 | 9 | 104/112 (93%) | 104 (100%) | 0 | 100 | 100 |
| 12 | A0 | 176/190 (93%) | 175 (99%) | 1 (1%) | 86 | 92 |
| 13 | A1 | 253/291 (87%) | 252 (100%) | 1 (0%) | 91 | 94 |
| 14 | A2 | 99/101 (98%) | 97 (98%) | 2 (2%) | 55 | 73 |
| 15 | A3 | 63/166 (38%) | 63 (100%) | 0 | 100 | 100 |
| 16 | A4 | 494/609 (81%) | 490 (99%) | 4 (1%) | 81 | 89 |
| 18 | AB | 192/249 (77%) | 192 (100%) | 0 | 100 | 100 |
| 19 | AC | 115/143 (80%) | 115 (100%) | 0 | 100 | 100 |
| 20 | AD | 283/357 (79%) | 282 (100%) | 1 (0%) | 91 | 94 |
| 21 | AE | 104/107 (97%) | 104 (100%) | 0 | 100 | 100 |
| 22 | AF | 178/209 (85%) | 178 (100%) | 0 | 100 | 100 |
| 23 | AG | 264/342 (77%) | 264 (100%) | 0 | 100 | 100 |
| 24 | AH | 125/180 (69%) | 125 (100%) | 0 | 100 | 100 |
| 25 | AI | 104/147 (71%) | 104 (100%) | 0 | 100 | 100 |
| 26 | AJ | 93/118 (79%) | 93 (100%) | 0 | 100 | 100 |
| 27 | AK | 91/113 (80%) | 91 (100%) | 0 | 100 | 100 |
| 28 | AL | 152/226 (67%) | 152 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|---------------|------------|----------|-------------|-----|
| 29 | AM | 95/113 (84%) | 95 (100%) | 0 | 100 | 100 |
| 30 | AN | 93/115 (81%) | 93 (100%) | 0 | 100 | 100 |
| 31 | AO | 166/230 (72%) | 166 (100%) | 0 | 100 | 100 |
| 32 | AP | 86/123 (70%) | 86 (100%) | 0 | 100 | 100 |
| 33 | AQ | 77/79 (98%) | 77 (100%) | 0 | 100 | 100 |
| 34 | AR | 229/318 (72%) | 227 (99%) | 2 (1%) | 78 | 87 |
| 35 | AS | 115/164 (70%) | 115 (100%) | 0 | 100 | 100 |
| 36 | AT | 150/157 (96%) | 148 (99%) | 2 (1%) | 69 | 82 |
| 37 | AU | 149/174 (86%) | 148 (99%) | 1 (1%) | 84 | 90 |
| 38 | AV | 315/364 (86%) | 314 (100%) | 1 (0%) | 92 | 95 |
| 39 | AW | 84/158 (53%) | 84 (100%) | 0 | 100 | 100 |
| 40 | AX | 307/351 (88%) | 305 (99%) | 2 (1%) | 84 | 90 |
| 41 | AY | 104/357 (29%) | 104 (100%) | 0 | 100 | 100 |
| 42 | AZ | 79/95 (83%) | 79 (100%) | 0 | 100 | 100 |
| 44 | XD | 190/245 (78%) | 189 (100%) | 1 (0%) | 88 | 93 |
| 45 | XE | 259/290 (89%) | 259 (100%) | 0 | 100 | 100 |
| 46 | XF | 217/262 (83%) | 217 (100%) | 0 | 100 | 100 |
| 47 | XH | 86/228 (38%) | 86 (100%) | 0 | 100 | 100 |
| 48 | XI | 194/232 (84%) | 194 (100%) | 0 | 100 | 100 |
| 49 | XJ | 133/150 (89%) | 131 (98%) | 2 (2%) | 65 | 80 |
| 50 | XK | 155/156 (99%) | 155 (100%) | 0 | 100 | 100 |
| 51 | XL | 98/124 (79%) | 98 (100%) | 0 | 100 | 100 |
| 52 | XM | 245/249 (98%) | 244 (100%) | 1 (0%) | 91 | 94 |
| 53 | XN | 188/211 (89%) | 188 (100%) | 0 | 100 | 100 |
| 54 | XO | 133/150 (89%) | 133 (100%) | 0 | 100 | 100 |
| 55 | XP | 125/155 (81%) | 125 (100%) | 0 | 100 | 100 |
| 56 | XQ | 220/256 (86%) | 220 (100%) | 0 | 100 | 100 |
| 57 | XR | 118/126 (94%) | 117 (99%) | 1 (1%) | 81 | 89 |
| 58 | XS | 145/180 (81%) | 145 (100%) | 0 | 100 | 100 |
| 59 | XT | 146/176 (83%) | 144 (99%) | 2 (1%) | 67 | 81 |
| 60 | XU | 126/135 (93%) | 126 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-------------------|--------------|----------|-------------|-----|
| 61 | XV | 179/191 (94%) | 177 (99%) | 2 (1%) | 73 | 85 |
| 62 | XW | 91/119 (76%) | 89 (98%) | 2 (2%) | 52 | 71 |
| 63 | XX | 219/229 (96%) | 218 (100%) | 1 (0%) | 88 | 93 |
| 64 | XY | 161/223 (72%) | 161 (100%) | 0 | 100 | 100 |
| 65 | XZ | 111/147 (76%) | 110 (99%) | 1 (1%) | 78 | 87 |
| 66 | a | 93/133 (70%) | 93 (100%) | 0 | 100 | 100 |
| 67 | b | 130/186 (70%) | 130 (100%) | 0 | 100 | 100 |
| 68 | c | 241/288 (84%) | 240 (100%) | 1 (0%) | 91 | 94 |
| 69 | d | 196/274 (72%) | 196 (100%) | 0 | 100 | 100 |
| 70 | e | 188/236 (80%) | 186 (99%) | 2 (1%) | 73 | 85 |
| 71 | f | 128/188 (68%) | 128 (100%) | 0 | 100 | 100 |
| 72 | g | 122/148 (82%) | 122 (100%) | 0 | 100 | 100 |
| 73 | h | 103/148 (70%) | 103 (100%) | 0 | 100 | 100 |
| 74 | i | 86/110 (78%) | 86 (100%) | 0 | 100 | 100 |
| 75 | j | 68/97 (70%) | 68 (100%) | 0 | 100 | 100 |
| 76 | k | 80/90 (89%) | 80 (100%) | 0 | 100 | 100 |
| 77 | l | 74/116 (64%) | 74 (100%) | 0 | 100 | 100 |
| 78 | m | 54/113 (48%) | 54 (100%) | 0 | 100 | 100 |
| 79 | o | 80/87 (92%) | 80 (100%) | 0 | 100 | 100 |
| 80 | p | 117/181 (65%) | 117 (100%) | 0 | 100 | 100 |
| 81 | q | 141/178 (79%) | 140 (99%) | 1 (1%) | 84 | 90 |
| 82 | r | 138/169 (82%) | 138 (100%) | 0 | 100 | 100 |
| 85 | s | 326/381 (86%) | 326 (100%) | 0 | 100 | 100 |
| 86 | t1 | 41/158 (26%) | 40 (98%) | 1 (2%) | 49 | 69 |
| 86 | t2 | 29/158 (18%) | 29 (100%) | 0 | 100 | 100 |
| 86 | t3 | 29/158 (18%) | 29 (100%) | 0 | 100 | 100 |
| 86 | t4 | 28/158 (18%) | 28 (100%) | 0 | 100 | 100 |
| 86 | t5 | 28/158 (18%) | 28 (100%) | 0 | 100 | 100 |
| 86 | t6 | 26/158 (16%) | 26 (100%) | 0 | 100 | 100 |
| All | All | 12397/16507 (75%) | 12359 (100%) | 38 (0%) | 92 | 95 |

5 of 38 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-------|------|
| 61 | XV | 152 | ARG |
| 70 | e | 273 | ARG |
| 62 | XW | 56 | MET |
| 65 | XZ | 152 | LYS |
| 86 | t1 | 21[A] | LEU |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 33 | AQ | 27 | ASN |
| 85 | s | 207 | HIS |
| 40 | AX | 347 | ASN |
| 67 | b | 129 | GLN |
| 40 | AX | 54 | ASN |

5.3.3 RNA [i](#)

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 11 | XA | 1490/1561 (95%) | 266 (17%) | 6 (0%) |
| 17 | AA | 916/954 (96%) | 158 (17%) | 3 (0%) |
| 43 | XB | 54/72 (75%) | 10 (18%) | 0 |
| 83 | r1 | 0/4 | - | - |
| 84 | r3 | 0/75 | - | - |
| All | All | 2460/2666 (92%) | 434 (17%) | 9 (0%) |

5 of 434 RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 11 | XA | 1672 | C |
| 11 | XA | 1681 | G |
| 11 | XA | 1685 | C |
| 11 | XA | 1689 | C |
| 11 | XA | 1692 | A |

5 of 9 RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 17 | AA | 1048 | C |
| 17 | AA | 1234 | C |
| 11 | XA | 2602 | U |
| 11 | XA | 2961 | C |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 11 | XA | 2962 | C |

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

79 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 |
| 84 | Y5P | r3 | 20 | 84 | 14,19,20 | 3.13 | 3 (21%) | 18,26,29 | 0.58 | 0 |
| 84 | Y5P | r3 | 13 | 84 | 14,19,20 | 3.13 | 4 (28%) | 18,26,29 | 0.64 | 0 |
| 83 | Y5P | r1 | 49 | 83 | 14,19,20 | 3.14 | 3 (21%) | 18,26,29 | 0.57 | 0 |
| 84 | P5P | r3 | 74 | 84 | 16,23,24 | 0.97 | 1 (6%) | 14,33,36 | 2.03 | 3 (21%) |
| 84 | P5P | r3 | 14 | 84 | 16,23,24 | 0.95 | 1 (6%) | 14,33,36 | 2.02 | 3 (21%) |
| 84 | P5P | r3 | 8 | 84 | 16,23,24 | 0.95 | 1 (6%) | 14,33,36 | 1.99 | 3 (21%) |
| 84 | P5P | r3 | 23 | 84 | 16,23,24 | 0.95 | 1 (6%) | 14,33,36 | 2.00 | 3 (21%) |
| 84 | Y5P | r3 | 64 | 84 | 14,19,20 | 3.13 | 3 (21%) | 18,26,29 | 0.58 | 0 |
| 84 | Y5P | r3 | 24 | 84 | 14,19,20 | 3.13 | 3 (21%) | 18,26,29 | 0.61 | 0 |
| 84 | Y5P | r3 | 32 | 84 | 14,19,20 | 3.14 | 3 (21%) | 18,26,29 | 0.56 | 0 |
| 84 | P5P | r3 | 57 | 84 | 16,23,24 | 0.94 | 1 (6%) | 14,33,36 | 1.93 | 3 (21%) |
| 84 | P5P | r3 | 44 | 84 | 16,23,24 | 0.96 | 1 (6%) | 14,33,36 | 1.97 | 3 (21%) |
| 84 | P5P | r3 | 11 | 84 | 16,23,24 | 0.95 | 1 (6%) | 14,33,36 | 1.98 | 3 (21%) |
| 84 | P5P | r3 | 43 | 84 | 16,23,24 | 0.94 | 1 (6%) | 14,33,36 | 1.97 | 3 (21%) |
| 84 | P5P | r3 | 3 | 84 | 16,23,24 | 0.95 | 1 (6%) | 14,33,36 | 1.99 | 3 (21%) |
| 84 | Y5P | r3 | 72 | 84 | 14,19,20 | 3.10 | 3 (21%) | 18,26,29 | 0.65 | 0 |
| 84 | Y5P | r3 | 28 | 84 | 14,19,20 | 3.13 | 3 (21%) | 18,26,29 | 0.59 | 0 |
| 84 | P5P | r3 | 45 | 84 | 16,23,24 | 0.95 | 1 (6%) | 14,33,36 | 1.95 | 3 (21%) |
| 84 | P5P | r3 | 68 | 84 | 16,23,24 | 0.95 | 1 (6%) | 14,33,36 | 1.99 | 3 (21%) |
| 84 | Y5P | r3 | 70 | 84 | 14,19,20 | 3.13 | 3 (21%) | 18,26,29 | 0.59 | 0 |
| 84 | P5P | r3 | 22 | 84 | 16,23,24 | 0.95 | 1 (6%) | 14,33,36 | 1.98 | 3 (21%) |
| 83 | Y5P | r1 | 48 | 83 | 14,19,20 | 3.13 | 3 (21%) | 18,26,29 | 0.57 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 84 | Y5P | r3 | 17 | 84 | 14,19,20 | 3.16 | 3 (21%) | 18,26,29 | 0.56 | 0 |
| 84 | Y5P | r3 | 39 | 84 | 14,19,20 | 3.13 | 3 (21%) | 18,26,29 | 0.59 | 0 |
| 84 | Y5P | r3 | 50 | 84 | 14,19,20 | 3.15 | 3 (21%) | 18,26,29 | 0.58 | 0 |
| 84 | P5P | r3 | 51 | 84 | 16,23,24 | 0.96 | 1 (6%) | 14,33,36 | 1.99 | 3 (21%) |
| 84 | Y5P | r3 | 65 | 84 | 14,19,20 | 3.13 | 3 (21%) | 18,26,29 | 0.63 | 0 |
| 84 | Y5P | r3 | 73 | 84 | 14,19,20 | 3.11 | 3 (21%) | 18,26,29 | 0.54 | 0 |
| 84 | P5P | r3 | 10 | 84 | 16,23,24 | 0.95 | 1 (6%) | 14,33,36 | 1.98 | 3 (21%) |
| 84 | Y5P | r3 | 47 | 84 | 14,19,20 | 3.14 | 3 (21%) | 18,26,29 | 0.60 | 0 |
| 84 | Y5P | r3 | 61 | 84 | 14,19,20 | 3.13 | 3 (21%) | 18,26,29 | 0.56 | 0 |
| 84 | Y5P | r3 | 69 | 84 | 14,19,20 | 3.13 | 3 (21%) | 18,26,29 | 0.53 | 0 |
| 84 | P5P | r3 | 42 | 84 | 16,23,24 | 0.96 | 1 (6%) | 14,33,36 | 1.99 | 3 (21%) |
| 83 | Y5P | r1 | 46 | 83 | 14,19,20 | 3.13 | 3 (21%) | 18,26,29 | 0.62 | 0 |
| 83 | Y5P | r1 | 47 | 83 | 14,19,20 | 3.12 | 3 (21%) | 18,26,29 | 0.56 | 0 |
| 84 | Y5P | r3 | 33 | 84 | 14,19,20 | 3.13 | 3 (21%) | 18,26,29 | 0.58 | 0 |
| 84 | Y5P | r3 | 67 | 84 | 14,19,20 | 3.13 | 3 (21%) | 18,26,29 | 0.58 | 0 |
| 84 | Y5P | r3 | 49 | 84 | 14,19,20 | 3.14 | 3 (21%) | 18,26,29 | 0.56 | 0 |
| 84 | Y5P | r3 | 53 | 84 | 14,19,20 | 3.15 | 3 (21%) | 18,26,29 | 0.58 | 0 |
| 84 | Y5P | r3 | 63 | 84 | 14,19,20 | 3.14 | 3 (21%) | 18,26,29 | 0.57 | 0 |
| 84 | Y5P | r3 | 40 | 84 | 14,19,20 | 3.13 | 3 (21%) | 18,26,29 | 0.59 | 0 |
| 84 | P5P | r3 | 19 | 84 | 16,23,24 | 0.96 | 1 (6%) | 14,33,36 | 2.01 | 3 (21%) |
| 84 | Y5P | r3 | 1 | 84 | 18,20,20 | 2.78 | 3 (16%) | 25,29,29 | 0.67 | 0 |
| 84 | Y5P | r3 | 59 | 84 | 14,19,20 | 3.14 | 3 (21%) | 18,26,29 | 0.57 | 0 |
| 84 | Y5P | r3 | 34 | 84 | 14,19,20 | 3.13 | 3 (21%) | 18,26,29 | 0.58 | 0 |
| 84 | Y5P | r3 | 16 | 84 | 14,19,20 | 3.13 | 3 (21%) | 18,26,29 | 0.60 | 0 |
| 84 | P5P | r3 | 21 | 84 | 16,23,24 | 0.95 | 1 (6%) | 14,33,36 | 1.96 | 3 (21%) |
| 84 | Y5P | r3 | 54 | 84 | 14,19,20 | 3.14 | 3 (21%) | 18,26,29 | 0.59 | 0 |
| 84 | P5P | r3 | 15 | 84 | 16,23,24 | 0.97 | 1 (6%) | 14,33,36 | 1.96 | 3 (21%) |
| 84 | P5P | r3 | 46 | 84 | 16,23,24 | 0.96 | 1 (6%) | 14,33,36 | 1.99 | 3 (21%) |
| 84 | Y5P | r3 | 12 | 84 | 14,19,20 | 3.12 | 3 (21%) | 18,26,29 | 0.56 | 0 |
| 84 | P5P | r3 | 37 | 84 | 16,23,24 | 0.96 | 1 (6%) | 14,33,36 | 1.98 | 3 (21%) |
| 84 | Y5P | r3 | 62 | 84 | 14,19,20 | 3.14 | 3 (21%) | 18,26,29 | 0.59 | 0 |
| 84 | Y5P | r3 | 2 | 84 | 14,19,20 | 3.13 | 3 (21%) | 18,26,29 | 0.57 | 0 |
| 84 | P5P | r3 | 29 | 84 | 16,23,24 | 0.95 | 1 (6%) | 14,33,36 | 2.00 | 3 (21%) |
| 84 | Y5P | r3 | 41 | 84 | 14,19,20 | 3.13 | 3 (21%) | 18,26,29 | 0.56 | 0 |
| 84 | Y5P | r3 | 60 | 84 | 14,19,20 | 3.13 | 3 (21%) | 18,26,29 | 0.59 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 84 | P5P | r3 | 6 | 84 | 16,23,24 | 0.95 | 1 (6%) | 14,33,36 | 2.01 | 3 (21%) |
| 84 | Y5P | r3 | 56 | 84 | 14,19,20 | 3.13 | 3 (21%) | 18,26,29 | 0.64 | 0 |
| 84 | P5P | r3 | 48 | 84 | 16,23,24 | 0.95 | 1 (6%) | 14,33,36 | 1.99 | 3 (21%) |
| 84 | P5P | r3 | 55 | 84 | 16,23,24 | 0.95 | 1 (6%) | 14,33,36 | 1.96 | 3 (21%) |
| 84 | Y5P | r3 | 25 | 84 | 14,19,20 | 3.14 | 3 (21%) | 18,26,29 | 0.60 | 0 |
| 84 | P5P | r3 | 26 | 84 | 16,23,24 | 0.95 | 1 (6%) | 14,33,36 | 2.00 | 3 (21%) |
| 84 | P5P | r3 | 18 | 84 | 16,23,24 | 0.95 | 1 (6%) | 14,33,36 | 2.01 | 3 (21%) |
| 84 | Y5P | r3 | 58 | 84 | 14,19,20 | 3.13 | 4 (28%) | 18,26,29 | 0.66 | 0 |
| 84 | P5P | r3 | 9 | 84 | 16,23,24 | 0.98 | 1 (6%) | 14,33,36 | 1.98 | 3 (21%) |
| 84 | Y5P | r3 | 7 | 84 | 14,19,20 | 3.11 | 3 (21%) | 18,26,29 | 0.62 | 0 |
| 84 | P5P | r3 | 31 | 84 | 16,23,24 | 0.94 | 1 (6%) | 14,33,36 | 1.97 | 3 (21%) |
| 84 | P5P | r3 | 35 | 84 | 16,23,24 | 0.95 | 1 (6%) | 14,33,36 | 1.99 | 3 (21%) |
| 84 | P5P | r3 | 17(A) | 84 | 16,23,24 | 0.93 | 1 (6%) | 14,33,36 | 2.01 | 3 (21%) |
| 84 | P5P | r3 | 66 | 84 | 16,23,24 | 0.94 | 1 (6%) | 14,33,36 | 2.01 | 3 (21%) |
| 84 | Y5P | r3 | 38 | 84 | 14,19,20 | 3.13 | 3 (21%) | 18,26,29 | 0.57 | 0 |
| 84 | P5P | r3 | 4 | 84 | 16,23,24 | 0.96 | 1 (6%) | 14,33,36 | 2.00 | 3 (21%) |
| 84 | P5P | r3 | 30 | 84 | 16,23,24 | 0.95 | 1 (6%) | 14,33,36 | 1.99 | 3 (21%) |
| 84 | P5P | r3 | 52 | 84 | 16,23,24 | 0.95 | 1 (6%) | 14,33,36 | 1.99 | 3 (21%) |
| 84 | P5P | r3 | 71 | 84 | 16,23,24 | 0.95 | 1 (6%) | 14,33,36 | 1.98 | 3 (21%) |
| 84 | Y5P | r3 | 27 | 84 | 14,19,20 | 3.14 | 3 (21%) | 18,26,29 | 0.55 | 0 |
| 84 | Y5P | r3 | 36 | 84 | 14,19,20 | 3.11 | 3 (21%) | 18,26,29 | 0.59 | 0 |
| 84 | P5P | r3 | 5 | 84 | 16,23,24 | 0.95 | 1 (6%) | 14,33,36 | 2.01 | 3 (21%) |

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 |
|-----|------|-------|-----|------|---------|-----------|---------|
| 84 | Y5P | r3 | 20 | 84 | - | 1/7/33/34 | 0/2/2/2 |
| 84 | Y5P | r3 | 13 | 84 | - | 5/7/33/34 | 0/2/2/2 |
| 83 | Y5P | r1 | 49 | 83 | - | 3/7/33/34 | 0/2/2/2 |
| 84 | P5P | r3 | 74 | 84 | - | 0/3/25/26 | 0/3/3/3 |
| 84 | P5P | r3 | 14 | 84 | - | 1/3/25/26 | 0/3/3/3 |
| 84 | P5P | r3 | 8 | 84 | - | 0/3/25/26 | 0/3/3/3 |
| 84 | P5P | r3 | 23 | 84 | - | 0/3/25/26 | 0/3/3/3 |
| 84 | Y5P | r3 | 64 | 84 | - | 1/7/33/34 | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|------------|---------|
| 84 | Y5P | r3 | 24 | 84 | - | 1/7/33/34 | 0/2/2/2 |
| 84 | Y5P | r3 | 32 | 84 | - | 1/7/33/34 | 0/2/2/2 |
| 84 | P5P | r3 | 57 | 84 | - | 1/3/25/26 | 0/3/3/3 |
| 84 | P5P | r3 | 44 | 84 | - | 0/3/25/26 | 0/3/3/3 |
| 84 | P5P | r3 | 11 | 84 | - | 0/3/25/26 | 0/3/3/3 |
| 84 | P5P | r3 | 43 | 84 | - | 1/3/25/26 | 0/3/3/3 |
| 84 | P5P | r3 | 3 | 84 | - | 3/3/25/26 | 0/3/3/3 |
| 84 | Y5P | r3 | 72 | 84 | - | 2/7/33/34 | 0/2/2/2 |
| 84 | Y5P | r3 | 28 | 84 | - | 1/7/33/34 | 0/2/2/2 |
| 84 | P5P | r3 | 45 | 84 | - | 0/3/25/26 | 0/3/3/3 |
| 84 | P5P | r3 | 68 | 84 | - | 0/3/25/26 | 0/3/3/3 |
| 84 | Y5P | r3 | 70 | 84 | - | 1/7/33/34 | 0/2/2/2 |
| 84 | P5P | r3 | 22 | 84 | - | 0/3/25/26 | 0/3/3/3 |
| 83 | Y5P | r1 | 48 | 83 | - | 1/7/33/34 | 0/2/2/2 |
| 84 | Y5P | r3 | 17 | 84 | - | 3/7/33/34 | 0/2/2/2 |
| 84 | Y5P | r3 | 39 | 84 | - | 1/7/33/34 | 0/2/2/2 |
| 84 | Y5P | r3 | 50 | 84 | - | 4/7/33/34 | 0/2/2/2 |
| 84 | P5P | r3 | 51 | 84 | - | 2/3/25/26 | 0/3/3/3 |
| 84 | Y5P | r3 | 65 | 84 | - | 1/7/33/34 | 0/2/2/2 |
| 84 | Y5P | r3 | 73 | 84 | - | 1/7/33/34 | 0/2/2/2 |
| 84 | P5P | r3 | 10 | 84 | - | 0/3/25/26 | 0/3/3/3 |
| 84 | Y5P | r3 | 47 | 84 | - | 2/7/33/34 | 0/2/2/2 |
| 84 | Y5P | r3 | 61 | 84 | - | 3/7/33/34 | 0/2/2/2 |
| 84 | Y5P | r3 | 69 | 84 | - | 3/7/33/34 | 0/2/2/2 |
| 84 | P5P | r3 | 42 | 84 | - | 0/3/25/26 | 0/3/3/3 |
| 83 | Y5P | r1 | 46 | 83 | - | 5/7/33/34 | 0/2/2/2 |
| 83 | Y5P | r1 | 47 | 83 | - | 5/7/33/34 | 0/2/2/2 |
| 84 | Y5P | r3 | 33 | 84 | - | 1/7/33/34 | 0/2/2/2 |
| 84 | Y5P | r3 | 67 | 84 | - | 1/7/33/34 | 0/2/2/2 |
| 84 | Y5P | r3 | 49 | 84 | - | 3/7/33/34 | 0/2/2/2 |
| 84 | Y5P | r3 | 53 | 84 | - | 3/7/33/34 | 0/2/2/2 |
| 84 | Y5P | r3 | 63 | 84 | - | 3/7/33/34 | 0/2/2/2 |
| 84 | Y5P | r3 | 40 | 84 | - | 3/7/33/34 | 0/2/2/2 |
| 84 | P5P | r3 | 19 | 84 | - | 2/3/25/26 | 0/3/3/3 |
| 84 | Y5P | r3 | 1 | 84 | - | 1/10/34/34 | 0/2/2/2 |
| 84 | Y5P | r3 | 59 | 84 | - | 4/7/33/34 | 0/2/2/2 |
| 84 | Y5P | r3 | 34 | 84 | - | 3/7/33/34 | 0/2/2/2 |
| 84 | Y5P | r3 | 16 | 84 | - | 2/7/33/34 | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-------|------|---------|-----------|---------|
| 84 | P5P | r3 | 21 | 84 | - | 3/3/25/26 | 0/3/3/3 |
| 84 | Y5P | r3 | 54 | 84 | - | 1/7/33/34 | 0/2/2/2 |
| 84 | P5P | r3 | 15 | 84 | - | 0/3/25/26 | 0/3/3/3 |
| 84 | P5P | r3 | 46 | 84 | - | 1/3/25/26 | 0/3/3/3 |
| 84 | Y5P | r3 | 12 | 84 | - | 1/7/33/34 | 0/2/2/2 |
| 84 | P5P | r3 | 37 | 84 | - | 0/3/25/26 | 0/3/3/3 |
| 84 | Y5P | r3 | 62 | 84 | - | 1/7/33/34 | 0/2/2/2 |
| 84 | Y5P | r3 | 2 | 84 | - | 3/7/33/34 | 0/2/2/2 |
| 84 | P5P | r3 | 29 | 84 | - | 0/3/25/26 | 0/3/3/3 |
| 84 | Y5P | r3 | 41 | 84 | - | 1/7/33/34 | 0/2/2/2 |
| 84 | Y5P | r3 | 60 | 84 | - | 1/7/33/34 | 0/2/2/2 |
| 84 | P5P | r3 | 6 | 84 | - | 0/3/25/26 | 0/3/3/3 |
| 84 | Y5P | r3 | 56 | 84 | - | 4/7/33/34 | 0/2/2/2 |
| 84 | P5P | r3 | 48 | 84 | - | 1/3/25/26 | 0/3/3/3 |
| 84 | P5P | r3 | 55 | 84 | - | 2/3/25/26 | 0/3/3/3 |
| 84 | Y5P | r3 | 25 | 84 | - | 3/7/33/34 | 0/2/2/2 |
| 84 | P5P | r3 | 26 | 84 | - | 2/3/25/26 | 0/3/3/3 |
| 84 | P5P | r3 | 18 | 84 | - | 2/3/25/26 | 0/3/3/3 |
| 84 | Y5P | r3 | 58 | 84 | - | 1/7/33/34 | 0/2/2/2 |
| 84 | P5P | r3 | 9 | 84 | - | 0/3/25/26 | 0/3/3/3 |
| 84 | Y5P | r3 | 7 | 84 | - | 3/7/33/34 | 0/2/2/2 |
| 84 | P5P | r3 | 31 | 84 | - | 2/3/25/26 | 0/3/3/3 |
| 84 | P5P | r3 | 35 | 84 | - | 0/3/25/26 | 0/3/3/3 |
| 84 | P5P | r3 | 17(A) | 84 | - | 3/3/25/26 | 0/3/3/3 |
| 84 | P5P | r3 | 66 | 84 | - | 2/3/25/26 | 0/3/3/3 |
| 84 | Y5P | r3 | 38 | 84 | - | 1/7/33/34 | 0/2/2/2 |
| 84 | P5P | r3 | 4 | 84 | - | 3/3/25/26 | 0/3/3/3 |
| 84 | P5P | r3 | 30 | 84 | - | 0/3/25/26 | 0/3/3/3 |
| 84 | P5P | r3 | 52 | 84 | - | 0/3/25/26 | 0/3/3/3 |
| 84 | P5P | r3 | 71 | 84 | - | 0/3/25/26 | 0/3/3/3 |
| 84 | Y5P | r3 | 27 | 84 | - | 1/7/33/34 | 0/2/2/2 |
| 84 | Y5P | r3 | 36 | 84 | - | 1/7/33/34 | 0/2/2/2 |
| 84 | P5P | r3 | 5 | 84 | - | 2/3/25/26 | 0/3/3/3 |

The worst 5 of 167 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 84 | r3 | 17 | Y5P | C6-C5 | 10.59 | 1.52 | 1.33 |
| 84 | r3 | 27 | Y5P | C6-C5 | 10.59 | 1.52 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 84 | r3 | 32 | Y5P | C6-C5 | 10.56 | 1.52 | 1.33 |
| 84 | r3 | 59 | Y5P | C6-C5 | 10.55 | 1.52 | 1.33 |
| 84 | r3 | 1 | Y5P | C6-C5 | 10.54 | 1.52 | 1.33 |

The worst 5 of 108 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 84 | r3 | 42 | P5P | N1-C2-N3 | -6.00 | 119.97 | 127.65 |
| 84 | r3 | 11 | P5P | N1-C2-N3 | -5.97 | 120.01 | 127.65 |
| 84 | r3 | 48 | P5P | N1-C2-N3 | -5.97 | 120.01 | 127.65 |
| 84 | r3 | 66 | P5P | N1-C2-N3 | -5.97 | 120.01 | 127.65 |
| 84 | r3 | 51 | P5P | N1-C2-N3 | -5.97 | 120.02 | 127.65 |

There are no chirality outliers.

5 of 124 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 83 | r1 | 46 | Y5P | C4'-C5'-O5'-P |
| 83 | r1 | 46 | Y5P | C3'-C4'-C5'-O5' |
| 83 | r1 | 47 | Y5P | C3'-C4'-C5'-O5' |
| 83 | r1 | 48 | Y5P | O4'-C1'-N1-C2 |
| 84 | r3 | 3 | P5P | O4'-C4'-C5'-O5' |

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 205 ligands modelled in this entry, 202 are monoatomic - leaving 3 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 |
| 89 | H8Q | XA | 5143 | - | 77,80,80 | 1.08 | 5 (6%) | 103,115,115 | 1.34 | 15 (14%) |
| 90 | DOL | XA | 5144 | - | 43,50,50 | 3.48 | 15 (34%) | 51,70,70 | 2.66 | 10 (19%) |
| 91 | GTP | AX | 500 | - | 26,34,34 | 1.13 | 2 (7%) | 32,54,54 | 1.53 | 6 (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 |
|-----|------|-------|------|------|---------|---------------|---------|
| 89 | H8Q | XA | 5143 | - | - | 31/83/127/127 | 0/8/8/8 |
| 90 | DOL | XA | 5144 | - | - | 16/58/77/77 | 0/2/3/3 |
| 91 | GTP | AX | 500 | - | - | 8/18/38/38 | 0/3/3/3 |

The worst 5 of 22 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 90 | XA | 5144 | DOL | C28-C29 | 9.91 | 1.55 | 1.32 |
| 90 | XA | 5144 | DOL | C22-C23 | 9.51 | 1.56 | 1.32 |
| 90 | XA | 5144 | DOL | C19-C20 | 7.30 | 1.57 | 1.34 |
| 90 | XA | 5144 | DOL | C6-N5 | 6.38 | 1.49 | 1.34 |
| 90 | XA | 5144 | DOL | C26-N25 | 6.38 | 1.48 | 1.34 |

The worst 5 of 31 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 90 | XA | 5144 | DOL | O40-S39-O41 | -14.97 | 101.12 | 118.19 |
| 90 | XA | 5144 | DOL | C24-N25-C26 | -5.00 | 113.94 | 122.03 |
| 90 | XA | 5144 | DOL | C23-C22-C20 | -4.38 | 119.27 | 125.89 |
| 91 | AX | 500 | GTP | PA-O3A-PB | -3.92 | 119.36 | 132.83 |
| 89 | XA | 5143 | H8Q | O41-C34-C33 | 3.84 | 122.03 | 110.83 |

There are no chirality outliers.

5 of 55 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|---------------|
| 89 | XA | 5143 | H8Q | C2-C1-N13-C14 |
| 89 | XA | 5143 | H8Q | C2-C1-N13-C18 |
| 89 | XA | 5143 | H8Q | O1-C1-N13-C14 |
| 89 | XA | 5143 | H8Q | O1-C1-N13-C18 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 89 | XA | 5143 | H8Q | C33-C34-O41-C43 |

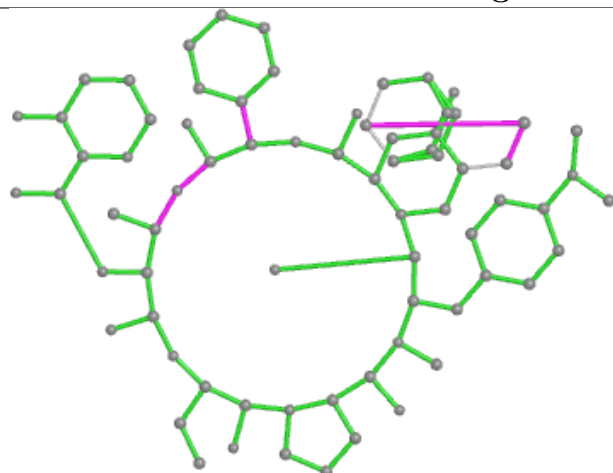
There are no ring outliers.

3 monomers are involved in 8 short contacts:

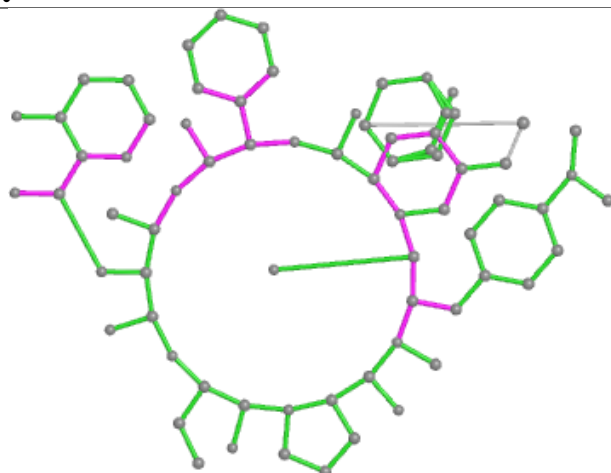
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 89 | XA | 5143 | H8Q | 3 | 0 |
| 90 | XA | 5144 | DOL | 4 | 0 |
| 91 | AX | 500 | GTP | 1 | 0 |

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.

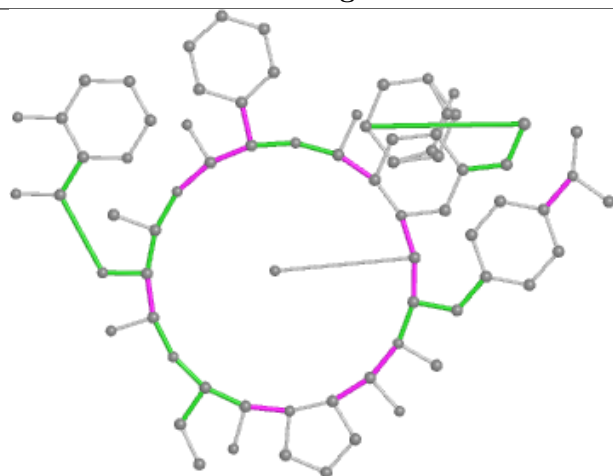
Ligand H8Q XA 5143



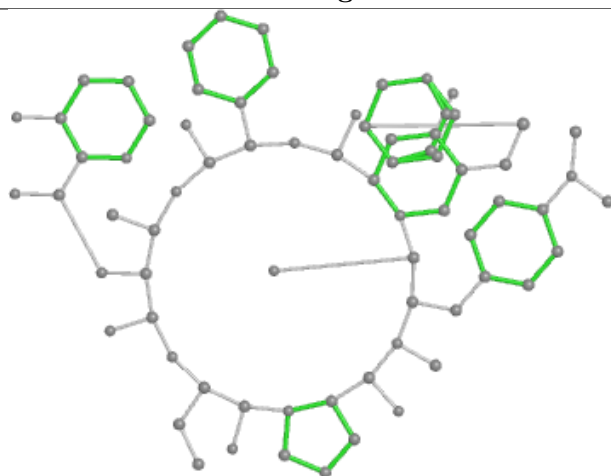
Bond lengths



Bond angles

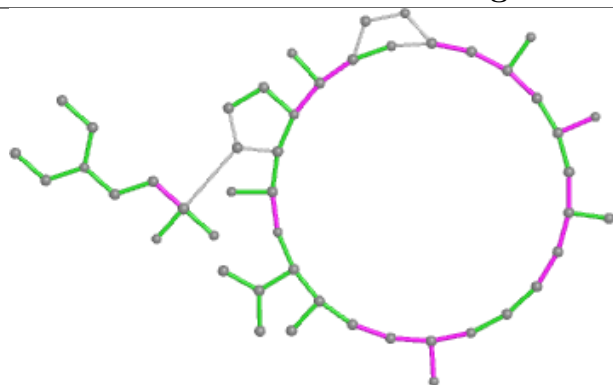


Torsions

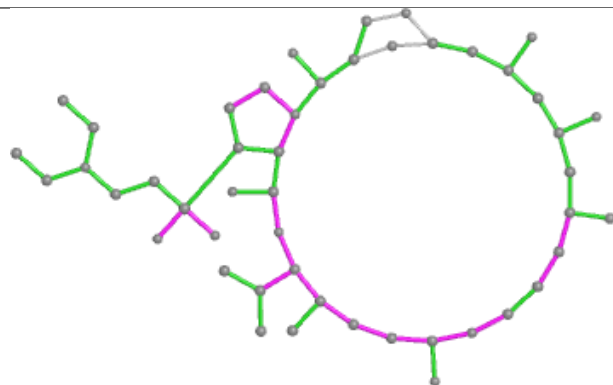


Rings

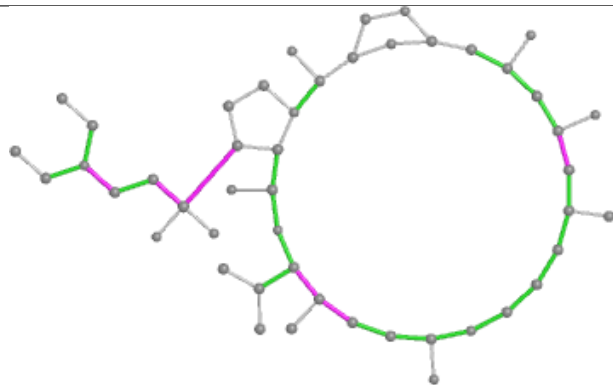
Ligand DOL XA 5144



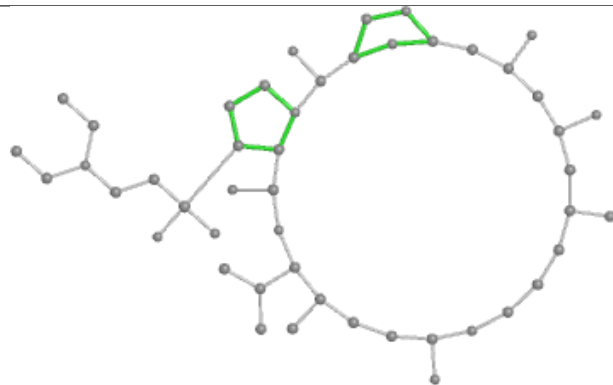
Bond lengths



Bond angles

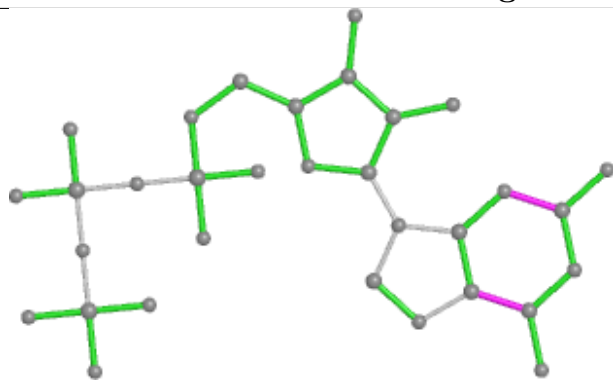


Torsions

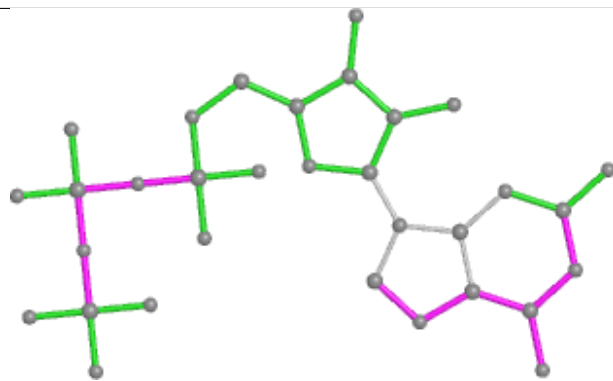


Rings

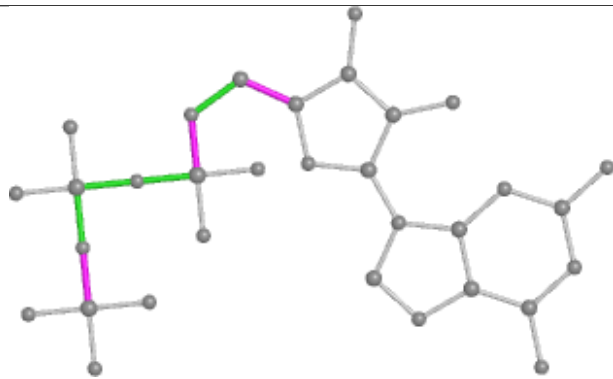
Ligand GTP AX 500



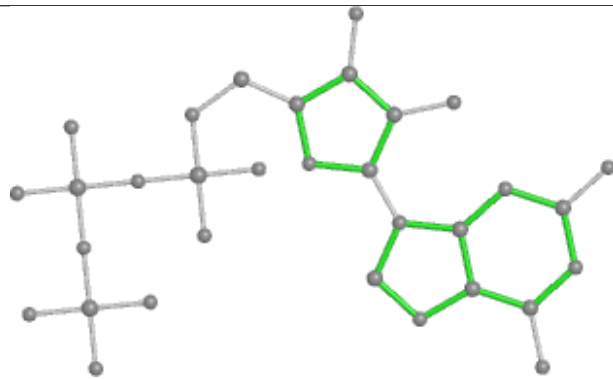
Bond lengths



Bond angles



Torsions



Rings

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 |
|-----|-------|------------------|
| 16 | A4 | 2 |
| 8 | 7 | 2 |
| 82 | r | 1 |
| 38 | AV | 1 |
| 6 | 5 | 1 |
| 72 | g | 1 |

The worst 5 of 8 chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1 | A4 | 537:ARG | C | 538:ASP | N | 6.17 |
| 1 | 7 | 285:ASN | C | 286:LEU | N | 6.12 |
| 1 | r | 134:ARG | C | 135:LEU | N | 5.70 |
| 1 | AV | 269:SER | C | 270:PRO | N | 4.50 |
| 1 | 7 | 185:LEU | C | 186:ASP | N | 3.18 |

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-11392. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal surface views

This section was not generated.

6.5 Mask visualisation

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

7 Map analysis ⓘ

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

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation ⓘ

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

9 Map-model fit

This section was not generated.